UNIWERSYTET
MIKOŁAJA KOPERNIKA
W TORUNIU
Wydział Chemii

mgr Jadwiga Musiał

Nowe podejście w izolowaniu i identyfikacji związków psychoaktywnych (dopalaczy) w materiale biologicznym

Rozprawa doktorska
w dziedzinie nauk ścisłych i przyrodniczych
w dyscyplinie nauki chemiczne

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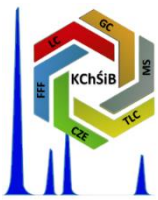

Toruń 2024

A new approach for isolation and identification psychoactive compounds (designer drugs) in biological material

Praca powstała w wyniku realizacji programu Doktorat wdrożeniowy w ramach zatrudnienia w Instytucie Genetyki Sądowej w Bydgoszczy

Badania współfinansowane ze środków Europejskiego Funduszu Rozwoju Regionalnego w ramach Programu Operacyjnego Inteligentny Rozwój (POIR.01.01.01-00-0023/16, *Opracowanie innowacyjnego testu Next Generation Drug Clear Test (NGDC Test) do wykrywania tzw. Dopalaczy we włosach, krwi i moczu*

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Spis treści

Wykaz skrótów i oznaczeń

(+)-Norpseudoephedrine - α-[(1S)-1-aminoetylo]-benzenometanol; katyna
1-AI - 1-aminoindan
1-OH-MDAI - 1-hydroksy-5,6-metylenodioksy-2-aminoindan
2,3-DCPP - 2,3-dichlorfenylpiperazyna
2,3-DMEC - 2,3-dimetyloetkatynon
2,3-DMMC - 2,3-dimetylometkatynon
2,3-ethylone isomer - 2,3-metylenodioksy-α etyloaminopropiofenon
2,3-MDMA - 2,3-metylenodioksymetylamfetamina
2,3-MDPV - 2,3-metylenodioksypyrowaleron
2,4,5-trimethoxyamphetamine - 2,4,5-trimetoksy-α-metylo-benzenoetanoamina
2,4-DMEC - 1-(2,4-dimetylfenylo)-2-(etyloamino)propan-1-on
2,4-DMMC - 1-(2,4-dimetylfenylo)-2-(metyloamino)-1-propanon
2,5-DMMA - 2,5-dimetoksy-N,α-dimetylo-benzenoetanoamina
25B-NBF - 4-bromo-N-[(2-fluorofenylo)metylo]-2,5-dimetoksy-benzenoetanoamina
25C-NBF - 4-chloro-N-[(2-fluoropfenylo)metylo]-2,5-dimetoksy-benzenoetanoamina
25C-NBOH - 2-[[[2-(4-chloro-2,5-dimetoksyfenylo)etylo]amino]metylo]-fenol
25C-NBOMe - 2-(4-chloro-2,5-dimetoksyfenylo)-N-(2-metoksybenzylo)etanoamina
25D-NBOMe - 2,5-dimetoksy-N-[(2-metoksyfenylo)metylo]-4-metylo-benzenoetanoamina
25E-NBOMe - 4-etyl-2,5-dimetoksy-N-[(2-metoksyfenylo)metylo]-benzenoetanoamina
25G-NBOMe - 2,5-dimetoksy-N-[(2-metoksyfenylo)metylo]-3,4-dimetylo-benzenoetanoamina
25H-NBOMe - 2-(2,5-dimetoksyfenylo)-N-(2-metoksybenzylo)etanoamina
25-I-NB2OMe - 2-(4-jodo-2,5-dimetoksyfenylo)-N-[(2-metoksyfenylo)metylo]ethanoamina
25I-NB3OMe - 2-(4-jodo-2,5-dimetoksyfenylo)-N-(3-metoksybenzylo)etanoamina
25I-NB4OMe - 2-(4-jodo-2,5-dimetoksyfenylo)-N-(4-metoksybenzylo)etano-1-amina
25I-NBF - N-(2-fluorobenzylo)-2-(4-jodo-2,5-dimetoksyfenylo)etanoamina
25I-NBMD - N-(1,3-benzodioksol-4-ylmetylo)-2-(4-jodo-2,5-dimetoksyfenylo)etanoamina
25I-NBOH - 2-(((4-jodo-2,5-dimetoksyfenetylo)amino)metylo)fenol
25N-NBOMe - 2,5-dimetoksy-N-[(2-metoksyfenylo)metylo]-4-nitro-benzenoetanoamina
25T2-NBOMe - 4-(tioetylo)-2,5-dimetoksy-N-[(2-metoksyfenylo)metylo]benzenoetanoamina
25T-NBOMe - 2,5-dimetoksy-N-[(2-metoksyfenylo)metylo]-4-(tiometylo)-benzenoetanoamina
2-AI - 2-aminoindan
2-amino-1-phenylbutane - α-etylo-benzenoetanoamina
2-BA - 2-bromo-α-metylo-benzenoetanoamina; 2-bromoamfetamina
2-bromomethamphetamine - 1-(2-bromofenylo)-n-metylpropano-2-amina
2-CA - 2-chloro-α-metylo-benzenoetanamina;2-chloroamfetamina
2C-B - 4-Bromo-2,5-dimetoksyfenyloetyloamina
2C-B FLY - 8-bromo-2,3,6,7-tetrahydro-benzo[1,2-b:4,5-b']difurano-4-etanoamina
2C-C - 2,5-Dimetoksy-4-chlorofenyloetyloamina
2C-D - 2,5-Dimetoksy-4-metylofenyloetyloamina
2C-G - 3,4-Dimetyl-2,5-dimetoksyfenyloenetyloamina
2C-I - 2,5-Dimetoksy-4-jodofenyloetyloamina
2C-P - 2,5-Dimetoksy-4-propylfenyloetyloamina
2C-T-7 - 2,5-Dimetoksy-4-propyltiofenyloetyloamina
2C-TFM - 2,5-dimetoksy-4-(trifluorometylo)-benzenoetanoamina
2-DPMP - 2-(difenylometylo)-piperidyna; desoksypipradol
2-FA - 2-fluoro-α-metylo-benzenoetanoamina; 2-fluoroamfetamina

2-FEC - 2-(etyloamino)-1-(2-fluorofenylo)-1-propanon

2-FIC - 1-amino-1-(2-fluorofenylo)-2-propanon

2-FMA - 2-fluoro-N-α-dimetylo-benzenoetanamina

2-FMC - 1-(2-fluorofenylo)-2-(metyloamino)propan-1-on; 2-fluorometkatynon

2-IA - 2-jodo-α-metylo-benzenoetanoamina; 2-jodoamfetamina

2-MA - 2-metoksy-α-metylo-benzenoetanoamina; 2-metoksyamfetamina

2-MAPB - N,α-dimetylo-2-benzofuranetanoamina

2-MeOMA - 2-metoksy-N,α-dimetylo-benzenoetanoamina; 2-metoksymetamfetamina

2-MeOMC - 1-(2-metoksyfenylo)-2-(metyloamino)propan-1-on

2-methylamino-1-phenylbutane - α-etylo-N-metylo-benzenoetanoamina

2-METHYL-PBP - 2-(pyrrolidin-1-yl)-1-(o-tolylo)butan-1-on

2-METHYL-PPP - 1-(2-metylofenylo)-2-(1-pyrrolidinylo)-1-propanon

2-MMC - 2-(metyloamino)-1-(2-metylofenylo)-1-propanon; 2-metylmetkatynon

3,4-CTMP - 3,4-Dichlorometylfenidat

3,4-DMEC - 1-(3,4-dimetylfenylo)-2-(etyloamino)propan-1-on

3,4-DMMA - 3,4-dimetoksy-N,α-dimetylo-benzenoetanoamina

3,4-DMMC - 1-(3,4-dimetylfenylo)-2-(metyloamino)-1-propanon; 3,4-Dimetylmetkatynon

3,4-DMPV - 3',4'-Dimetoksy-α-pyrrolidinopentiofenon; 3,4-dimetoksy-alfa-PVP

3,4-EDMA - 1-(2,3-dihydrobenzo[b][1,4]dioksin-6-yl)-N-metylpropan-2-amina

3,4-EDMC - 1-(2,3-dihydro-1,4-benzodiokso-6-yl)-2-(metyloamino)-1-propanon

3,4-MDMA - N,α-dimetylo-1,3-benzodioksol-5-etanoamina

3,4-MDPA - α-metylo-N-propylo-1,3-benzodioksol-5-etanoamina

3,4-MDPHP - 1-(1,3-benzodioksol-5-yl)-2-(1-pyrrolidinyl)o-1heksanon

3,4-MDPV - 1-(1,3-benzodioksol-5-yl)-2-(1-pyrrolidinylo)-1-pentanon; 3,4-Metylenodioksypyrowaleron

3,4-methylenedioxy PV9 - 1-(1,3-benzodioksol-5-yl)-2-(1-pyrrolidinylo)-1-oktanon; 3,4-Metylenodioksy PV9

30C-NBOMe - 2-(4-chloro-2,5-dimetoksyfenylo)-N-(3,4,5-trimetoksybenzylo)etanoamina

3-BA - 3-bromo-α-metyl-benzenoetanoamina; 3-bromoamfetamina

3-BMA - 3-Bromometamfetamina

3-BMC - 1-(3-bromofenylo)-2-(metyloamino)-1-propanon; 3-bromometkatynon

3-CA - 3-chloro-α-metylo-benzenoetanoamina; 3-chloroamfetamina

3-CAF - kwas 1-(2-fluorofenyl)-1H-indazole-3-karboksylowy

3C-B-FLY - 8-bromo-2,3,6,7-tetrahydro-α-metyl-benzo[1,2-b:4,5-b']difuran-4-etanoamina

3-CMC - 1-(3-chlorofenylo)-2-(metyloamino)-1-propanon; 3-chlorometkatynon

3C-P - 3,5-dimetoksy-α-metyl-4-propoksy-benzenoetanoamina

3-desoxy-3,4-MDPV - 1-(2,3-dihydro-5-benzofuranylo)-2-(1-pyrrolidinylo)-1-pentanon

3-EMC - 1-(3-etylofenylo)-2-(metyloamino)-1-propanon; 3-etylmetkatynon

3-FA - 3-fluoro-α-metyl-benzenoetanoamina; 3-fluoroamfetamina

3-FEC - 2-(etyloamino)-1-(3-fluorofenylo)-1-propanon

3-fluoro-alfa-PPP - 1-(3-fluorofenylo)-2-(1-pyrrolidinylo)-1-propanon

3-FMA - 1-(3-fluorofenylo)-N-metylopropan-2-amina; 3-fluorometamfetamina

3-FMC - 1-(3-fluorofenylo)-2-(metyloamino)propan-1-on; 3-fluorometkatynon

3-hydroxybromazepam - 7-bromo-3-hydroksy-5-pyridin-2-yl-1,3-dihydro-1,4-benzodiazepin-2-on

3-hydroxyflunitrazepam - 5-(2-fluorofenylo)-1,3-dihydro-3-hydroksy-1-metylo-7-nitro-2H-1,4-benzodiazepin-2-on

3-IA - 3jodo-α-metylo-benzenoetanoamina; 3-jodoamfetamina

3-MA - 3-metoksy-α-metylo-benzenoetanoamina; 3-metoksyamfetamina

3-MEC - 2-(etyloamino)-1-(3-metylofenylo)-1-propanon

3-MeO PCP - 1-[1-(3-metoksyfenylo)cykloheksylo]-piperidina; 3-metoksyfencyklidyna

3-MeOMC - 1-(3-metoksyfenylo)-2-(metyloamino)propan-1-on
3-methyl-PPP - 1-(3-metylofenylo)-2-(1-pyrrolidinylo)-1-propanon
3-MMC - 2-(metyloamino)-1-(3-metylofenylo)-1-propanon; 3-metylmetkatynon
4,4'-DMAR - 4,5-dihydro-4-metylo-5-(4-metylofenylo)-2-oksazolamina
4'-methylhexedrone - 2-(metyloamino)-1-(p-tolyl)heksan-1-on; 4-Metylo-n-metyloheksanofenon
4-AcO-DET - 3-[2-(dietyloamino)etyl]-1H-indol-4-ol 4-octan
4-AcO-DMT - 3-[2-(dimetyloamino)etyl]-1H-indol-4-ol-4-octan
4-AcO-MET - 3-[2-(etylometyloamino)etyl]-1H-indol-4-ol 4-octan
4-APB - α-metylo-4-benzofuranoetanoamina
4-APDB - 2,3-dihydro-α-metylo-4-benzofuranoetanoamina
4-BA - 4-bromo-α-metylo-benzenoetanoamina; 4-bromoamfetamina
4-BMA - 1-(4-Bromofenylo)-n-metylopropan-2-amina;4-bromometamfetamina
4-BMC - 1-(4-bromofenylo)-2-(metyloamino)-1-propanoe; brefedron; 4-bromometkatynon
4-bromo-2,5-DMMA - 4-bromo-2,5-dimetoksy-N,α-dimetylo-benzenoetanoamina
4-CA - 4-chloro-α-metylo-benzenoetanoamina; 4-chloroamfetamina
4-CAB - 4-chloro-α-etylo-benzenoetanoamina
4-CEC - 1-(4-chlorofenylo)-2-(etyloamino)-1-propanon
4-chloro-alpha-PPP - 1-(4-chlorofenylo)-2-(1-pyrrolidinylo)-1-propanon
4-chloro-alpha-PVP - 1-(4-chlorofenylo)-2-(1-pyrrolidinylo)-1-pentanon
4-CMA - 4-chloro-N,α-dimetylo-benzenoetanoamina; 4-chlorometamfetamina
4-CMC - 1-(4-chlorofenylo)-2-(metyloamino)-1-propanon; 4-chlorometkatynon
4-EAPB - 1-(benzofuran-4-yl)-N-etylopropano-2-amina
4-ethyl-N,N-DMC - 2-(dimetyloamino)-1-(4-etylopfenylo)-1-propanon
4-FBP - 1-(4-fluorofenylo)-2-(metyloamino)-1-butanon; 4-fluorobufedron
4-FEC - 2-(etyloamino)-1-(4-fluorofenylo)-1-propanon
4-fluoro-α-PHPP - 1-(4-fluorofenylo)-2-(pyrrolidin-1-ylo)heptan-1-on; 4-fluoro PV8
4'-fluoro-α-PPP - 1-(4-fluorofenylo)-2-(1-pyrrolidinylo)-1-propanon
4-fluoro-α-PVP - 1-(4-fluorofenylo)-2-(1-pyrrolidinylo)-1-pentanon
4-FMA - 4-fluoro-N-α-dimetylo-benzenoetanoamina; 4-furometamfetamina
4-FMC - 1-(4-fluorofenylo)-2-(metyloamino)propan-1-on; 4-fluorometkatynon
4-FPD - 1-(4-fluorofenylo)-2-(metyloamino)pentan-1-on; 4-fluoropentedron
4-hydroxymidazolam - 8-chloro-6-(2-fluorofenylo)-1-metylo-4h-imidazo[1,5-a][1,4]benzodiazepin-4-ol
4-IA - 4-jodo-α-metylo-benzenoetanoamina; 4-jodoamfetamina
4-MA - α,4-dimetylo-benzenoetanoamina; 4-metylamfetamina
4-MAPB - 1-(benzofuran-4-ylo)-N-metylopropan-2-amina
4-MBC - 1-(4-metylofenylo)-2-[(fenylometylo)amino]-1-propanon; benzedron
4-MEAP - 2-(etyloamino)-1-(4-metylofenylo)-1-pentanon
4-MeO PCP - 1-[1-(4-metoksyfenylo)cykloheksylo]-piperidina
4-MeO PV8 - 1-(4-metoksyfenylo)-2-(pyrrolidin-1-ylo)heptan-1-on
4-MeO PV9 - 1-(4-metoksyfenylo)-2-(pyrrolidin-1-ylo)oktan-1-on
4-MeOPBP - 1-metoksyfenylo)-2-(pyrrolidin-1-ylo)butan-1-on
4-MeO-α-PVP - 1-(4-metoksyfenylo)-2-(1-pyrrolidinylo)-1-pentanon
4-methyl-alpha-ethylaminobutiophenone - 2-(etyloamino)-1-(4-metylofenylo)-1-butanon
4-methylcathinone - 2-Amino-1-(4-metylofenylo)-1-propanon
4-methyl-N,N-DMC - 2-(dimetyloamino)-1-(4-metylofenylo)-1-propanon
4-methyl-N-methylbuphedrone - 2-(dimetyloamino)-1-(4-metylofenylo)-1-butanon
4-methyl-PBP - 1-(4-metylofenylo)-2-(1-pyrrolidinylo)-1-butanon
4-methyl-α-ET - α-etylo-4-metylo-1H-indolo-3-etanoamina

4-MMA - N,α,4-trimetylo-benzenoetanoamina;4-metylmetamfetamina

4-MMC - 2-(metyloamino)-1-(4-metylofenylo)-1-propanon;4-metylmetkatynon

4-MPD - 2-(metyloamino)-1-(p-tolylo)pentan-1-on; 4metylpentedron

4-OH DiPT - 3-[2-[bis(1-metyloetylo)amino]etylo]-1H-indol-4-ol,

4-OH-MDAI - 4-hydroksy-5,6-metylenodioksy-2-aminoindan

5-APB - α-metylo-5-benzofuranoetanoamina

5-APDB - 2,3-dihydro-α-metylo-5-benzofuranoetanoamina

5-APDI - 2,3-dihydro-α-metylo-1H-indene-5-etanoamina

5-chloro-ABP - N-[(1S)-1-(aminokarbonylo)-2-metylopropylo]-1-(5-chloropentylo)-1H-indazol-3 karboksyamid; 5-chloro AB-PINACA

5-chloro-NNEI - 1-(5-chloropentylo)-N-1-naftalenylo-1H-indol-3-karboksyamid

5-EAPB - N-etylo-α-metylo-5-benzofuranoetanoamina

5F-ABICA - N-[(1S)-1-(aminokarbonylo)-2-metylopropylo]-1-(5-fluoropentylo)-1H-indol-3-karboksyamid

5F-AB-PINACA - N-[(1S)-1-(aminokarbonylo)-2-metylopropylo]-1-(5-fluoropentylo)-1H-indazol-3-karboksyamid

5F-ADB - 5F-MDMB-PINACA; N-[[1-(5-fluoropentylo)-1H-indazol-3-ylo]karbonylo]-3-metylo-D-walina, ester metylowy

5F-AMB - 5F-AMB-PINACA; N-[[1-(5-fluoropentylo)-1H-indazol-3-ylo]karbonylo]-L-walina, ester metylowy

5F-APINACA - N-((3s,5s,7s)-adamantan-1-ylo)-1-(5-fluoropentylo)-1H-indazol-3-karboksyamid

5-fluoro AMB-PICA (MMB2201) - N-[[1-(5-fluoropentylo)-1H-indol-3-ylo]karbonylo]-L-walina, ester metylowy

5-fluoro APP-PICA (PX-1) - (S)-N-(1-amino-1-okso-3-fenylopropan-2-ylo)-1-(5-fluoropentylo)-1H-indol-3-karboksamid

5-fluoro APP-PINACA (PX-2) - N-[(1S)-2-amino-2-okso-1-(fenylometylo)etylo]-1-(5-fluoropentylo)-1H-indazol-3-karboksyamid

5-fluoro MN-24 - 5-fluoro-NNEI; 1-(5-fluoropentylo)-N-(naftalen-1-ylo)-1H-indol-3-karboksamid

5-fluoro NIN (FUB-NPB-22) - chinolin-8-ylo-1-(4-fluorobenzylo)-1H-indazol-3-karboksylan

5-fluoro THJ - 1-(5-fluoropentylo)-N-8-chinolinylo-1H-indazol-3-karboksyamid

5-fluoro UR-144 (XLR-11) - (1-(5-fluoropentylo)-1H-indol-3-ylo)(2,2,3,3 tetrametylocyklopropylo)metanon

5-fluoro-2-ADB-PINACA isomer 2 - N-(1-amino-3S-metylo-1-oksopentan-2S-ylo)-2-(5-fluoropentylo)-2H-indazol-3-karboksyamid

5-fluoro-MN-18 - 1-(5-fluoropentylo)-N-1-naftalenylo-1H-indazol-3-karboksyamid

5-fluoro-SDB-006 - 1-(5-fluoropentylo)-N-(fenylometylo)-1H-indol-3-karboksyamid

5-fluro-PCN - 1-(5-Fluoropentylo)-N-(naftalen-1-ylo)-1H-pyrrolo(3,2-C)pyridino-3-karboksyamid

5F-NPB-22 - kwas 1-(5-fluoropentylo)-1H-Indazole-3-karboksylowy, 8-chinolinowy ester

5F-PB-22 - 1-(5-fluoropentylo)-8-chinolinowy ester -1H-indol-3-karboksylowwego kwasu

5-fluoro-pentyl-3-pyridinoylindole - [1-(5-fluoropentylo)-1H-indol-3-ylo]-3-pyridinylo-metanon

5F-SDB-005 - 1-(5-fluoropentylo)-1H-indazol-3-karboksylowego kwasu, 1-naftalenowy ester

5-HT - 5-hydroksytryptamina

5-IT - α-metylo-1H-indol-5-etanoamina

5-MAPB - N,α-dimetylo-5-benzofuranoetanoamina

5-MAPDB - 2,3-dihydro-N,α-dimetylo-5-benzofuranoetanoamina

5-MeO AMT - 5-metoksy-α-metylo-1H-indol-3-etanoamina

5-MeO DiPT - 5-metoksy-N,N-bis(1-metyloetylo)-1H-indol-3-etanoamina

5-MeO DMT - 5-metoksy-N,N-dimetylo-1H-indol-3-etanoamina

5-MeO MiPT - 5-metoksy-N-metylo-N-(1-metyloetylo)-1H-Indol-3-etanoamina

5-MeO-DALT - 5-metoksy-N,N-di-2-propen-1-ylo-1H-indol-3-etanoamina

5-MeO-α-ET - α -etylo-5-metoksy-1H-indol-3-etanoamina

5-methoxy methylone - 1-(7-metoksy-1,3-benzodioksol-5-ylo)-2-(metyloamino)-1-propanon

5-OH DMT - 3-[2-(dimetyloamino)ethylo]-1H-indol-5-ol

6-APB - α-metylo-6-benzofuranoetanoamina

6-APDB - 2,3-dihydro-α-metylo-6-benzofuranoetanoamina

6-bromo-MDMA - 1-(6-bromobenzo[d][1,3]dioksol-5-ylo)-N-metylopropan-2-amina

6-chloro-MDMA - 1-(6-chlorobenzo[d][1,3]dioksol-5-ylo)-N-metylopropan-2-amina

6-EAPB - N-etylo-α-metylo-6-benzofuranetanoamina

6-IT - α-metylo-1H-indole-6-etanoamina

6-MAM - (5α,6α)-7,8-didehydro-4,5-epoksy-17-metylo-morfinan-3,6-diol; 6-monoacetylomorfina

6-MAPB - N,α-dimetylo-6-benzofuranoetanoamina

7-aminoclonazepam - 7-amino-5-(2-chlorofenylo)-1,3-dihydro-2H-1,4-benzodiazepin-2-on

7-aminodesmethylflunitrazepam - 7-Amino-5-(o-fluorofenylo)-1,3-dihydro-2H-1,4 benzodiazepin-2-on

7-aminoflunitrazepam - 7-amino-5-(2-fluorofenylo)-1,3-dihydro-1-metylo-2H-1,4-benzodiazepin-2-on

7-aminonitrazepam - 7-amino-5-fenylo-1,3-dihydro-1,4-benzodiazepin-2-on

7-APB - α-metylo-7-benzofuranoetanoamina

7-APDB - 2,3-dihydro-α-metylo-7-benzofuranoetanoamina

A-796260 - [1-[2-(4-morfinylo)etylo]-1H-indol-3-ylo](2,2,3,3-tetrametylocyklopropylo)-metanon

A-834735 - [1-[(tetrahydro-2H-pyran-4-ylo)metylo]-1H-indol-3-ylo](2,2,3,3-tetrametylocyklopropylo)-metanon

A-836339 - [N(Z)]-N-[3-(2-metoksyetylo)-4,5-dimetylo-2(3H)-thiazolyliden]-2,2,3,3-tetrametylo-cyklopropanokarboksyamid

AB-001 - (1s,3s)-adamantan-1-ylo(1-pentylo-1H-indol-3-ylo)metanon

AB005 -[1-[(1-metylo-2-piperidinylo)metylo]-1H-indol-3-ylo](2,2,3,3-tetrametylocyklopropylo)-metanon

AB-CHMINACA - N-[(1S)-1-(aminokarbonylo)-2-metylopropylo]-1-(cykloheksylometylo)-1H-indazol-3-karboksyamid

AB-FUBINACA - N-[(1S)-1-(aminokarbonylo)-2-metylopropylo]-1-[(4-fluorofenylo)metylo]-1H-indazol-3-karboksamid

AB-FUBINACA 2-fluorobenzyl isomer - N-[(1S)-1-(aminokarbonylo)-2-metylopropylo]-1-[(2-fluorofenylo)metylo]-1H-indazol-3-karboksyamid

AB-FUBINACA 3-fluorobenzyl isomer - N-[(1S)-1-(aminokarbonylo)-2-metylopropylo]-1-[(3-fluorofenylo)metylo]-1H-indazol-3-karboksyamid

AB-PINACA - (S)-N-(1-amino-3-metylo-1-oksobutan-2-ylo)-1-pentylo-1H-indazol-3-karboksyamid

Ac-DHAI - N-acetyl-5,6-dihydroksy-2-aminoindan

Acetaminophen (paracetamol) - N-(4-hydroksyfenyl)-acetamid

Ac-HMAI - N-acetyl-5-hydroksy-6-metoksy-2-aminoindan

ACN - acetonitryl

ADB-FUBINACA - N-[1-(aminokarbonyl)-2,2-dimetylopropylo]-1-[(4-fluorofenylo)metylo]-1H-indazole-3-karboksyamid

ADB-PINACA - N-[1-(aminokarbonylo)-2,2-dimetylopropylo]-1-pentylo-1H-indazol-3-karboksyamid

ADB-PINACA isomer 1 - N-(1-amino-2,3-dimetylo-1-oksobutan-2-yl)-1-pentylo-1H-indazol-3-karboksyamid

ADB-PINACA isomer 2 - N-((2S,3S)-1-amino-3-metyl-1-oksopentan-2-yl)-1-pentyl-1H-indazol-3-carboksamid

ADB-PINACA isomer 3 - (S)-N-(1-amino-1-oksoheksan-2-yl)-1-pentyl-1H-indazol-3-karboksyamid

ADB-PINACA isomer 4 - (S)-N-(1-amino-4-metyl-1-oksopentan-2-yl)-1-pentyl-1H-indazol-3-karboksyamid

AFB-48 - 1-[(4-fluorofenylo)metylo]-N-tricyklo[3.3.1.13,7]dec-1-yl-1H-indazol-3-karboksyamid

AH-7921 - 3,4-dichloro-N-[[1-(dimetyloamino)cykloheksyl]metylo]-benzamid

Alfa-ethylaminopentiophenone - 2-(etyloamino)-1-fenyl-1-pentanon

Alfa-propylaminopentiophenone - 1-fenylo-2-(propyloamino)-1-pentanon

Allylescalin - 3,5-dimetoksy-4-(2-propen-1-yloksy)-benzenoetanoamina

Alpha-dimethylaminopentiophenone - 2-(dimetyloamino)-1-fenylo-1-pentanon

Alpha-ethylaminohexanophenone - 2-(etyloamino)-1-fenyl-1-heksanon

Alpha-hydroxymidazolam - 8-chloro-6-(2-fluorofenyl)-4H-imidazo[1,5-a][1,4]benzodiazepin-1-metanol

Alpha-methyltryptamine - alfa-metylo-1H-indol-3-etanoamina

Alpha-phtalimidopropiophenone - 2-(1-okso-1-fenylopropan-2-yl)isoindol-1,3-dion

Alprazolam - 8-chloro-1-metylo-6-fenylo-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepina

AM1220 - [1-[(1-metylo-2-piperidinylo)metylo]-1H-indol-3-yl]-1-naftalenylo-metanon

AM-1248 - [1-[(1-metylo-2-piperidinylo)metylo]-1H-indol-3-yl]tricyklo[3.3.1.13,7]dec-1-yl-metanon

AM-2201 - [1-(5-fluoropentylo)-1H-indol-3-yl]-1-naftalenylo-metanon

AM2201 8-quinolinyl carboxamide - 1-(5-fluoropentylo)-N-8-quinolinylo-1H-indol-3-karboksyamid

AM2201 adamantyl analog - [1-(5-fluoropentyl)-1H-indol-3-yl]tricyclo[3.3.1.13,7]dec-1-yl-metanon

AM2232 - 3-(1-naftalenylokarbonylo)-1H-Indol-1-pentanonitryl

AM678 - 1-naftalenylo(1-pentylo-1H-indol-3-yl)-metanon

AMB-PICA - N-[(1-pentylo-1H-indol-3-yl)karbonylo]-L-walina, ester metylowy

Amitriptyline - 3-(10,11-dihydro-5H-dibenzo[a,d]cyklohepten-5-yliden)-N,N-dimetylo-1-propanamina

Amphetamine - α-metylo-benzenoetanoamina

APICA (JWH-018 adamantyl carboxamide) - 1-pentylo-N-tricyklo[3.3.1.13,7]dec-1-yl-1H-indol-3-karboksyamid

Atenolol - 4-[2-hydroksy-3-[(1-metyloetylo)amino]propoksy]-benzenoacetamid

Atrazine - 6-chloro-N2-etylo-N4-(1-metyloetylo)-1,3,5-triazyno-2,4-diamina

Azacyclonol - α,α-difenyl-4-piperidinometanol

Ba 34276 (maprotiline) - N-metylo-9,10-etanoantracen-9(10H)-propanamina

BB-22 - ester 8-chinolinylowy kwasu 1-(cykloheksylometylo)-1H-indolo-3-karboksylowego

BCP - 1-(1-benzo[b]tien-2-ylcykloheksylo)-piperidyna; benocyklidyna

BD 98 (phenazepam) - 7-bromo-5-(2-chlorofenylo)-1,3-dihydro-2H-1,4-benzodiazepin-2-on

BDB - α-etylo-1,3-benzodioksol-5-etanoamina

Benzocaine - ester etylowy kwasu 4-amino benzoesowego

Benzoylecgonine - kwas (1R,2R,3S,5S)-3-(benzoiloksy)-8-metylo-8-azabicyklo[3.2.1]octane-2-karboksylowy

Benzydamine - N,N-dimetylo-3-[[1-(fenylometylo)-1H-indazol-3-yl]oksy]-1-propanamina

BIM-018 (JWH 018 benzimidazole analog) - naftalen-1-yl(1-pentylo-1H-benzo[d]imidazol-2-yl)metanon

bk-2C-B - 2-amino-1-(4-bromo-2,5-dimetoksyfenyl)-etanon

bk-DMBDP - 1-(1,3-benzodioksol-5-yl)-2-(dimetyloamino)-1-pentanon; N,N-dimetylopentylon

bk-EBDB - 1-(benzo[d][1,3]dioksol-4-yl)-2-(etyloamino)butan-1-on; eutylon

bk-MBDB - 1-(1,3-benzodioksol-5-yl)-2-(metyloamino)-1-butanon; butylon

bk-MDA - 3,4-Metylenodioksykatynon

bk-MDDMA - 1-(1,3-benzodioksol-5-yl)-2-(dimetyloamino)-1-propanon; dimetylon

bk-MDMA - 1-(1,3-benzodioksol-5-yl)-2-(metyloamino)-1-propanon; metylon

BMPEA - β-metylo-benzenoetanoamina

BRL29060A (paroxetine) - 3S,4R)-3-[(1,3-benzodioksol-5-yloksy)metyl0]-4-(4-fluorofenylo)-piperidyna

Bromo-DRAGON-FLY - 8-bromo-α-metylo-benzo[1,2-b:4,5-b']difuran-4-etanoamina

Buprenorphine - αS,5α,7α)-17-(cyklopropylometylo)-α-(1,1-dimetyloetylo)-4,5-epoksy-18,19-dihydro-3-hydroksy-6-metoksy-α-metylo-6,14-etenomorfinan-7-metanol

Bupropion - 1-(3-chlorofenyl)-2-[(1,1-dimetyloetylo)amino]-1-propanon

Camfetamine - N-Metylo-3-fenylonorbornan-2-amina

Carbamazepine - 5H-Dibenzo[b,f]azepino-5-karboksyamid

Cathinone - (2S)-2-amino-1-fenylopropan-1-on

CBD - 2-[1R-3-metylo-6R-(1-metyloetenylo)-2-cykloheksen-1-yl]-5-pentylo-1,3-benzenodiol

CBL-018 - naftalen-1-yl 1-pentylo-1H-indol-3-karboksylat

CBL-2201 (NM2201) - ester 1-naftalenowy kwasu 1-(5-fluoropentylo)-1H-indol-3-karboksylowego,

CE - energia zderzeń

CI 1008 (pregabalin) - kwas 3S-(aminometylo)-5-metylo-heksanowy

CI2201 - (4-chloro-1-naftalenylo)[1-(5-fluoropentylo)-1H-indol-3-yl]-metanon
CI-581 (ketamina) - 2-(2-chlorofenyl)-2-(metyloamino)-cykloheksanon
CI-634 (tiletamine) - 2-(etyloamino)-2-(2-tienylo)-cykloheksanon
Clobazam - 7-Chloro-1-metylo-5-fenylo-1H-1,5-benzodiazepin-2,4(3H,5H)-dion
Clomipramine - 3-chloro-10,11-dihydro-N,N-dimetylo-5H-dibenz[b,f]azepin-5-propanoamina
Clonazepam - 5-(2-chlorofenyl)-1,3-dihydro-7-nitro-2H-1,4-benzodiazepin-2-on
Cocaethylene - kwas (1R,2R,3S,5S)-3-(benziloksy)-8-metylo-8-azabicyklo[3.2.1]octan-2-karboksylowy
Cocaine - kwas (1R,2R,3S,5S)-3-(benzoiloksy)-8-(metylo)-8-azabicyklo[3.2.1]octan-2-karboksylowy
Codeine - (5α,6α)-7,8-didehydro-4,5-epoksy-3-metoksy-17-metylo-morfinan-6-ol
CRA-13 - 1-naftalenylo[4-(pentyloksy)-1-naftalenylo]-metanon
CUMYL-PICA - N-(1-metylo-1-fenyloetylo)-1-pentylo-1H-indol-3-karboksyamid
CXP - potencjał wyjściowy
D2PM - α,α-difenylo-2R-pyrrolidinometanol
DBZP - 1,4-dibenzylpiperazyna
Demoxepam - 4-tlenek 7-Chloro-5-fenyl-1,3-dihydro-2H-1,4-benzodiazepin-2-onu
DEP - 1-(1,2-difenyloetylo)-piperidyna; difenidyna
Desalkylflurazepam - 7-chloro-5-(2-fluorofenylo)-1,3-dihydro-2H-1,4-benzodiazepin-2-on
Deschloroetizolam - 2-etylo-9-metylo-4-fenylo-6H-tieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepina
Desipramine - 5-[3-(Metyloamino)propylo]-5H-dibenz[b,f]azepina
Desmethylflunitrazepam - 5-(2-fluorofenylo)-1,3-dihydro-7-nitro-2H-1,4-benzodiazepin-2-one
Desomorphine - 4,5α-epoksy-17-metylo-morfinian-3-ol
Desoxy-D2PM - 2-(difenylometylo)-pyrrolidyna
DHAI - 5,6-dihydroksy-2-aminoindan
Diazepam - 7-chloro-1,3-dihydro-1-metylo-5-fenylo-2H-1,4-benzodiazepin-2-on
Diclazepam - 7-chloro-5-(2-chlorofenylo)-1,3-dihydro-1-metylo-2H-1,4-benzodiazepin-2-on
Diethylcathinone (amfepramone) - 2-(dietyloamino)-1-fenylo-1-propanon
Dihydrocodeine - 4,5α-epoksy-3-metoksy-17-metylo-morfinian-6α-ol
Dimethocaine - 3-(dietyloamino)-2,2-dimetylo-1-(4-aminobenzoesano)-1-propanol
DiPT - N,N-bis(1-metyloetylo)-1H-indol-3-etanoamina
DL-4662 - 1-(3,4-dimetoksyfenylo)-2-(etyloamino)pentan-1-on
DL-ephedrone (methcathinone) - 2-(metyloamino)-1-fenylo-1-propanon
DMMA - 4-metylo-2-heksanoamina; metylheksanamina
DOI - 4-jodo-2,5-dimetoksy-alfa-metylo-benzenoetanoamina
Dothiepin - (3Z)-3-(6H-benzo[c][1]benzotiepin-11-yliden)-N,N-dimetylopropan-1-amina
Doxepin - 3-(dibenz[b,e]oksepin-11(6H)-yliden)-N,N-dimetylo-1-propanamina
DP - potencjał rozgrupowania klastrów
DPH - 2-(difenylometoksy)-N,N-dimetylo-etanoamina; difenhydramina
DXM - (9α,13α,14α)-3-metoksy-17-metylo-morfinan; dekstrometorfan
E-4 (RCS-4) - (4-metoksyfenylo)(1-pentylo-1H-indol-3-yl)metanon
EAM-2201 - (4-etylo-1-naftalenylo)[1-(5-fluoropentylo)-1H-indol-3-yl]-metanon
EDDP - 5-etylo-3,4-dihydro-1,2-dimetylo-4,4-difenylo-2H-pirol
EG-2201 - [9-(5-fluoropentylo)-9H-karbazol-3-yl]-1-naftalenylo-metanon
EP - potencjał wejściowy
Ephylone - 1-(1,3-benzodioksol-5-yl)-2-(etyloamino)-1-pentanon; N-etylopentylon
Ergometrine - (6aR,9R)-N-[(2S)-1-hydroksypropan-2-yl]-7-metylo-6,6a,8,9-tetrahydro-4H-indolo[4,3-fg]chinolino-9-karboksyamide
ESI - jonizacja poprzez rozpraszanie (ang. electrospray ionization)
Estazolam - 8-chloro-6-fenylo-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepina

Etaqualone - 3-(2-etylofenylo)-2-metylo-4(3H)-chinazolinon

Ethcathinone metabolite - 2-(etyloamino)-1-fenylopropan-1-ol

Ethylphenidate - ester etylowy kwasu (αR,2R)-rel-α-fenylo-2-piperidynooctowego

Etizolam - 4-(2-chlorofenylo)-2-etylo-9-metylo-6H-tieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepina

FDU-PB-22 - ester naftalenylowy kwasu 1-[(4-fluorofenylo)metylo]-1H-indolo-3-karboksylowego

Fenfluramine - N-etylo-α-metylo-3-(trifluorometylo)-benzenoetanoamina

Fentanyl - N-fenylo-N-[1-(2-fenyloetylo)-4-piperidynylo]-propanoamid

Flubromazepam - 7-bromo-5-(2-fluorofenylo)-1,3-dihydro-2H-1,4-benzodiazepin-2-on

Fludiazepam - 7-chloro-5-(2-fluorofenyl)-1,3-dihydro-1-metylo-2H-1,4-benzodiazepin-2-on

Flumazenil - kwas 8-fluoro-5,6-dihydro-5-metylo-6-okso-4H-imidazo[1,5-a][1,4]benzodiazepino-3 karboksylowy

Flunitrazepam - 5-(2-fluorofenylo)-1,3-dihydro-1-metylo-7-nitro-2H-1,4-benzodiazepin-2-on

Fluoxetine - N-metylo-γ-[4-(trifluorometylo)fenoksy]-benzenopropanoamina

Flurazepam - 7-chloro-1-[2-(dietyloamino)etylo]-5-(2-fluorofenylo)-1,3-dihydro-2H-1,4-benzodiazepin-2-on

FPP - 1-(4-fluorofenylo)piperazyna

FUB-144 - [1-[(4-fluorofenylo)metylo]-1H-indol-3-ylo](2,2,3,3-tetrametylocyklopropylo)-methanon

Fubimina - [1-(5-fluoropentylo)benzimidazol-2-ylo](naftaleno-1-ylo)-metanon

FUB-JWH-018 - (1-(4-fluorobenzylo)-1H-indol-3-ylo)(naftalen-1-ylo)metanon

FUB-PB-22 - ester 8-chinolinolowy kwasu 1-[(4-fluorofenylo)metylo]-1H-indole-3-karboksylowego

Fu-F - N-fenylo-N-[1-(2-fenyloetylo)-4-piperidinylo]-2-furanokarboksyamid; furanylfentanyl

F-α-POP - 1-(4-fluorofenylo)-2-(1-pyrrolidinylo)-1-oktanon; 4-fluro PV9

GC-MS - chromatografia gazowa sprzężona ze spektrometrią mas (ang. gas chromatography coupled with mass spectrometry)

GHB - kwas 4-hydroksy-butanowy

Harmaline - 4,9-dihydro-7-metoksy-1-metylo-3H-pyrido[3,4-b]indol

Harmine - 7-metoksy-1-metylo-9H-pyrido[3,4-b]indol

HMAI - 5-hydroksy-6-metoksy-2-aminoindan

HU-210 - 3-(1,1'-dimetyloheptylo)-6aR,7,10,10aR-tetrahydro-1-hydroksy-6,6-dimetylo-6H-dibenzo[b,d]pyrano-9-metanol

Hydrocodone - 4,5α-epoksy-3-metoksy-17-metylo-morfinian-6-on

I-C6 (MT45) - 1-cykloheksylo-4-(1,2-difenyloetylo)-piperazina

ICI 204636 (quetiapine) - 2-[2-(4-dibenzo[b,f][1,4]tiazepin-11-ylo-1-piperazinyol)etoksy]-etanol

Imipramine - 10,11-dihydro-N,N-dimetylo-5H-dibenz[b,f]azepino-5-propanoamina

Isopentedrone - 1-(metyloamino)-1-fenylo-2-pentanon

JWH 018 indazole analog - 1-naftalenylo(1-pentylo-1H-indazol-3-ylo)-metanon

JWH-011 - [2-metylo-1-(1-metylohksylo)-1H-indol-3-ylo]-1-naftalenylo-metanon

JWH-016 - 1-butylo-2-methylo-1H-indol-3-ylo)-1-naftalenylo-metanon

JWH-020 - (1-heptylo-1H-indol-3-ylo)-1-naftalenylo-metanon

JWH-022 - 1-naftalenylo[1-(4-penten-1-ylo)-1H-indol-3-ylo]-metanon

JWH-031 - (1-heksylo-1H-pyrrol-3-ylo)-1-naftalenylo-metanon

JWH-071 - (1-etylo-1H-indol-3-ylo)-1-naftalenylo-metanon

JWH-073 - (1-butylo-1H-indol-3-ylo)-1-naftalenylo-metanon

JWH-080 - (1-butylo-1H-indol-3-ylo)(4-metoksy-1-naftalenylo)-metanon

JWH-081 - (4-metoksy-1-naftalenylo)(1-pentylo-1H-indol-3-ylo)-metanon

JWH-098 - (4-metoksy-1-naftalenylo)(2-metylo-1-pentylo-1H-indol-3-ylo)-metanon

JWH-116 - (2-etylo-1-pentylo-1H-indol-3-ylo)-1-naftalenylo-metanon

JWH-122 - (4-metylo-1-naftalenylo)(1-pentylo-1H-indol-3-ylo)-metanon

JWH-145 - 1-naftalenylo(1-pentylo-5-fenylo-1H-pirol-3-ylo)-metanon

JWH-146 - (1-heptylo-5-fenylo-1H-pirol-3-ylo)-1-naftalenylo-metanon

JWH-147 - (1-heksylo-5-fenylo-1H-pirol-3-ylo)-1-naftalenylo-metanon

JWH-149 - (4-metylo-1-naftalenylo)(2-metylo-1-pentylo-1H-indol-3-ylo)-metanon

JWH-167 - 1-(1-pentylo-1H-indol-3-ylo)-2-fenylo-etanon

JWH-175 - 3-(1-naftalenylometylo)-1-pentylo-1H-indol

JWH-182 - (1-pentylo-1H-indol-3-ylo)(4-propylo-1-naftalenylo)-metanon

JWH-193 - (4-metylo-1-naftalenylo)[1-[2-(4-morfolinylo)etylo]-1H-indol-3-ylo]-metanon

JWH-198 - (4-metoksy-1-naftalenylo)[1-[2-(4-morfolinylo)etylo]-1H-indol-3-ylo]-metanon

JWH-200 - [1-[2-(4-morfolinylo)etylo]-1H-indol-3-ylo]-1-naftalenylo-metanon

JWH-201 - 2-(4-metoksyfenylo)-1-(1-pentylo-1H-indol-3-ylo)-etanon

JWH-213 - (4-etylo-1-naftalenylo)(2-metylo-1-pentylo-1H-indol-3-ylo)-metanon

JWH-307 - [5-(2-fluorofenylo)-1-pentylo-1H-pirol-3-ylo]-1-naftalenylo-metanon

JWH-309 - 1-naftalenylo[5-(1-naftalenylo)-1-pentylo-1H-pirol-3-ylo]-metanon

JWH-368 - [5-(3-fluorofenylo)-1-pentylo-1H-pirol-3-ylo]-1-naftalenylo-metanon

JWH-369 - [5-(2-chlorofenylo)-1-pentylo-1H-pirol-3-ylo]-1-naftalenylo-metanon

JWH-412 - (4-fluoro-1-naftalenylo)(1-pentylo-1H-indol-3-ylo)-metanon

JWH-424 - (8-bromonaftalen-1-ylo)(1-pentylo-1H-indol-3-ylo)metanon

LAMPA - (8β)-9,10-didehydro-N,6-dimetylo-N-propylo-ergolino-8-karboksyamid

LC-HRMS - chromatografia cieczowa sprzężona z wysokorozdzielczą spektrometrią mas (ang. liquid chromatography coupled with high resolution mass spectrometry)

LC-MS/MS - chromatografia cieczowa sprzężona z tandemową spektrometrią mas (ang. liquid chromatography coupled with tandem mass spectrometry)

LOD – granica wykrywalności

Loprazolam - (2Z)-6-(2-Chlorofenylo)-2,4-dihydro-2-[(4-metylo-1-piperazinylo)metyleno]-8-nitro-1H-imidazo[1,2-a][1,4]benzodiazepin-1-on

LOQ - granica oznaczalności

Lormetazepam - 7-Chloro-5-(2-chlorofenylo)-3-hydroksy-1-metylo-1,3-dihydro-2H-1,4-benzodiazepin-2-on

LSD - dietyloamid kwasu lizergowego

MA - N,α-dimetylo-benzenoetanoamina; metamfetamina

M-ALPHA -1-metyloamino-1-(3,4-metylenodioksyfenylo)propan

MAM-2201 - [1-(5-fluoropentylo)-1H-indol-3-ylo](4-metylo-1-naftalenylo)-metanon

MBDB - α-etylo-N-metylo-1,3-benzodioksolo-5-etanoamina

MBZP - 1-metylo-4-(fenylometylo)-piperazina

mCPP - 1-(3-chlorofenylo)-piperazina

MDAI - 5,6-metylenodioksy-2-aminoindan

MDAT - 6,7-metylenodioksy-2-aminotetralina

MDBP -1-(3,4metylenodioksybenzylo)piperazyna

MDEA - N-etylo-alfa-metylo-1,3-benzodioksolo-5-etanoamina

MDEC - 1-(1,3-benzodioksol-5-ylo)-2-(etyloamino)-1-propanon; etylon

MDMB-CHMINACA - N-[[1-(cykloheksylometylo)-1H-indazol-3-ylo]karbonylo]-3-metylo-L-walina

MDPBP - 1-(1,3-benzodioksol-5-ylo)-2-(1-pirrolidinylo)-1-butanon

Meclonazepam - (3S)-5-(2-chlorofenylo)-1,3-dihydro-3-metylo-7-nitro-2H-1,4-benzodiazepin-2-on

Medazepam - 7-chloro-1-metylo-1,3-dihydro-2H-1,4-benzodiazepina

Memantine - 1-amino-3,5-dimetyloadamantan

MeOH - metanol

MeOPP - 1-(4-metoksyfenylo)piperazyna

Mepirapim - (4-metylo-1-piperazinylo)(1-pentylo-1H-indol-3-ylo)-metanon

Meprobamate - ester 2-metylo-2-propylotrimetylenowy kwasu karbaminowego

Methadone - 6-(dimetyloamino)-4,4-difenylo-3-heptanon

Methandienone - (17β)-17-hydroksy-17-metyloandrosta-1,4-dien-3-on

Methohexital - 5-Allilo-1-metylo-5-(1-metylo-pent-2-ynylo)-pirymidyno-2,4,6-trion

Methylphenidate - kwas 2-Piperidynooctowy

Mexedrone - 3-metoksy-2-(metyloamino)-1-(p-tolilo)propan-1-on

Mianserin - (±)-2-metylo-1,2,3,4,10,14b-heksahydrodibenzo[*c*,*f*]piperazyno[1,2-*a*]azepina

Midazolam - 8-chloro-6-(2-fluorofenylo)-1-metylo-4H-imidazo[1,5-a][1,4]benzodiazepina

Mitragynine - ester metylowy kwasu (αE,2S,3S,12bS)-3-etylo-1,2,3,4,6,7,12,12b-oktahydro-8-metoksy-α-(metoksymetyleno)-indolo[2,3-a]chinolizyno-2-actowego

MMAI - 2,3-dihydro-5-metoksy-6-metylo-1H-indeno-2-amina

MMB-CHMINACA - N-[[1-(cykloheksylometylo)-1H-indol-3-ylo]karbonylo]-3-metylo-L-walina

MN-18 - N-1-naftalenylo-1-pentylo-1H-indazolo-3-karboksyamid

MN-24 (NNEI) - N-1-naftalenylo-1-pentylo-1H-indolo-3-karboksyamid

MN-25-2-methyl derivative - 7-metoksy-2-metylo-1-[2-(4-morfolinylo)etylo]-N-[(1S,2S,4R)-1,3,3-trimetylobicyklo[2.2.1]hept-2-ylo]-1H-indolo-3-karboksyamid

MO-AMB - 1-metoksy-3,3-dimetylo-1-oksobutan-2-yl

Morphine - 7,8-didehydro-4,5α-epoksy-17-metylo-morfinian-3,6α-diol

MPBP - 4'-Metylo-alfa-pirrolidynobutiofenon

MTTA - 3,4-dihydro-2-[(metyloamino)metylo]-1(2H)-naftalenon; meftetramina

MXE - 2-(etyloamino)-2-(3-metoksyfenylo)-cykloheksanon

MXP - 1-(1-(2-metoksyfenylo)-2-fenyloetylp)piperydyna; metoksyfenidyna

N,N-DMC - 2-(dimetyloamino)-1-fenylo-1-propanon

N-acetyl-3,4-MDMC - N-[2-(1,3-benzodioksol-5-ylo)-1-metylo-2-oksoetylo]-N-metylo-acetamid

N-benzylnorbutylone - N-benzyl-(3,4-metylenodioksyfenylo)-2-aminobutan-1-on

N-desmethylclobazam (norclobazam) - 8-chloro-1-fenylo-1H-1,5-benzodiazepin-2,4(3H,5H)-dion

N-desmethylclomipramine (norclomipramine) - 3-chloro-10,11-dihydro-N-metylo-5H-dibenz[b,f]azepino-5-propanoamina

N-desmethylketamine (norketamine) - 2-amino-2-(2-chlorofenylo)-cykloheksanon

NEB - 2-(etyloamino)-1-fenylobutan-1-on; n-etylobufedron

N-ethyl-n-methylcathinone - 2-(etylo(metylo)amino)-1-fenylopropan-1-on

N-ethylnordazepam - 7-chloro-1-etylo-5-fenylo-3H-1,4-benzodiazepin-2-on

N-ethylnorketamine - 2-(2-chlorofenylo)-2-(etyloamino)-cykloheksanon

N-ethyloxazepam - N-etylo-9-chloro-4-hydroksy-6-fenylo-2,5-diazabicyklo[5.4.0]undeka-5,8,10,12-tetraen-3-on

NIH 10522 (meperidine) - ester etylowy kwasu 1-metylo-4-fenylo-4-piperydinokarboksylowego

Nitracaine - 3-(dietyloamino)-2,2-dimetylopropylo-4-nitrobenzoesan

NM2AI - N-metylo-2-amino-indan (N-metylo-2,3-dihydro-1H-inden-2-amina)

N-methyl-PEA - N-metylo-2-fenyloetyloamina

NMT - N-metylo-1H-indolo-3-etanoamina

Nortriptyline - 3-(10,11-dihydro-5H-dibenzo[a,d]cyklohepten-5-ylideno)-N-metylo-1-propanoamina

NPA - α-metylo-N-propylo-benzenoetanoamina

NPS - nowe substancje psychoaktywne (ang. New Psychoactive Substances)

NRG-1 - 1-(2-naftalenylo)-2-(1-pirrolidynylo)-1-pentanon

NRG-3 - 2-(metyloamino)-1-(naftalen-2-ylo)pentan-1-on

NSC 111388 (methaqualone) - 2-metylo-3-(2-metylofenylo)-4(3H)-chinazolinon

NSC 169448 (oksazepam) - 7-chloro-1,3-dihydro-3-hydroksy-5-fenylo-2H-1,4-benzodiazepin-2-on

NSC 19045 (oksymorfon) - (5α)-4,5-epoksy-3,14-dihydroksy-17-metylo-morfinian-6-on

NSC 246303 (temazepam) - 7-chloro-1,3-dihydro-3-hydroksy-1-metylo-5-fenylo-2H-1,4-benzodiazepin-2-on

NSC 27110 (propylhexedrine) - N,α-dimetylo-cykloheksanoetanoamina

NSC 277179 (prazepam) - 7-chloro-1-(cyklopropylometylo)-1,3-dihydro-5-fenylo-2H-1,4-benzodiazepin-2-on

NSC 279758 (lorazepam) - 7-chloro-5-(2-chlorofenylo)-1,3-dihydro-3-hydroksy-2H-1,4-benzodiazepin-2-on

NSC 29847 (ibogaine) - 12-metoksy-ibogamina

NSC 40030 (lidokaina) - 2-(dietyloamino)-N-(2,6-dimetylofenylo)-acetamid

NSC 58775 (nitrazepam) - 1,3-dihydro-7-nitro-5-fenylo-2H-1,4-benzodiazepin-2-on

NSC 63795 (n,n-dmt) - N,N-dimetylo-1H-indolo-3-etanoamina

NSC 74772 - N,N-dimetylo-2-[1-fenylo-1-(2-pirydinylo)etoksy]monoetanoamina; doksylamina

NSC 91523 (propranolol) - 1-[(1-metyloetylo)amino]-3-(1-naftalenyloksy)-2-propanon

NSC 9848 (phenobarbital) - 5-etylo-5-fenylo-2,4,6(1H,3H,5H)-pirymidinotrion

NSC169914 (prolintane) - 1-[1-(fenylometylo)butylo]-pirrolidyna

o-CPP - orto-chlorofenylopiperazyna

Octacaine - Butanamid, 3-(dietyloamino)-N-fenylobutanoamid

O-PCE - 2-(etyloamino)-2-fenylo-cykloheksanon; deschloro-n-etylo-ketamina

ORG-28611 - [1-(cykloheksylometylo)-7-metoxy-1H-indol-3-ylo](3,4-dimetylo-1-piperazynylo)-metanon

PCMPA - N-(3-metoksypropylo)-1-fenylo-cykloheksanoamina

PCP - 1-(1-fenylocykloheksylo)-piperydyna; fencyklidyna

pCPP - 1-(4-chlorofenylo)piperazyna

PCPr - 1-fenylo-N-propylo-cykloheksanoamina

Pentedrone - 2-(metyloamino)-1-fenylo-1-pentanon

Pentedrone metabolite - α-[(1R)-1-(metyloamino)butylo]-benzenometanol

Pentylone (bk-MBDP) - 2-(metyloamino)-3',4'-(metylenodioksy)-walerofenon

Phentermine - α,α-dimetylo-benzenoetanoamina

Phenytoin - 5,5-difenylo-2,4-imidazolidinodion

PMEA -N-etylo-4-metoksy-alfa-metylo-benzenoetanoamina; n-etylo-4-metoksyamfetamina

PMMA - 4-metoksy-N,α-dimetylo-benzenoetanoamina; 4-metoksymetamfetamina

PMMC - 1-(4-metoksyfenylo)-2-(metyloamino)-1-propanon; metedron

Procaine - 4-aminobenzoesan 2-(dietyloamino)etylu

Promethazine - N,N,α-trimetylo-10H-fenotiazyna-10-etanoamina

Propafenone - 1-[2-[2-hydroksy-3-(propyloamino)propoksy]fenylo]-3-fenylo-1-propanon

PSB-SB-1202 - 5-metoksy-3-[(2-metoksyfenylo)metylo]-7-pentylo-2H-1-benzopyran-2-on

PTI-1 - N,N-dietylo-2-(1-pentylo-1H-indol-3-ylo-4-tiazolometanoamina

PTI-2 - N-(2-metoksyetylo)-N-(1-metyloetylo)-2-(1-pentylo-1H-indol-3-ylo)-4-tiazolometanoamina

PV4 - 2-(pirrolidyn-1-ylo)-1-(p-tolilo)heksan-1-on; 4-metylo-PHP

Pyrazolam - 8-bromo-1-metylo-6-(2-pirydynylo)-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepina

QUPIC (PB-22) - Ester 8-chinolinylowy kwasu 1-pentylo-1H-indolo-3-karboksylowego

RH-34 - 3-[2-[[(2-metoksyfenylo)metylo]amino]etylo]-2,4(1H,3H)-chinazolinodion

Ro 5-3453 (nimetazepam) - 1,3-dihydro-1-metylo-7-nitro-5-fenylo-2H-1,4-benzodiazepin-2-on

Ro 8-4650 - 4-(3,4-dichlorofenylo)-1,2,3,4-tetrahydro-7-metoksy-2-metylo-izochinolina diklofensina

SCB - syntetyczne kannabinoidy

Scopolamine - 3-hydroksy-2-fenylpropanian 9-metylo-3-oksa-9-azatricyklo[3.3.1.$0^{2,4}$]nonan-7-ylu

SDB-005 - 1-pentylo-1H-indazolo-3-karboksylan naftalen-1-ylu

SDB-006 - 1-pentylo-N-(fenylometylo)-1H-indolo-3-karboksyamid

Sertraline - (1S,4S)-4-(3,4-dichlorofenylo)-1,2,3,4-tetrahydro-N-metylo-1-naftalenoamina

SGT-67 - 1-(5-fluoropentylo)-N-(1-metylo-1-fenyloetylo)-1H-indolo-3-karboksyamid; 5-fluoro-CUMYL-PICA

Sildenafil - 1-[4-etoksy-3-(6,7-dihydro-1-metylo-7-okso-3-propylo-1*H*-pirazolo[4,3-*d*]-pirymidyn-5-ylo)fenylosulfonylo]-4-metylopiperazyna

STS-135 (5F-APICA) - 1-(5-fluoropentylo)-N-tricyklo[3.3.1.13,7]dec-1-ylo-1H-indolo-3-karboksyamid

SWGTOX – Naukowa Grupa Robocza ds. Toksykologii Sądowej (ang. Scientific Working Group for Forensic Toxicology)

Tapentadol - 3-[(1R,2R)-3-(dimetyloamino)-1-etylo-2-metylopropylo]-fenol

Tetracaine - 4-(butyloamino)benzoesan 2-(dimetyloamino)etylu

TFMPP - 1-(3-trifluorometylofenylo)piperazyna

THC - 6aR,7,8,10aR-tetrahydro-6,6,9-trimetylo-3-pentylo-6H-dibenzo[b,d]pyran-1-ol

THCCOOH - (-)-11-Nor-9-karboksy-delta9-THC

Thiopropamine - α-metylo-2-tiofenoetanoamina

THJ - 1-pentylo-N-(chinolin-8-ylo)-1H-indazolo-3-karboksyamid

THJ-2201 (5-fluoro THJ-018) - [1-(5-fluoropentylo)-1H-indazol-3-yol]-1-naftalenylo-metanon

TMPEA - 3,4,5-trimetoksy-benzenoetanoamina; meskalina

Tramadol (CG 315) - el-2R-[(dimetyloamino)metylo]-1R-(3-metoksyfenylo)-cykloheksanol

Trazodone - 2-[3-[4-(3-chlorofenylo)-1-piperazynylo]propylo]-1,2,4-triazolo[4,3-a]pirydyn-3(2H)-on

Triazolam (U-33030) - 8-chloro-6-(2-chlorofenylo)-1-metylo-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepina

Trimipramine - 10,11-dihydro-N,N,β-trimetylo-5H-dibenz[b,f]azepino-5-propanoamina

U-47700 - trans-3,4-dichloro-N-[2-(dimetyloamino)cykloheksylo]-N-metylo-benzamid

UGT - glukuronylotransferaza

UNODC - Biuro Narodów Zjednoczonych ds. Narkotyków i Przestępczości (ang. United Nations Office on Drugs and Crime)

UR-12 - 7-metoksy-1-[2-(4-morfolinylo)etylo]-N-[(1S,2S,4R)-1,3,3-trimetylobicyklo[2.2.1]hept-2-ylo]-1H-indolo-3-karboksyamid

UR-144 (KM-X1) - (1-pentylo-1H-indol-3-ylo)(2,2,3,3-tetrametylocyklopropylo)-metanon

UR-144 metabolite (XLR11 N-(4-hydroxypentyl) metabolite) - (1-(4-hydroksypentylo)-1H-indol-3-ylo)(2,2,3,3-tetrametylocyklopropylo)metanon

W-15 - 4-chloro-N-[1-(2-fenyloetylo)-2-piperydynylideno]-benzenosulfonoamid

WIN 14,833 (stanozolol) - 17α-metylo-2'H-5α-androst-2-eno[3,2-c]pirazol-17β-ol;

WIN 48,098 (pravadoline) - (4-metoksyfenylo)[2-metylo]-1-[2-(4-morfolinylo)etylo]-1H-indol-3-ylo]-metanon

WIN 54,461 - [6-bromo-2-metylo-1-[2-(4-morfolinylo)etylo]-1H-indol-3-ylo](4-metoksyfenylo)-metanon

WIN 55,212-2 - (11R)-2-metylo-11-[(morfolin-4-ylo)metylo]-3-(naftaleno-1-karbonylo)-9-oksa-1-azatricyklo[6.3.1.04,12]dodeka-2,4 (12),5,7-tetraen

XLR12 - (2,2,3,3-tetrametylocyklopropylo)[1-(4,4,4-trifluorobutylo)-1H-indol-3-ylo]-metanon

Yangonin - 4-metoksy-6-[(1E)-2-(4-metoksyfenylo)etenylo]-2H-piran-2-on

Zaleplon (CL 284,846) - N-[3-(3-cyjanopirazolo[1,5-a]pirymidyn-7-ylo)fenylo]-N-etyloacetamid

Zolpidem (SL 80-0750) - N,N,6-trimetylo-2-(4-metylofenylo)-imidazo[1,2-a]pirydyno-3-acetamid

Zopiclone (RP 27267) - (*RS*)-4-metylopiperazyno-1-karboksylan 6-(5-chloropirydyn-2-ylo)-5-okso-7*H*-pirolo[3,4-*b*]pirazyn-7-ylu

Zuclopenthixol - (*Z*)-2-{4-[3-(2-chloro-9*H*-tioksanten-9-ylideno)propylo]piperazyn-1-ylo}etanol

α-ET - α-etylo-1H-indolo-3-etanoamina; alfa-etylotryptamina

α-naphyrone - 1-(naftalen-1-ylo)-2-(pirrolidyn-1-ylo)pentan-1-on;

α-PBP - 1-fenylo-2-(1-pirrolidynylo)-1-butanon

α-PHP -1-fenylo-2-(1-pirrolidynylo)-1-heksanon

α-PHPP (PV8) - 1-fenylo-2-(1-pirrolidynylo)-1-heptanon

α-PipBP - 1-fenylo-2-(1-piperidynylo)-1-butanon

α-POP (PV9) - 1-fenylo-2-(1-pirrolidynylo)-1-oktanon

α-PPP - 1-fenylo-2-(1-pirrolidynylo)-1-propanon

α-PVP -1-fenylo-2-(1-pirrolidynylo)-1-pentanon

α-PVT -2-(1-pirrolidynylo)-1-(2-tienylo)-1-pentanon

1 Wprowadzenie

W ostatnich latach ciągle rosnącego zainteresowania substancjami psychoaktywnymi, które według Biura Narodów Zjednoczonych ds. Narkotyków i Przestępczości (UNODC) są klasyfikowane jako substancje nadużywające w postaci czystej lub w preparacie, które nie są objęte jednolitą konwencją o środkach odurzających z 1961 roku lub konwencją o substancjach psychotropowych z roku 1971. Mianem *nowe* oznacza się substancje, które pojawiły się na rynku nielegalnie i są używane w celach rekreacyjnych, a nie medycznych [1]. Tego typu substancje nazywane są również dopalaczami, działają na układ nerwowy podobnie jak klasyczne narkotyki (środki psychoaktywne), które podlegają surowym przepisom jednostek rządowych i są uwzględnione w konwencji o kontroli narkotyków [2].

Pojawiające się w nielegalnej sprzedaży *nowe* substancje psychoaktywne są ogromnym zagrożeniem dla zdrowia i życia zażywających je osób. Producenci tego typu substancji podejmują działania mające na celu ominięcie przepisów prawa poprzez modyfikowanie już nam znanych substancji psychoaktywnych, dzięki czemu wprowadzają do sprzedaży co raz to nowe dopalacze, które stanowią ogromne zagrożenie dla zdrowia i życia osób je zażywających. Im więcej modyfikacji strukturalnych zostanie przeprowadzonych w cząsteczce, tym trudniej jest ją jednoznacznie zidentyfikować i objąć restrykcjami prawnymi. Dzięki takim działaniom producentom udaje się uniknąć konsekwencji prawnych związanych z ich wytwarzaniem, rozprowadzaniem, a także uszczerbkiem na zdrowiu czy nawet śmiercią osób je zażywających, a co za tym idzie zwiększa się ich dostępność na nielegalnych rynkach [3]. Dodatkowym zagrożeniem dla zdrowia i życia jest fakt, iż nowe substancje psychoaktywne (NPS) często produkowane są w nieodpowiednich warunkach, przez co czystość i skład tych substancji często pozostaje nieznany [4].

Ogromna liczba dostępnych na rynku NPS to bardzo duże wyzwanie dla laboratoriów analitycznych. Ze względu na ilość analitów często stosuje się najpierw metody przesiewowe, a dopiero później próbkę podaje się analizie metodą konfirmacyjną w celu jednoznacznej identyfikacji analitu i wyznaczenia jego zawartości. Do metod przesiewowych zaliczają się między innymi metody immunochemiczne, które wciąż są stosowane przez wielu badaczy [5-18]. Niewątpliwą zaletą tych metod jest ich prostota i szybkość, jednakże wyniki uzyskiwane za pomocą tych metod często okazują się fałszywie pozytywne lub fałszywie negatywne ze względu na ich niską czułość i specyficzność [**D1**]. Dokładniejszą, co raz częściej stosowaną metodą analizy jest chromatografia gazowa sprzężona ze spektrometrią mas (GC-MS) [19-23].

Mimo, że metody te charakteryzują się niższą granicą wykrywalności (LOD) niż metody immunochemiczne [19], to nadal można napotkać wiele problemów analitycznych podczas ich stosowania. Jednym z nich jest konieczność upochodnienia badanych związków, co wydłuża czas analizy, zwiększa koszt jednostkowy, a także generuje utratę analitów i obniżenie wartości odzysku dla poszczególnych analitów [19]. Wychodząc naprzeciw tym problemom badacze stosują do oznaczania tych związków chromatografię cieczową sprzężoną z tandemową spektrometrią mas (LC-MS/MS) [24-33]. Technika ta umożliwia oznaczanie wielu substancji psychoaktywnych w toku jednej analizy, jednak w celu pełnej analizy toksykologicznej próbek biologicznych konieczne jest opracowanie nowych procedur umożliwiających identyfikację NPS. Poszukuje się takich rozwiązań analitycznych, które pozwolą oznaczyć wiele różnych grup związków w jednym i krótkim czasie, redukując koszty jednostkowej analizy oraz ilość odpadów, które są toksyczne [**D1**].

Substancje psychoaktywne, leki i ich metabolity stanowią obszerną grupę analitów w analizach toksykologicznych. Biorąc pod uwagę złożoność procesu przygotowania próbek do analizy oraz identyfikacji tak zróżnicowanych pod względem fizykochemicznym związków, widzimy niebagatelne wyzwanie dla laboratoriów toksykologicznych. Istnieje potrzeba opracowania metodyk analitycznych pozwalających na przygotowanie próbek z matryc biologicznych różniących się zawartością związków współwystępujących z jak największą efektywnością izolowania wszystkich badanych analitów oraz umożliwiające ich jednoznaczną identyfikację w możliwie krótkim czasie.

Niniejsza rozprawa doktorska wychodzi naprzeciw wyżej wspominanym problemom analitycznym i dotyczy opracowania metod pozwalających na identyfikację i ilościowe oznaczenie ponad 500 substancji psychoaktywnych, leków i ich metabolitów izolowanych z próbek krwi, moczu i włosów z wykorzystaniem techniki LC-MS/MS. Przeprowadzone badania wymagały opracowania selektywnej, a zarazem efektywnej metody ekstrakcji wybranych analitów z różnych matryc biologicznych oraz doboru warunków rozdzielania z wykorzystaniem chromatografii cieczowej i parametrów pracy spektrometru mas do ich identyfikacji. Opracowane procedury badawcze zostały poprawnie zweryfikowane poprzez udział w badaniach biegłości, co pozwoliło na wdrożenie ich do rutynowych analiz toksykologicznych w Instytucie Genetyki Sądowej w Bydgoszczy [**D4**].

Podstawę rozprawy doktorskiej stanowi cykl tematycznie spójnych publikacji, które ukazały się w specjalistycznych czasopismach naukowych o zasięgu międzynarodowym oraz zgłoszenie patentowe:

[**D1**] **Jadwiga Musiał**, Jakub Czarny, Renata Gadzała-Kopciuch, *Overview of analytical methods for determining novel psychoactive substances, drugs and their metabolites in biological samples*, Critical Reviews in Toxicology, 2022, 52:3, 239-258, https://doi.org/10.1080/10408444.2022.2091424, IF=6,184

[**D2**] **Jadwiga Musiał**, Jolanta Powierska-Czarny, Jakub Czarny, Michał Raczkowski, Natalia Galant, Bogusław Buszewski, Renata Gadzała-Kopciuch, *One-step extraction and determiantion of 513 psychoactive substances, drugs, and their metabolites from hair by LC-MS/MS*, Archives of Toxicology, 2022, 96:2927-2933, https://doi.org/10.1007/s00204-022-03343-w, IF=6,168

[**D3**] Jakub Czarny, **Jadwiga Musiał**, Jolanta Powierska-Czarny, Natalia Galant, Michał Raczkowski, Bogusław Buszewski, Renata Gadzała-Kopciuch, *Validation of a simple and quick method for determination of psychoactive substances, drugs and their metabolites from human blood by LC-MS/MS*, Microchemical Journal, 2022, 182: 107922, ISSN 0026-265X, https://doi.org/10.1016/j.microc.2022.107922, IF=5,304

[**D4**] Jolanta Powierska-Czarny, Jakub Czarny, Radosław Zbytniewski, Michał Raczkowski, Natalia Galant, **Jadwiga Musiał**., *Sposób wykrywania związków psychoaktywnych w próbkach biologicznych oraz zastosowanie tego sposobu do wykrywania substancji psychoaktywnych*, Zgłoszenie patentowe - Numer P.441164 UP

[**D5**] Jakub Czarny, **Jadwiga Musiał**, Jolanta Powierska-Czarny, Michał Raczkowski, Natalia Galant, Bogusław Buszewski, Renata Gadzała-Kopciuch, *Determination of 465 psychoactive substances, drugs and their metabolites in urine by LC-MS/MS*, Analytical Methods, 2024, https://doi.org/10.1039/D4AY00777H, IF=2,7

2 Cele i założenia rozprawy doktorskiej

Nadrzędnym celem rozprawy doktorskiej było opracowanie procedur analitycznych pozwalających na oznaczanie, jak największej liczby substancji psychoaktywnych, leków i ich metabolitów w toku jednego postępowania analitycznego i krótkim czasie w matrycach biologicznych takich jak: krew [**D3**], mocz [**D5**] i włosy [**D2**]. Badania realizowane w ramach pracy doktorskiej miały na celu wdrożenie opracowanych procedur badawczych do rutynowych analiz pod kątem identyfikacji substancji psychoaktywnych, leków i ich metabolitów w próbkach krwi, moczu i włosów w laboratorium Instytutu Genetyki Sądowej w Bydgoszczy.

Cel rozprawy realizowano poprzez:

- opracowanie efektywnej metody izolowania wybranych analitów należących do grupy substancji psychoaktywnych, ich metabolitów i leków z próbek krwi, moczu i włosów,
- dobór warunków chromatograficznych rozdzielenia wybranych substancji psychoaktywnych poprzez wybór odpowiedniego składu fazy ruchomej oraz rodzaju kolumny chromatograficznej, dobór parametrów identyfikacji badanych związków za pomocą spektrometru mas,
- walidacja opracowanych procedur analitycznych,
- weryfikacja metodyki postępowania analitycznego w badaniach międzylaboratoryjnych (badania biegłości),
- wdrożenie opracowanych metodyk analitycznych do rutynowych analiz w Instytucie Genetyki Sądowej w Bydgoszczy.

Do przeprowadzenia eksperymentów wykorzystano wzorce analityczne każdej z badanych substancji. Wszystkie anality wykorzystano do stworzenia mieszaniny analitów, która służyła do wzbogacania próbek biologicznych podczas przeprowadzanych badań. Do identyfikacji analitów wykorzystano tandemową spektrometrię mas (MS/MS) z jonizacją poprzez elektrorozpylanie w trybie jonów dodatnich i ujemnych. Analizy przeprowadzano w trybie monitorowania par MRM, po dwie pary dla każdego z analitów. Opracowane procedury poddano procesowi walidacji zgodnie z wytycznymi Naukowej Grupy Roboczej ds. Toksykologii Sądowej (ang. *Scientific Working Group for Forensic Toxicology* - SWGTOX).

3 Problem badawczy

3.1 Metabolizm substancji psychoaktywnych

Ze względu na ogromną ilość znanych już nowych substancji psychoaktywnych Biuro Narodów Zjednoczonych ds. Narkotyków i Przestępczości (ang. *United Nations Office on Drugs and Crime* - UNODC) podzieliło je na kilka grup. Wśród nich znajdują się: aminoindany, benzodiazepiny, pochodne fentanylu, lizergamidy, nitrazeny, substancje typu fencyklidyny, fenetylaminy, fenidaty, fenmetrazyny, piperazyny, substancje pochodzenia roślinnego, syntetyczne kannabinoidy, syntetyczne katynony, tryptaminy oraz inne substancje [34]. Odrębną grupę stanowią klasyczne narkotyki obejmujące: amfetaminy, opiaty i opioidy, kannabinoidy, katynony oraz barbiturany. Należy zaznaczyć, że analizy toksykologiczne tych psychoaktywnych substancji w próbkach biologicznych to nie tylko oznaczenie substancji macierzystej, ale przede wszystkim identyfikacja metabolitów zażytych substancji psychoaktywnych w celu weryfikacji wyników pochodzących z różnych matryc oraz podjęcia odpowiednich działań medycznych czy prawnych.

W trakcie badań zajmowano się substancjami należącymi do każdej z powyższych grup. Metabolizm wielu z tych substancji jest już dobrze poznany. Najlepiej zbadany jest metabolizm benzodiazepin, które należą do najczęściej przepisywanych leków na całym świecie. Pomimo wspólnego elementu strukturalnego (5-fenylo-1,3-dihydrobenzo[e][1,4]diazepina) benzodiazepiny różnią się właściwościami farmakokinetycznymi i metabolicznymi. Wykazują działanie anksjolityczne, uspokajające, nasenne, amnestyczne, przeciwpadaczkowe oraz zwiotczające mięśnie [35]. Czas działania danej benzodiazepiny jest ściśle związany z ilością metabolitów, które z niej powstają. Metabolizm tej grupy związków obejmuje dwa główne szlaki metaboliczne: utlenianie i glukuronidację. Benzodiazepiny o dłuższym czasie działania zwykle najpierw ulegają utlenieniu pod wpływem cytochromu P450 (CYP), w wyniku czego powstają aktywne metabolity, które następnie muszą ulec glukuronidacji w celu usunięcia z organizmu [36]. Natomiast benzodiazepiny, które ulegają bezpośredniej glukuronidacji, co prowadzi do powstania nieaktywnych i szybko wydalanych metabolitów, charakteryzują się krótkim czasem działania [37]. Szczegółowe ścieżki metabolizmu związków należących do tej grupy opisywało wielu badaczy [36-44]. Głównymi związkami z grupy benzodiazepin wykrywanymi we krwi są diazepam i nordiazepam, natomiast w przypadku próbek moczu są to oksazepam i temazepam, które ulegają reakcji sprzęgania z kwasem glukuronowym i zostają wydalone z moczem z identyczną szybkością z jaką powstają [45]. Dlatego kluczowe

jest wykrywanie tych substancji zarówno we krwi, jak i w próbkach moczu, co umożliwia potwierdzenie ich zażycia nawet po zakończeniu procesów metabolicznych w organizmie.

Kolejną z dobrze zbadanych grup są aminoindany. Jednym z najczęściej spotykanych związków należących do tej grupy jest MDAI, który wykazuje działanie serotoninergiczne. MDAI pojawił się na nielegalnym rynku jako substytut zakazanych leków stymulujących i entaktogennych, dlatego też uwzględniono go w badaniach. Szlak metaboliczny tej substancji jest dobrze znany [46-49] i dowodzi, że jest on wydalany z moczem głównie w postaci niezmienionej, co narzuca konieczność identyfikacji tej substancji w próbkach moczu. Warto zwrócić uwagę również na NM2AI, którego metabolizm został opisany w jednej z prac [50]. Badania potwierdziły konieczność analizowania zarówno NM2AI, jak i jego metabolitu 2AI w próbkach toksykologicznych. Oba te anality zostały wprowadzone do badań w naszym laboratorium.

Bardzo istotnymi w analizach toksykologicznych są te z NPS, które są wprowadzane do obrotu na skutek modyfikacji strukturalnych tych dobrze znanych i nielegalnych substancji psychoaktywnych. Procesy metaboliczne tych substancji nie są jeszcze zbyt dobrze znane. W pracy przeglądowej [**D1**] skoncentrowano się na analizie procesów związanych z używaniem kilku grup często stosowanych substancji psychoaktywnych. Poza tym, omówiono grupy, które są istotne pod względem toksykologicznym, ale jeszcze nie zostały uwzględnione w regulacjach prawnych. W opisywanych metodach badawczych skupiono się na piperazynach, kannabinoidach i ich syntetycznych pochodnych oraz opioidach i opiatach.

Piperazyny, które stanowią jedną z nowych grup narkotyków, dzielą się na dwie klasy: N-benzylpiperazyna (BZP) i jej analog MDBP oraz fenylopiperazyny (mCPP, TFMPP i MeOPP) [51]. Wytwarzane są one w celu obejścia przepisów prawa poprzez modyfikację struktury chemicznej niektórych produktów naturalnych lub innych zabronionych już narkotyków, a następnie sprzedawane w internecie pod nazwami takimi jak: *Rapture, Frenzy, Bliss, Charge, Herbal ecstasy, A2, Legal X* i *Legal E* [51]. Piperazyny są łatwo wchłaniane z przewodu pokarmowego, część wchłoniętej substancji jest metabolizowana i usuwana z moczem. Dopalacze pochodzące od piperazyny są metabolizowane głównie w wątrobie. Ze względu na fakt, iż fenelopiperazyny są metabolizowane w większym stopniu niż benzylopiperazyny, dlatego też są one wydalane prawie wyłącznie w postaci metabolitów [52]. Jako główny metabolit mCPP zidentyfikowano para-hydroksy-mCPP powstały na skutek aromatycznej hydroksylacji. Związek ten w postaci niezmienionej występował w małych ilościach [51]. Głównym produktem metabolizmu TFPP (związek strukturalnie podobny do mCPP) jest hydroksy-TFMPP, który następnie ulega częściowej glukuronidacji lub

siarczanowaniu. Natomiast degradacja heterocyklu piperazyny poprzez podwójną N-dealkilację powoduje powstanie N-(3-trifluorometylofenylo)etylenodiaminy lub 3-trifluorometyloaniliny. Hydroksylowany metabolit hydroksy-TFMPP prowadzi do powstania N-(hydroksy-3-trifluorometylofenylo)etylenodiaminy lub hydroksy-3-trifluorometyloaniliny [53,54].

W przypadku kannabinoidów, które są reprezentowane między innymi przez THC, metabolizm odbywa się głównie w wątrobie, za pośrednictwem izoenzymów CYP2C9, CYP2C19, CYP3A4 cytochromu P450 (CYP450) [55]. THC jest metabolizowany głównie do 11-hydroksy-THC (11-OH-THC) i 11-karboksy-THC(11-COOH-THC), który ulega glukuronidacji [56], a następnie jest wydalany z kałem i moczem [57,58]. Dlatego tak ważne jest uwzględnienie tych analitów w badaniach toksykologicznych. Syntetyczne kannabinoidy (SCB) to klasa nielegalnych narkotyków, zwykle przegotowanych na bazie matrycy ziołowej, które są palone jak marihuana [59]. Sprzedawane są one pod nazwami takimi jak: *K2* czy *SPICE* i opisane zwrotami - *nie do spożycia przez ludzi*. Często sprzedawane jako syntetyczna marihuana są unikalnymi substancjami chemicznymi [59]. Nielegalni producenci zmotywowani do dalszych działań ciągle zmieniają struktury SCB w celu uniknięcia przepisów i identyfikacji w standardowych testach narkotykowych. Konsument nigdy nie ma pewności jaki skład ma zakupiony *K2* czy *SPICE* i jakie będą konsekwencje jego zażycia. Do tej pory w Stanach Zjednoczonych zidentyfikowano ponad 50 specyficznych SCB, ale większość z nich jest biochemicznie sklasyfikowana jako aminoalkiloindole, cykloheksylofenole, benzoiloindole lub analogi Δ9-THC [59]. Ze względu na wzrost zainteresowania tą grupą związków ich metabolizm jest w ostatnim czasie szybko rozwijającym się obszarem naukowym. Wykazano, że kolejność powstawania metabolitów jest taka, że najpierw związki te są utleniane przez cytochromy P450, a następnie sprzęgane z kwasem glukuronowym przez klasę enzymów UDP – glukuronylotransferazy (UGT), co jest niezbędnym procesem do usunięcia tych substancji z organizmu [60]. Jednym z popularnych syntetycznych kannabinoidów jest JWH-018. Zaobserwowano, że jego metabolity są wydalane prawie całkowicie w postaci koniugatów glukuronidowych [61]. Przeprowadzone również dla innych związków (JWH-073, JWH-250) badania potwierdziły powstawanie metabolitów zawierających pojedynczą grupę hydroksylową jako głównych metabolitów, które ulegały glukuronidacji w celu eliminacji z moczem ludzkim [62, 63].

Opiaty definiuje się jako pochodne alkaloidów opium, z których najważniejszymi przedstawicielami są morfina, kodeina i heroina [64]. Heroina jest szybko metabolizowana przez hydrolizę/deacetylację do 6-AM, a następnie do morfiny, odpowiedzialna za ten proces

jest acetylocholinoesteraza erytrocytów i osoczowa butyrylocholinoesteraza [64]. Powyższe informacje wskazują na konieczność analizy zarówno morfiny, jak i 6-AM w celu potwierdzenia lub wykluczenia zażycia nie tylko morfiny ale i heroiny.

Badania nad metabolizmem substancji psychoaktywnych pozwalają na rozwój metod toksykologicznych zarówno pod kątem analitycznym, jak i retrospektywnym. Tak szeroki zakres analiz substancji psychoaktywnych oraz możliwość zastosowania metod badawczych do różnych matryc biologicznych daje ogromne możliwości poznania szlaków metabolicznych, a co za tym idzie identyfikacji nowych substancji psychoaktywnych pojawiających się na nielegalnym rynku.

3.2 Analiza substancji psychoaktywnych i ich metabolitów oraz leków w materiale biologicznym

W ostatnich latach substancje psychoaktywne stały się zamiennikiem dla alkoholu. Sprzedawane w postaci środków nie do spożycia o nazwach takich jak: dopalacze, sole do kąpieli czy chemikalia badawcze [46]. Niepokojący jest fakt, że zażywają je coraz młodsi ludzie, którzy nie zdają sobie sprawy z konsekwencji stosowania tego typu substancji dla ich organizmu. Ponadto, działania prawne podjęte w celu ograniczenia dostępności tego typu środków w legalnej sprzedaży skutkują wprowadzaniem kolejnych dopalaczy, które są modyfikacjami strukturalnymi już znanych i nielegalnych substancji psychoaktywnych. Dzięki temu handlarze wprowadzają do sprzedaży dopalacze, które są poza zasięgiem organów ścigania. Ten aspekt jest szczególnie ważny w analizie NPS. Bardzo istotne jest jednoznaczne identyfikowanie pojawiających się na rynku nowości i zgłaszanie ich do wpisania na listę środków zakazanych.

Analiza substancji psychoaktywnych w próbkach biologicznych staje się ogromnym wyzwaniem dla laboratoriów, które muszą stale rozwijać swoje metody by móc wykryć co raz to nowe NPS pojawiające się na rynku. Wstępnie próbki poddaje się analizie przesiewowej wykorzystując w tym celu testy immunochemiczne [12, 14, 17, 18]. Jednakże zwykle granica oznaczalności (LOQ) tych metod jest zbyt wysoka na wykrycie pozostałości NPS w organizmie. Ponadto, testy te zazwyczaj są dedykowane dla konkretnych grup analitów, co wymusza większą liczbę analiz pod kątem różnych grup NPS, co generuje dodatkowe koszty, odpady, a także znacznie wydłuża czas analiz, które trzeba potem potwierdzić metodami konfirmacyjnymi. Wychodząc naprzeciw powyższym problemom opracowywane są nowe metody oparte na chromatografii gazowej [9, 19, 65, 66] i chromatografii cieczowej [31-33,67-71], które są coraz częściej stosowane w laboratoriach. W przypadku połączenia chromatografii

gazowej ze spektrometrią mas (GC-MS) plusem jest obniżenie LOQ względem metod immunochemicznych, jednakże należy zwrócić uwagę na konieczność dodatkowego etapu jakim jest derywatyzacja w celu zwiększenia liczby wykrywanych analitów [19]. Biorąc pod uwagę powyższe ograniczenia techniki GC-MS oraz oznaczanie dużej ilości analitów w toku jednego postępowania analitycznego, chromatografia cieczowa sprzężona ze spektrometrią mas wydaje się być bardziej uniwersalną techniką umożliwiającą oznaczenie NPS.

Do analizy substancji psychoaktywnych przy użyciu MS wykorzystuje się najczęściej tryb jonizacji ESI w jonizacji dodatniej [24-31,67,68,70], a w przypadku niektórych analitów również ujemnej [29]. Natomiast jeśli chodzi o proces rozdzielenia analitów na kolumnie chromatograficznej to największe zastosowanie ma kolumna z wypełnieniem oktadecylowym [25,27-29,31,33,67,68,70]. Fazami ruchomymi zazwyczaj są mieszaniny wody i rozpuszczalnika organicznego, którym zwykle jest metanol [24,26,29,33,70] lub acetonitryl [25,27,28,30,31,35,68]. Spotyka się również kolumny z sorbentem fenyloheksylowym [26] czy bifenylowym [30]. Ze względu na metodę jonizacji stosuje się modyfikatory do faz ruchomych np. mrówczan amonu [28,70], kwas octowy [30], kwas mrówkowy [24-29,31,67,68,70], które zwiększają efektywność procesu jonizacji. Podczas opracowywania metody rozdzielania NPS należy zwrócić szczególną uwagę na izomeryi bardzo podobne strukturalnie anality, które są pochodnymi tego samego zakazanego narkotyku. Konieczna staje się więc weryfikacja czy otrzymany wynik nie jest sumą izomerów. Przy analizie tak dużej liczby substancji podczas jednej analizy, konieczne jest takie dobranie warunków rozdzielenia, aby związki o takich samych wartościach par MRM były wstanie zostać jednoznacznie zidentyfikowane.

Jednym z najważniejszych etapów oznaczania NPS jest przygotowanie próbki. Analizie poddaje się próbki krwi, moczu, włosów, a także śliny. Każda z tych matryc wymaga indywidualnego podejścia i uwzględnienia występujących utrudnień w celu dobrania najefektywniejszego procesu ekstrakcji. Materiały biologiczne są bardzo złożonymi matrycami, a składniki takie jakie białka, fosfolipidy i sole muszą zostać usunięte z próbki przed analizą. W przypadku krwi są to białka, które zwykle są strącane za pomocą acetonitrylu. Natomiast jeśli chodzi o próbki moczu poddaje się je procesowi hydrolizy, do którego zazwyczaj stosuje się β-glukuronidazę, co ułatwia oznaczenie wolnych metabolitów substancji psychoaktywnych [72]. W przypadku analizy NPS najczęściej spotyka się metody wykorzystujące technikę ekstrakcji do fazy stałej (SPE) [24, 25, 27-29,33]. Anality ekstrahowane są do rozpuszczalnika, a próbka nanoszona jest na sorbent, następnie przemywa się sorbent odpowiednim rozpuszczalnikiem w celu usunięcia składników zakłócających pochodzących z matrycy, a zaadsorbowane anality eluuje się za pomocą selektywnych

rozpuszczalników [73,74]. Mimo ogromnej zalety SPE jaką jest możliwość łatwej automatyzacji, co pozwala na skrócenie czasu pracy i zmniejszenie ilości odpadów [72], nadal poszukuje się mniej skomplikowanych i tańszych metod izolowania NPS z próbek biologicznych. Dane dotyczące metod przygotowania próbek, zebrane w pracy przeglądowej [**D1**] potwierdzają, że wyodrębniając kilka grup NPS przy zastosowaniu jednego rodzaju koluminek SPE, zakres wartości odzysków mieści się w szerokim przedziale wartości (2-128,5 %). Sugeruje to konieczność zastosowania kilku kolumienek dla jednej próbki w celu wyizolowania każdego z analitów, co znacznie zwiększa koszty i wydłuża czas trwania badań. Ponadto, procedura ta wymaga znacznie większej ilości próbki, co nie stwarza większych problemów w przypadku moczu, ale w przypadku próbek krwi jest to trudne do wykonania. Wychodząc naprzeciw problemom napotykanym podczas zastosowania techniki SPE, można powrócić do klasycznej ekstrakcji w układzie ciecz-ciecz (LLE). Daje ona możliwość wyizolowania znacznie większej liczby analitów stosując rozpuszczalniki takie jak: acetonitryl (ACN)[31], octan butylu [76], chloroform [19], czy też mieszaniny: n-heksan-octan etylu [26], 1-chlorobutan:dichlorometan z octanem etylu [30], a także ACN z mrówczanem amonu [32]. W przypadku LLE również istnieje możliwość automatyzacji procesu choć jest to trudniejsze do osiągnięcia niż w przypadku SPE. Pomimo wysokich kosztów odczynników i dużej ilości szkodliwych odpadów, możliwość zminiaturyzowania, automatyzacji, uzyskanie niskich wartości LOQ i wysokich odzysków dla każdej z grup analizowanych NPS są zdecydowanymi zaletami LLE. Ogromną zaletą jest to, że można zastosować LLE również w przypadku innych matryc biologicznych, co daje ogromne możliwości kompleksowej analizy.

Wraz ze wzrostem zainteresowania NPS wśród społeczeństwa, a także koniecznością przeciwdziałania rozprzestrzeniania się pozornie bezpiecznych dopalaczy. Zagrażają one zdrowiu i życiu dlatego też, istotne jest opracowanie szybkiej, specyficznej, charakteryzującej się niskimi wartościami LOD i LOQ, wysokim odzyskiem, a także możliwością szybkiej rozbudowy i automatyzacji procedury analitycznej. Zapewni to możliwie krótki czas analizy obszernej liczby analitów w próbce. Istotne jest również łatwe przystosowanie opracowanej metodyki do innych matryc biologicznych (niejednokrotnie pochodzące od jednego pacjenta), aby móc analizować je pod kątem NPS dając możliwość pełnej analizy i poznania procesów metabolicznych tych niezbadanych jeszcze związków.

Wdrożenie opracowanych procedur analitycznych w Instytucie Genetyki Sądowej w Bydgoszczy, będących efektem badań niniejszej rozprawy doktorskiej, pozwoliło na

rozwiązanie problemów dotyczących analizy NPS. Wyeliminowanie SPE i rozcieńczenia próbek, a także duża liczba analitów identyfikowana w krótkim czasie, obniżenie wartości LOD i LOQ oraz możliwość automatyzacji i rozszerzania procedur o kolejne substancje psychoaktywne pozwoli na dalszy rozwój toksykologii, zwiększenie nie tylko ilości klientów Instytutu, ale także liczby substancji zakazanych, a co za tym idzie zwiększenie bezpieczeństwa społeczeństwa.

3.3 Metody przygotowania próbek biologicznych do jakościowej i ilościowej analizy substancji psychoaktywnych, leków i ich metabolitów

Opracowana metoda LC-MS/MS została wykorzystana do rozdzielenia i analizy ilościowej ponad 500 substancji psychoaktywnych (w tym leków oraz NPS) oraz ich metabolitów w próbkach biologicznych (włosy [**D1**], krew [**D3**], mocz [**D5**]). Studia literaturowe związane z metodami przygotowania próbek, zebrane zostały w pracy przeglądowej [**D1**]. Zazwyczaj analizowane są próbki moczu i krwi jednakże, coraz większą uwagę poświęca się również analizie próbek włosów. Ze względu na niską inwazyjność pobierania próbek włosów, zyskuje ona coraz większą popularność wśród rodziców czy w zakładach pracy. Każda z matryc wymaga odpowiedniego przygotowania próbki w celu uzyskania możliwie najwyższych odzysków zawartych w próbce analitów. Biorąc pod uwagę czas przygotowania próbek, ich objętość, koszty oraz możliwość przyszłej automatyzacji podjęto próbę opracowania ekstrakcji umożliwiającej szybką, specyficzną, możliwie tanią, nisko odpadową oraz uniwersalną metodę przygotowania próbek. Zaletą opracowanych metod była łatwość przystosowania ich do innej matrycy i poszerzenia zakresu badań o kolejne anality, aby móc podążać za ciągle rozwijającym się rynkiem NPS. Opracowane procedury pozwoliły na wdrożenie nowych procedur [**D4**] w Instytucie Genetyki Sądowej (IGS) w Bydgoszczy umożliwiając większą liczbę analiz w krótszym czasie, co wiąże się także z niższymi kosztami i większą liczbą zleconych badań.

3.3.1 Próbki krwi [D3]

Najczęściej badanymi próbkami trafiającymi do laboratorium IGS są próbki krwi. Właśnie z tego powodu to od tej matrycy rozpoczęto prace badawcze dotyczące niniejszej rozprawy doktorskiej. Próbki krwi zwykle poddawane są ekstrakcji SPE, jednakże ze względu na ilość analitów oraz fakt, że konieczne byłoby zastosowanie kilku kolumienek SPE posiadających różne adsorbenty odpowiednie dla poszczególnych grup analitów zdecydowano się sprawdzić inne metody. Podjęto próbę izolowania badanych analitów za pomocą różnych kombinacji techniki QuEChERS, jednakże uzyskiwane wyniki nie pozwoliły na zastosowanie

tej metody, ze względu na duże starty anlitów. W kolejnym etapie podjęto próby opracowania klasycznej metody ekstrkacji - LLE, co daje możliwość wyizolowania analitów w jednym toku analitycznym, co znacznie zmniejsza koszty przygotowania próbki. Umożliwia analizę znacznie większej liczby próbek w ciągu doby, a także zmniejsza potrzebną ilość materiału biologicznego do badań.

Analizowanym materiałem była krew pobrana od pracowników laboratorium deklarujących brak przyjmowania badanych analitów. Podczas opracowywania metody oznaczania analitów podjęto próbę przygotowania krzywych wzorcowych w MeOH. Jednakże ze względu na duży wpływ matrycy oraz chęć rozszerzenia metody o kolejne związki oraz matryce przygotowano krzywe kalibracyjne w matrycy. Ze względu na znaczący wpływ matrycy podjęto próbę rozcieńczenia próbek rzeczywistych zamiast ich wzbogacania w ostatnim etapie przygotowania próbki. Pozwoliło to na uzyskanie czystszych ekstraktów, które nie zanieczyszczają dodatkowo aparatu, a także pozwalają uzyskać niższe wartości LOQ dzięki zmniejszeniu wpływu matrycy. Każdą próbkę analizowano dwukrotnie. Jako wzorzec wewnętrzny użyto atrazyny, ze względu na pewność, że nie wystąpi ona w próbkach rzeczywistych, a także ze względu na jej wysoką stabilność. W każdej serii analiz badano dwie próbki z dodatkiem badanych analitów o stężeniach 2 i 10 ng/ml, krzywą wzorcową w matrycy, wzorzec w roztworze MeOH o stężeniu 10 ng/ml oraz próbkę zerową. Wszystkie roztwory wzorców analitycznych przygotowywano metodą kolejnych rozcieńczeń.

Przygotowanie próbek wzbogaconych

Do probówki typu Eppendorf o objętości 2 ml dodano odpowiednie objętości roztworów zawierających wszystkie anality (*MASTERMIXA*): 1) o stężeniu 2 ng/ml było to 100 µl *MASTERMIXA* o stężeniu 10 ng/ml, 2) 10 ng/ml było to 50 µl *MASTERMIXA* o stężeniu 100 ng/ml, następnie do probówek dodano 20 µl roztworu atrazyny o stężeniu 2500 ng/ml. Kolejnym etapem było dodatnie 500 µl próbki krwi nie zawierającej badanych analitów oraz 500 µl ACN z buforem (przygotowanym poprzez dodanie po 20 µl mrówczanu amonu i kwasu mrówkowego do kolby miarowej o objętości 100 ml i uzupełnienie ACN do kreski). Tak przygotowaną próbkę ujednorodniono, a następnie wytrząsano w temperaturze 21°C przez 10 minut z prędkością 1400 rpm. W kolejnym etapie próbkę umieszczono na 10 minut w zamrażarce, a następnie wirowano 5 minut (2000 rpm). Otrzymany roztwór znad osadu przefiltrowano. Na tym etapie sprawdzono czy kolejne zamrożenie próbki na 10 minut wpłynie na jakość ekstraktu. Stwierdzono, że etap ten nie ma wpływu na próbkę, a więc usunięto ten

dodatkowy etap z procedury. Tak otrzymaną próbkę wirowano przez 1 minutę (10 000 rpm). Z otrzymanego w ten sposób ekstraktu pobrano 50 µl do fiolki i dodano 450 µl fazy ruchomej (A:B, 90:10 v/v; gdzie A - 2mM mrówczan amonu w wodzie z 0,1% dodatkiem kwasu mrówkowego; B - 2mM mrówczan amonu w metanolu z 0,1% dodatkiem kwasu mrówkowego) i umieszczono w podajniku automatycznym.

Przygotowanie krzywej wzorcowej w matrycy

Do czterech próbówek typu Eppendorf dodano po 500 µl krwi, następnie dodano 500 µl ACN z buforem (przygotowanego jak w przypadku próbek z dodatkiem wzorca). Tak przygotowaną próbkę ujednorodniono, a następnie wytrząsano w 21°C przez 10 minut z prędkością 1400 rpm. W kolejnym etapie próbkę umieszczono na 10 minut w zamrażarce, a następnie odwirowano w wirówce przez 5 minut (2000 rpm). Otrzymany roztwór znad osadu przeniesiono na filtr wirówkowy (0,2 µm). Tak otrzymaną próbkę odwirowano przez 1 minutę w 10 000 rpm. Do ośmiu fiolek dodano po 10 µl roztworu atrazyny o stężeniu 2500 ng/ml, 50 µl odpowiedniej mieszaniny zawierającej wszystkie anality (zawsze jest to stężenie dziesięć razy wyższe niż punkt krzywej, a więc odpowiednio 0,05; 0,1; 0,5; 1; 5; 10; 20; 50 ng/ml) 50 µl otrzymanego ekstraktu oraz 390 µl fazy ruchomej (A:B 90:10 v/v; gdzie A - 2mM mrówczan amonu w wodzie z 0,1% dodatkiem kwasu mrówkowego; B - 2mM mrówczan amonu w metanolu z 0,1% dodatkiem kwasu mrówkowego). Stężenia punktów do krzywej wzorcowej z uwzględnieniem 20 krotnego rozcieńczenia wynoszą: 0,5, 1, 5, 10, 50, 100, 200 oraz 500 ng/ml.

Przygotowanie próbki zerowej

Próbkę zerową przygotowano na bazie wcześniej uzyskanego ekstraktu z krwi (roztwór acetonitrylu z buforem). Do fiolki dodano 10 µl roztworu atrazyny o stężeniu 250 ng/ml, 50 µl ekstraktu z krwi oraz 440 µl fazy ruchomej (A:B, 90:10 v/v; gdzie A - 2mM mrówczan amonu w wodzie z 0,1% dodatkiem kwasu mrówkowego; B - 2mM mrówczan amonu w metanolu z 0,1% dodatkiem kwasu mrówkowego).

Przygotowanie wzorca w metanolu

Wzorzec w metanolu przygotowano poprzez dodanie do fiolki 10 µl roztworu atrazyny o stężeniu 500 ng/ml, 50 µl *MASTERMIXA* o stężeniu 100 ng/ml oraz 440 µl fazy ruchomej (A:B 90:10 v/v).

W kolejnym etapie prac sprawdzono stabilność otrzymanych ekstraktów. Wykonano to poprzez analizę próbek archiwalnych. Otrzymane wyniki potwierdziły stabilność analitów i zostały wprowadzone do rutynowych analiz jako dodatkowa forma kontroli.

Opracowana metoda izolowania NPS z próbek krwi została wprowadzona do rutynowych analiz w laboratorium Instytutu Genetyki Sądowej [**D4**].

3.3.2 Próbki włosów [D2]

Kolejną matrycą do badań w zakresie rozprawy doktorskiej było opracowanie metody ekstrakcji wybranych analitów z próbek włosów. Wstępne przygotowanie polegało na pocięciu włosów na 1 cm fragmenty. Tak przygotowane próbki poddano przemyciu. Na tym etapie sprawdzono dwa sposoby przemywania: przemywanie mieszaniną etanolu i dichlorometanu oraz samym dichlorometanem. Ze względu na fakt, że zastosowanie samego dichlorometanu pozwoliło uzyskać wyniki zbliżone do częściej stosowanego wspomnianego etanolu i dichlorometanu, jednocześnie eliminując jeden z rozpuszczalników, a co za tym idzie i ilość odpadów pozostano przy tym sposobie przemywanie próbek włosów.

Próbkę włosów o długości 1 cm ścięto do korpusu strzykawki o objętości 5 ml, nałożono na końcówkę strzykawki filtr zabezpieczający przed utratą włosów, a następnie trzykrotnie przemyto otrzymaną próbkę 3 ml dichlorometanu i wytrząsano jak w przypadku próbek krwi. W kolejnym etapie włosy suszono na bibule przez 10 minut w temperaturze pokojowej (sprawdzano również suszenie w suszarce przez 10 minut w temperaturze 30°C) jednakże straty analitów były większe niż w przypadku bibuły), a następnie poddano próbkę sproszkowaniu przy użyciu jednej kulki proszkującej i 15 000 rpm w czasie 5 minut. Na tym etapie testowano najpierw wersję bez proszkowania włosów jednakże wyniki odzysków były niskie i niepowtarzalne, a ekstrakt nie do końca oczyszczony z zanieczyszczeń. W efekcie tych badań postanowiono sprawdzić wpływ proszkowania włosów na wyniki. Testowano różną ilość i wielkość kulek, jako wystarczające okazało się zastosowanie już jednej kulki o średnicy 25 mm. Kolejnym etapem prac było dobranie odpowiedniej naważki sproszkowanego materiału badanego do dalszych etapów przygotowania próbki do analizy. Powtarzalne wyniki otrzymano w przypadku 20 mg sproszkowanych włosów. Włosy odważano do próbówki typu Eppendorf, do której w kolejnym etapie dodano 20 µl roztworu atrazyny o stężeniu 2,5 µg/ml oraz 500 µl MeOH (tak jak w przypadku próbek krwi sprawdzono również ACN jednakże w przypadku próbek włosów z MeOH pozwolił uzyskać lepsze wyniki). Tak przygotowaną próbkę wytrząsano przez 1 godzinę w temperaturze 21 °C i 12 000 rpm, a następnie wymrażano przez

10 minut. Następnie próbkę odwirowano przez 5 minut (2000 rpm) i przefiltrowano. Z tak otrzymanego ekstraktu pobrano 50 µl i dodano do niego 450 µl fazy ruchomej (A:B, 90:10 v/v; gdzie A - 2mM mrówczan amonu w wodzie z 0,1% dodatkiem kwasu mrówkowego; B - 2mM mrówczan amonu w metanolu z 0,1% dodatkiem kwasu mrówkowego) dla rozcieńczenia 10-krotnego oraz 200 µl ekstraktu oraz 200 µl fazy ruchomej (A:B, 90:10 v/v; gdzie A - 2mM mrówczan amonu w wodzie z 0,1% dodatkiem kwasu mrówkowego; B - 2mM mrówczan amonu w metanolu z 0,1% dodatkiem kwasu mrówkowego) dla 2-krotnego rozcieńczenia. Próbkę ponownie umieszczono w zamrażarce na 10 minut (etap ten tak jak w przypadku poprzednich matryc po weryfikacji okazał się nie wnosić zmian i w procedurze został pominięty). Następnie próbkę umieszczono w wirówce na 3 minuty 10 000 rpm, a z otrzymanego ekstraktu pobrano 200 µl do fiolki o zmniejszonej objętości.

Przygotowanie próbki wzbogaconej

W przypadku próbki z dodatkiem wzorca na początku pracy do sproszkowanych włosów dodano oprócz atrazyny i MeOH jeszcze 20 µl mieszaniny wzorców zawierającego wszystkie anality o stężeniu 200 ng/ml, co odpowiada stężeniu 0,2 ng/mg włosa w badanej próbce.

Przygotowanie krzywej wzorcowej w matrycy

Próbkę włosów nie zawierających badanych analitów o długości 1 cm ścięto do strzykawki o objętości 5 ml, następnie trzykrotnie przemyto otrzymaną próbkę 3 ml dichlorometanu i nałożono na strzykawkę filtr nieprzepuszczający włosów i wytrząsano jak w przypadku próbek krwi. W kolejnym etapie suszono włosy na bibule przez 10 minut w temperaturze pokojowej, a następnie poddano próbkę sproszkowaniu przy użyciu jednej kulki proszkującej i obrotach 15 000 rpm w czasie 5 minut. Do dwóch próbówek typu Eppendorf odważono po 20 mg sproszkowanych włosów i dodano do nich 500 µl MeOH. Próbówkę z próbką wytrząsano przez 1 godzinę w temperaturze 21 °C i 12 000 rpm, a następnie wymrażano przez 10 minut. Następnie próbkę odwirowano przez 5 minut (2000 rpm) i przeniesiono na koszyczek z filtrem (0,2µm). Z tak otrzymanego ekstraktu pobrano do 8 fiolek po 50 µl ekstraktu, 10 µl roztworu atrazyny o stężeniu 500 ng/ml, 50 µl odpowiedniej mieszaniny zawierającej wszystkie anality (zawsze jest to stężenie dziesięć raz wyższe niż punkt krzywej a więc odpowiednio 0,5 ng/ml, 1 ng/ml, 5 ng/ml, 10 ng/ml, 50 ng/ml, 100 ng/ml, 200 ng/ml, 500 ng/ml) oraz 390 µl fazy ruchomej (A:B, 90:10 v/v; gdzie A - 2mM mrówczan amonu w wodzie z 0,1% dodatkiem kwasu mrówkowego; B - 2mM mrówczan amonu w metanolu z 0,1% dodatkiem kwasu mrówkowego).

Przygotowanie próbki zerowej

W przypadku próbki zerowej wykorzystujemy ekstrakt z włosów przygotowanych dla krzywej wzorcowej w matrycy. Z otrzymanego ekstraktu pobrano do fiolki 50 µl ekstraktu, 10 µl roztworu atrazyny o stężeniu 500 ng/ml oraz 450 µl fazy ruchomej (A:B, 90:10 v/v; gdzie A - 2mM mrówczan amonu w wodzie z 0,1% dodatkiem kwasu mrówkowego; B - 2mM mrówczan amonu w metanolu z 0,1% dodatkiem kwasu mrówkowego).

Przygotowanie wzorca w metanolu

W przypadku wzorca w metanolu postępowano tak jak w przypadku analiz próbek krwi.

Opracowana metoda izolowania NPS z próbek włosów została wprowadzona do rutynowych analiz w laboratorium Instytutu Genetyki Sądowej [**D4**].

3.3.3 Próbki moczu [D5]

W ramach kolejnych prac podjęto próbę przystosowania opisanej w punkcie 3.3.1 metody do analizy próbek moczu. Biorąc pod uwagę metabolizm NPS należy zwrócić uwagę na produkty powstające podczas tego procesu - glukuronidy i siarczany. W celu weryfikacji opracowanej metody analizy moczu sprawdzono, czy konieczne jest użycie enzymu β-glukuronidazy do procesu dekoniugaacji. Uzyskane wyniki potwierdziły przypuszczenia, że w próbkach moczu występują wystarczające ilości niezwiązanych analitów co oznacza, że nie jest konieczne stosowanie tego enzymu do wszystkich próbek. Jednak w celu badania ścieżek metabolicznych i identyfikacji wszystkich metabolitów istnieje możliwość łatwego wprowadzenia dodatkowego etapu z użyciem enzymu β-glukuronidazy. Tak jak w przypadku próbek krwi analizie poddawana jest seria próbek: wzorzec, próbka zerowa, próbki rzeczywiste oraz próbki z dodatkiem wzorca umożliwiające przygotowanie krzywych wzorcowych w matrycy. Dla tej matrycy przygotowano dwa rozcieńczenia próbki: 10-krotne oraz 100-krotne ze względu na zróżnicowany poziom stężeń powstających metabolitów, szczególnie w przypadku benzodiazepin.

Przygotowanie próbek z dodatkiem wzorca

Do probówki typu Eppendorf o objętości 2 ml dodano 50 µl roztworu zawierającego wszystkie anality (*MASTERMIXA*) o stężeniu 500 ng/ml, następnie do probówek dodano 20 µl roztworu atrazyny o stężeniu 2500 ng/ml. Kolejnym etapem było dodatnie 250 µl próbki moczu nie zawierającego badanych analitów oraz 200 µl ACN z buforem (przygotowanym poprzez dodanie po 20 µl mrówczan amonu i kwasu mrówkowego do kolby miarowej

o objętości 100 ml i uzupełnienie ACN). Tak przygotowaną próbkę mieszano na mieszadle typu Vortex, a następnie wytrząsano w 21°C przez 10 minut z prędkością 1400 rpm. W kolejnym etapie próbkę umieszczono na 10 minut w zamrażarce, a następnie umieszczono w wirówce na 5 minut (2000 rpm). Roztwór przefiltrowano przez filtr wirówkowy (0,2µm). Tak otrzymaną próbkę odwirowano przez 1 minutę w 10 000 rpm. Z otrzymanego w ten sposób ekstraktu pobrano 100 µl do fiolki w i dodano 400 µl fazy ruchomej (A:B 90:10 v/v; gdzie A - 2mM mrówczan amonu w wodzie z 0,1% dodatkiem kwasu mrówkowego; B - 2mM mrówczan amonu w metanolu z 0,1% dodatkiem kwasu mrówkowego) i umieszczono w podajniku automatycznym, a w przypadku 100-krotnego rozcieńczenia pobrano 10 µl ekstraktu z moczu oraz 490 µl fazy ruchomej (A:B 90:10 v/v; gdzie A - 2mM mrówczan amonu w wodzie z 0,1% dodatkiem kwasu mrówkowego; B - 2mM mrówczan amonu w metanolu z 0,1% dodatkiem kwasu mrówkowego) i również umieszczono fiolkę w podajniku automatycznym.

Przygotowanie krzywej wzorcowej w matrycy

Do trzech próbówek typu Eppendorf dodano po 250 µl moczu nie zawierającego badanych analitów, następnie dodano 250 µl ACN z buforem (przygotowanego jak w przypadku próbek fortyfikowanych). Dalej postępowano tak jak w przypadku krzywej wzorcowej w matrycy opisanej w punkcie 3.3.1 do etapu otrzymania ekstraktu z moczu. W przypadku 10-krotnego rozcieńczenia do ośmiu fiolek dodajemy po 10 µl atrazyny o stężeniu 1000 ng/ml, 50 µl odpowiedniej mieszaniny zawierającego wszystkie anality (zawsze jest to stężenie dziesięć raz wyższe niż punkt krzywej a więc odpowiednio, 0,5, 1, 5, 10, 50, 100, 200, 500 ng/ml), 100 µl otrzymanego ekstraktu oraz 340 µl fazy ruchomej (A:B, 90:10 v/v). W przypadku 100-krotnego rozcieńczenia do ośmiu fiolek dodajemy po 10 µl roztworu atrazyny o stężeniu 100 ng/ml, 50 µl odpowiedniego zawierającego wszystkie anality (zawsze jest to stężenie dziesięć raz wyższe niż punkt krzywej, a więc odpowiednio, 0,5, 1, 5, 10, 50, 100, 200, 500 ng/ml), 10 µl otrzymanego ekstraktu oraz 430 µl fazy ruchomej (A:B 90:10 v/v).

Przygotowanie próbki zerowej

Do przygotowania próbki zerowej wykorzystano ekstrakt moczu otrzymany podczas przygotowania krzywej wzorcowej w matrycy. W przypadku 10-krotnego rozcieńczenia do fiolki dodajemy 10 µl atrazyny o stężeniu 1000 ng/ml, 100 µl ekstaktu z moczu oraz 390 µl fazy ruchomej (A:B 90:10 v/v; gdzie A - 2mM mrówczan amonu w wodzie z 0,1% dodatkiem

kwasu mrówkowego; B - 2mM mrówczan amonu w metanolu z 0,1% dodatkiem kwasu mrówkowego). W przypadku 100-krotnego rozcieńczenia do fiolki dodajemy 10 µl atrazyny o stężeniu 100 ng/ml, 10 µl ekstaktu z moczu oraz 480 µl fazy ruchomej (A:B 90:10 v/v).

Przygotowanie wzorca w roztworze MeOH:

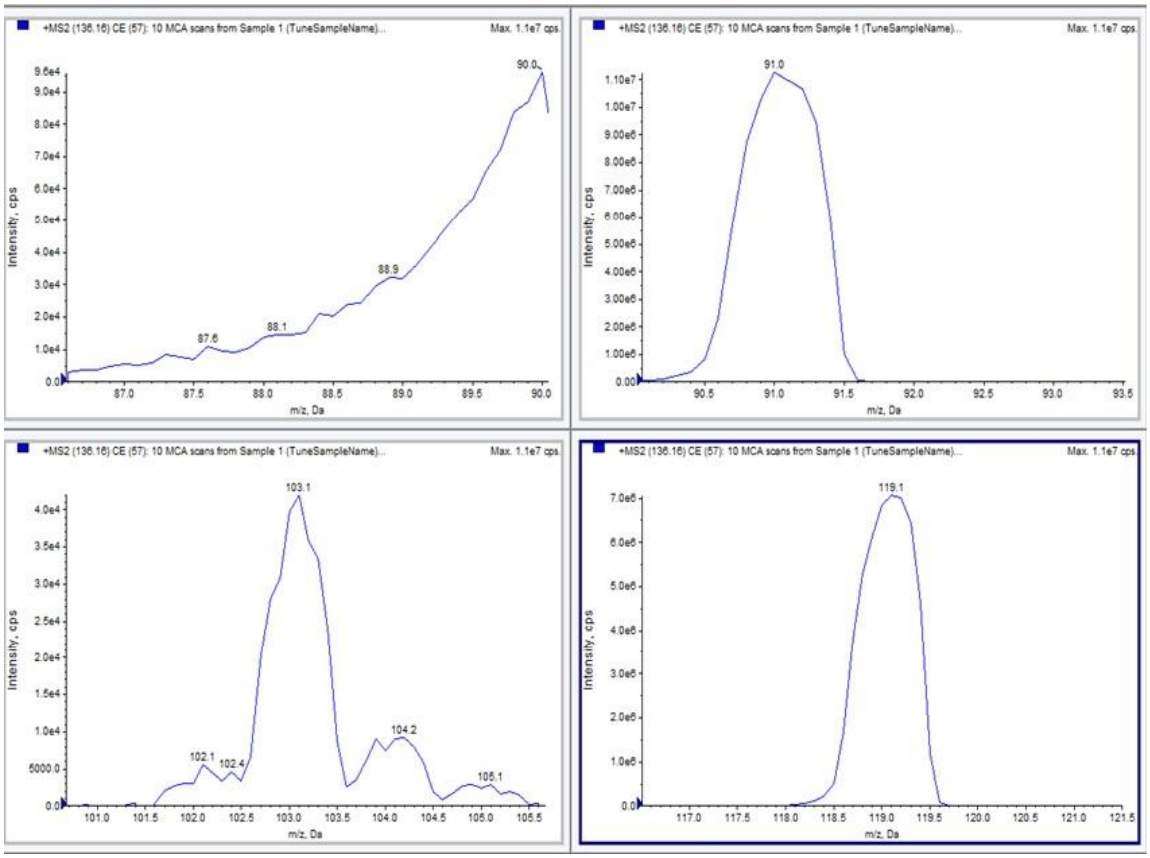
W przypadku wzorca w metanolu postępujemy tak jak w przypadku analiz próbek krwi.

Stabilność, analogiczne do próbek krwi stabilność sprawdzono poprzez analizę próbek archiwalnych, otrzymane wyniki potwierdziły stabilność analitów i zostały wprowadzone do rutynowych analiz jako dodatkowa forma kontroli serii analiz.

Opracowana metoda izolowania NPS z próbek moczu została wprowadzona do rutynowych analiz w laboratorium Instytutu Genetyki Sądowej [**D4**].

3.4 Zastosowanie chromatografii cieczowej sprzężonej z tandemową spektrometrią mas do opracowania procedury oznaczania ponad 500 substancji psychoaktywnych, leków i ich metabolitów w matrycach biologicznych

Pierwszym etapem prac był dobór parametrów spektrometru mas dla każdego z analitów, w celu uzyskania możliwie najwyższej czułości dla identyfikowanych związków. Optymalizację ustawień spektrometru przeprowadzono pojedynczo dla każdego z analitów sprawdzając zarówno jonizację dodatnią, jak i ujemną. Dla każdego z analitów wybrano po dwie pary MRM oraz najkorzystniejsze wartości energii DP, EP, CE i CXP. Dla większości badanych NPS korzystniejsza okazała się jonizacja dodatnia. Wyjątkiem był fenobarbital oraz GHB. Otrzymane parametry dla wszystkich analitów przedstawiono w publikacjach [**D2, D3, D5**]. Przykładową optymalizację warunków dla jednego z analitów przedstawiono na rysunku 1.



Rysunek 1. Przykładowa optymalizacja warunków pracy spektrometru mas dla amfetaminay.

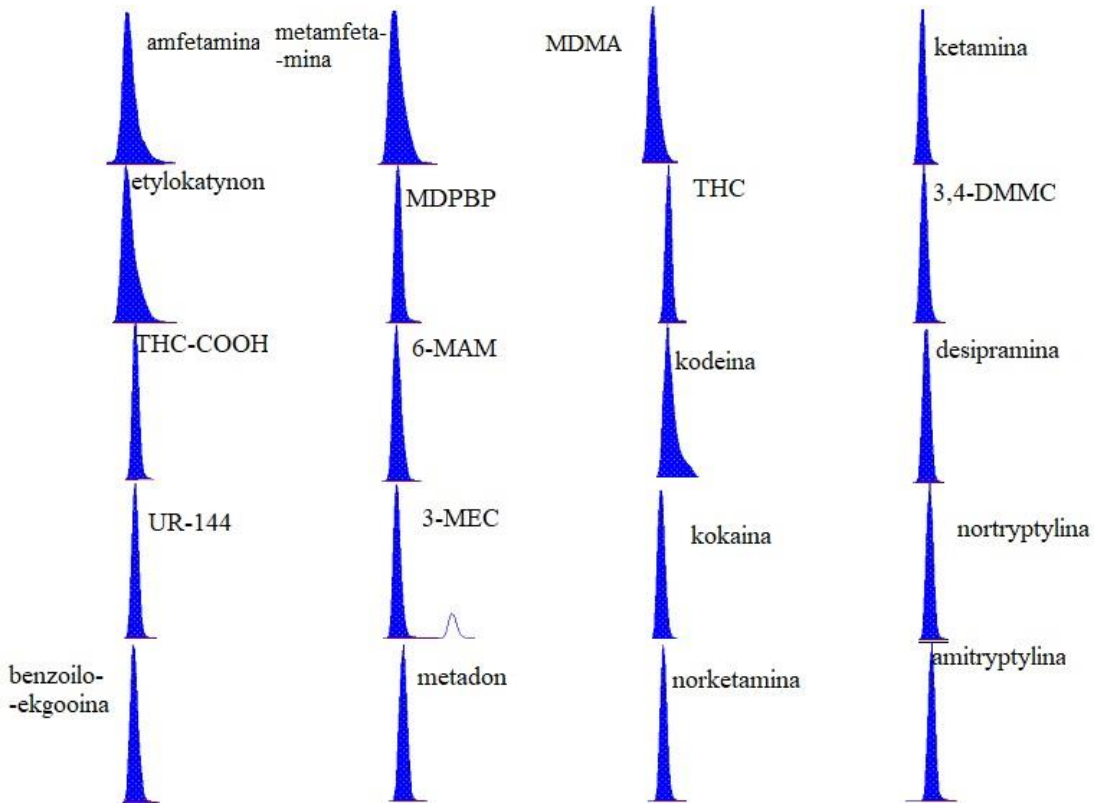
Kolejnym etapem prac był dobór warunków rozdzielenia chromatograficznego. W tym celu poddano testowaniu trzy kolumny chromatograficzne: Kinetex C18 3,0 x 100mm; 2,6 µm; Kinetex Biphenyl 3,0 x 100 mm; 2,6 µm oraz Kinetex Phenyl-Hexyl 3,0 x 100 mm; 2,6 µm w różnych wariantach składu fazy ruchomej oraz programów elucji gradientowej.

Nadrzędnym celem było rozdzielenie analitów będących izomerami szczególnie w przypadku katynonów np. 3-CMC i 4-CMC, których pary MRM po optymalizacji były identyczne. W celu osiągnięcia zadowalającego rozdzielenia analitów przeprowadzono badania stosując mieszaninę zawierającą mniejszą liczbę analitów, które potem zweryfikowano w oparciu o mieszaninę wszystkich badanych związków. Następnie dobrano skład fazy ruchomej używając odpowienidie ilości mrówczanu amonu (stężenie 2 mM oraz 5 mM). Otrzymane wyniki nie różniły się znacząco, więc pozostano przy pierwotnej wersji dodatku 2 mM mrówczanu amonu i 0,1 % kwasie mrówkowym w obu fazach. Kolejną zmienną był rozpuszczalnik organiczny użyty do przygotowania fazy B. Sprawdzono MeOH oraz ACN. Zastosowanie acetonitrylu nie poprawiło intensywności otrzymanych pików, ze względu na jego cenę oraz szkodliwość odpadów pozostano przy zastosowaniu MeOH. Warunki gradientu sprawdzono na czterech różnych programach gradientowych (Tabela 1) na kolumnie chromatograficznej Kinetex C18 (Phenomenex 3,0 x 100 mm; 2,6 μm).

Tabela 1. Programy elucji gradientowej zastosowane w analizie badanych związków.

Gradient 1		Gradient 2		Gradient 3		Gradient 4	
Czas [min]	Zawartość fazy B [%]	Czas [min]	Zawartość fazy B [%]	Czas [min]	Zawartość fazy B [%]	Czas [min]	Zawartość fazy B [%]
0,01	45	0,01	5	0,01	50	0	5
1	45	1	50	1	50	1	5
15	90	15	90	15	90	14	95
18	90	18	90	18	90	21	95
19,5	50	19,5	50	19,5	50	27	5
20	50	20	5	20	50	30	5

Najkorzystniejsze wyniki uzyskano dla programu elucji gradientowej nr 4. Pozwolił on na rozdzielenie prawie wszystkich analitów z wyjątkiem 3-MMC i 4-MMC, które w dalszych etapach analizowano jako sumę. Jako wynik przyjmowano wartość średnią z obu analitów. Ostatnim etapem było zweryfikowanie wybranego gradientu dla pozostałych kolumn: Kinetex Biphenyl 3,0 x 100 mm; 2,6 μm oraz Kinetex Phenyl-Hexyl 3,0 x 100 mm; 2,6 μm. Najkorzystniejsze rozdzielenie uzyskano dla pierwszej kolumny Kinetex C18 (Phenomenex 3,0 x 100 mm; 2,6 μm). Wyniki przeprowadzonych badań zamieszczono w publikacjach [**D2, D3, D5**]. Opracowana metodyka pozwoliła na rozdzielenie i identyfikację ponad 500 substancji. Do tej pory publikowane prace dotyczyły znacznie mniejszej liczby związków (około 200) [26-29,31]. Na Rysunku 2. przedstawiono piki otrzymane w wyniku selektywnego monitorowania wybranych reakcji jonowych (tryb MRM) dla wybranych analitów.



Rysunek 2. Przykładowe piki otrzymane w wyniku selektywnego monitorowania wybranych reakcji jonowych (tryb MRM) dla wybranych analitów.

3.5 Walidacja opracowanych procedur analitycznych

Walidację opracowanych metod analitycznych przeprowadzono zgodnie z wytycznymi SWGTOX (z ang. *Scientific Working Group for Forensic Toxicology*) [77]. Obejmowała ona wyznaczenie parametrów, takich jak:

- BIAS,
- precyzja,
- LOD,
- LOQ,
- liniowość,
- odzysk,
- wpływ matrycy,
- stabilność.

Wyniki otrzymane w procesie walidacji próbek włosów zostały zamieszczone w *Archives of Toxicology* **[D2]**, próbek krwi w *Microchemical Journal* [**D3**], natomiast próbek moczu w *Analytical Methods* – praca w redakcji **[D5].** Dla każdej z opracowanych procedur analitycznych kryteria walidacyjne zostały spełnione dla prawie wszystkich poddanych walidacji analitów. W przypadku krwi było to 520 z 522 analitów, dla próbek włosów 513 z 517 natomiast w przypadku ostatniej matrycy, którą jest mocz było to 465 z 477 substancji.

4 Wdrożenie opracowanych metod do rutynowych analiz w Instytucie Genetyki Sądowej w Bydgoszczy

Opracowane metody analityczne umożliwiły analizę ponad 500 substancji psychoaktywnych w tym NPS, leków i ich metabolitów w próbkach krwi i włosów oraz 465 w próbkach moczu i zostały wdrożone do rutynowych analiz w Instytucie Genetyki Sądowej w Bydgoszczy co potwierdza załączone do niniejszej rozprawy doktorskiej zgłoszenie patentowe [**D4**]. Opracowane metody pozwoliły na skrócenie czasu analizy pojedynczej próbki, obniżenie kosztów analiz, co umożliwia analizę większej liczby próbek. Dzięki wdrożeniu opracowanych metod laboratorium rozszerzyło swoją działalność, umożliwiając analizę większej liczby próbek, a co za tym idzie zwiększając liczbę zleceń. Konkurencyjność opracowanych metod pozwoliła na rozszerzenie liczby zleceniodawców Instytutu. Ponadto, uczestnictwo i sprawdzenie metod w badaniach biegłości dodatkowo jest kolejnym atutem dla Instytutu. Ponadto, opracowane metody pozwalają na identyfikację NPS wprowadzanych na rynek oraz ich klasyfikację do nowych przepisów prawnych, a co za tym idzie wprowadzenie ich na listę środków zakazanych co ma znaczący wpływ na zdrowie i życie.

Opracowaną metodę analizy próbek moczu wykorzystano podczas badań próbek pochodzących od kierowców. Badaniu poddano 70 próbek, jedynie w 18 z nich nie stwierdzono żadnego z analitów zawartych w opracowanej metodzie. W 21 próbkach wykryto paracetamol, który był najczęściej wykrywanym z analitów. Amfetamina została wykryta w 20 próbkach, GHB w 11 próbkach natomiast THCCOOH w 8. Natomiast w przypadku metamfetaminy i morfiny było to po 7 próbek, katyny, kodeiny i lidokainy po 5 próbek. Szczegółowe wyniki przeprowadzonych analiz przedstawiono w Tabeli 2. Przedstawione wyniki potwierdzają skuteczność metody dla próbek rzeczywistych, a co za tym idzie umożliwiają wyciągnięcie konsekwencji prawnych od osób badanych, co ma realny wpływ na zwiększenie bezpieczeństwa na drogach.

Tabela 2. Wyniki otrzymane dla próbek rzeczywistych moczu pochodzących od kierowców.

Ilość próbek w których wykryto analit	Analit	Zakres stężeń ng/ml	
		od	do
1	2,3-DICHLOROPHENYLPIPERAZINE (DCPP)	24,0	24,0
3	3,4-MDMA (3,4-METYLENODIOKSYMETAMFETAMINA)	10,5	180,1
3	3-CHLOROMETHCATHINONE (3-CMC)	23,5	13,8*
1	3-HYDROXYBROMAZEPAM	96,0	96,0
3	3-METHYLMETHCATHINONE (3-MMC) / 4-METHYLMETHCATHINONE (4-MMC)	12,8	24,9*
4	4-CHLOROMETHCATHINONE (4-CMC)	190,7	19,4*
1	4-METHYLCATHINONE (4-MC, NOR-MEFEDRON)	1365,7	1,4*
1	4-METYLOAMFETAMINA (4-METHYLAMPHETAMINE)	187,0	187,0
2	6-MAM (6-MONOACETYLOMORFINA)	176,1	738,8
3	7-AMINOKLONAZEPAM (7-AMINOCLONAZEPAM)	407,2	2,5*
2	ALPHA-ETHYLAMINOHEXANOPHENONE (ALFA-ETYLOAMINOHEKSANOFENON)	10,1	1,3*
2	ALPRAZOLAM	10,1	14,0
20	AMPHETAMINE (AMFETAMINA)	22,2	964,9*
1	AZACYCLONOL	126,5	126,5
4	BENZOYLECGONINE (BENZOILOEKGONINA)	16,9	51,3*
1	CARBAMAZEPINE (KARBAMAZEPINA)	1334,9	1,3*
5	CATHINE (KATYNA)	16,5	81,9
2	CLONAZEPAM (KLONAZEPAM)	21,4	31,0
1	COCAETHYLENE (KOKAETYLEN)	2272,3	2,3*
1	COCAINE (KOKAINA)	3309,7	3,3*
5	CODEINE (KODEINA)	62,5	8,3*
3	DEXTROMETHORPHAN (DEKSTROMETORFAN)	48,6	11,3*
3	DIAZEPAM	21,7	27,4
2	DIHYDROCODEINE (DIHYDROKODEINA)	309470,7	382,6*
1	DOKSEPINA (DOXEPIN)	330,3	330,3
4	EDDP	1821,2	8,0*
1	EUTYLONE (BK-EBDB) (EUTYLON)	29296,5	29,3*
1	FENTANYL	20,7	20,7
2	FLUOXETINE (FLUOKSETYNA)	85,7	1,4*
11	*GHB (KWAS GAMMA-HYDROKSYMASŁOWY)	10,4 µg/ml	29,5
2	HYDROCODONE (HYDROKODON)	1351,8	2,3*
1	KWETIAPINA (QUETIAPINE)	11,5	11,5
5	LIDOCAINE (LIDOKAINA)	14,6	438,5
4	METHADONE (METADON)	3014,6	6,3*
7	METHAMPHETAMINE (METAMFETAMINA)	18,3	17,2*
1	METHCATHINONE (METYLOKATYNON)	49,6	49,6
1	MIANSERIN (MIANSERYNA)	90,1	90,1
7	MORPHINE (MORFINA)	936,6	53,9*
3	NORDIAZEPAM (DESMETHYLDIAZEPAM)	16,1	91,2
2	OKSAZEPAM (OXAZEPAM)	89,3	238,3

22	PARACETAMOL	19,5	2333,8*
3	pCPP/mCPP/o-CPP	111,2	493,2
3	PREGABALINA (PREGABALIN)	99502,6	209,8*
1	PROPRANOLOL	70,2	70,2
1	SERTRALINA (SERTRALINE)	124,4	124,4
2	SILDENAFIL	173,2	301,4

*µg/ml

5 Dokumenty wchodzące w skład rozprawy doktorskiej

[D1] **Jadwiga Musiał**, Jakub Czarny, Renata Gadzała-Kopciuch, *Overview of analytical methods for determining novel psychoactive substances, drugs and their metabolites in biological samples*, Critical Reviews in Toxicology, 2022, 52:3, 239-258, https://doi.org/10.1080/10408444.2022.2091424, IF=6,184

W ostatnich latach obserwuje się wzrost zainteresowania substancjami psychoaktywnymi, ze szczególnym podkreśleniem tych dostępnych w sklepach internetowych. Dostępność tego typu substancji oraz korzystanie z nich jako alternatywy dla alkoholu czy narkotyków wpisanych na listę substancji zakazanych doprowadziła do zwiększenia liczby zatruć, zgonów, a także wypadków drogowych. Nowe substancje psychoaktywne (NPS) prowadzą do powstania ,etabolitów, które powodują wiele skutków ubocznych, co czyni je niebezpiecznymi dla zdrowia i życia już w niskich stężeniach. Powyższe fakty, a także chęć wyciągnięcia konsekwencji prawnych wobec osób nie tylko je zażywających, ale także tych które je produkują i wprowadzają do sprzedaży, spowodowały konieczność ich identyfikowania. To niezbędny etap, aby móc szybko podjąć działania ratujące życie w przypadku zatruć, wyciągnąć konsekwencje prawne zwłaszcza w przypadku wypadków drogowych popełnionych pod wpływem NPS, a także by dodawać je do listy substancji zakazanych.

Opracowanie metod analitycznych, które będą szybkie, proste, czułe i specyficzne, a także łatwe do rozszerzenia o kolejne anality stanowią ogromne wyzwanie dla laboratoriów. W pracy tej zwrócono uwagę na sposoby wprowadzenia do organizmu substancji psychoaktywnych, a także na mechanizmy jakim mogą ulegać w organizmie. Przedstawiono także szlaki metaboliczne dla przykładowych grup substancji psychoaktywnych. Jednakże, biorąc pod uwagę fakt, że oznaczanie tych substancji jest wyzwaniem dla laboratoriów skupiono się na stosowanych do tej pory metodach analitycznych. W pierwszej kolejności porównano metody przygotowania próbki do badań pod kątem substancji psychoaktywnych. Omówiono najczęściej stosowane metody takie jak: ekstrakcja do fazy stałej (SPE) czy ekstrakcja ciecz-ciecz (LLE), ale także te rzadziej stosowane np. z zastosowaniem polimerów z odciśniętą cząsteczką (MIPs). W przypadku SPE, podkreślono duże straty analitów podczas procesu przygotowania próbki, a także konieczność stosowania kilku sorbentów, by umożliwić wyizolowanie analitów należących do różnych grup substancji psychoaktywnych. Zwiększa to koszty etapu związanego z przygotowaniem próbek oraz ilość odpadów. Ponadto wymagane są duże objętości próbki. Mimo zalet tej metody, jakimi jest między innymi łatwość automatyzacji

procesu, ilość wad sugeruje podjęcie próby przygotowania próbki przy użyciu innej metody. Natomiast LLE charakteryzuje się dość dużą ilością stosowanych rozpuszczalników organicznych, ale istnieje możliwość miniaturyzacji, co byłoby korzystne w celu zmniejszenia ilości toksycznych odpadów. Odzyski są podobne do tych uyskanychza pomocą SPE, jednakże LLE daje możliwość ekstrakcji znacznie większej liczby analitów podczas jednego procesu. Na korzyść tej metody ma wpływ także niższa granica detekcji niż w przypadku SPE. Ostatnią z omówionych w pracy metod są wspomniane powyżej MIPy. Dają one duże możliwości analityczne. Mogą być szczególnie przydatne w przypadku izomerów, jednakże ze względu na konieczność oznaczanie bardzo dużej liczby analitów w szybkim czasie metoda ta nie jest najlepszą do rutynowych analiz. Zastosowanie jej wiązałoby się z dodatkowymi kosztami oraz wydłużeniem procesu ekstrakcji.

Kolejnym etapem analiz na jaki zwrócono uwagę w niniejszej pracy było metody rozdzielenia i detekcji NPS. W pierwszej kolejności zwrócono uwagę na metody immunochemiczne, które stosowane są jako metody przesiewowe. Niestety są one mało specyficzne, generują dużo wyników fałszywie dodatnich lub ujemnych. Są dedykowane konkretnym grupom analitów, a w przypadku NPS często są one nie wykrywane. Ponadto istnieje konieczność przeprowadzenia badań konfirmacyjnych, co zwiększa koszty i wydłuża czas trwania analiz. W pracy tej pochylono się także nad metodami takimi jak chromatografia gazowa sprzężona ze spektrometrią mas (GC-MS) oraz chromatografia cieczowa z zastosowaniem tego samego detektora (LC-MS). Wykazano, że metody te są znacznie lepiej przystosowane do analiz NPS. W publikacji przedstawiono porównanie tych metod, zwrócono także uwagę na wysokorozdzielczą spektrometrię mas (HR-MS) oraz metody elektrochemiczne. Spośród omówionych metod to LC-MS wydaje się najbardziej optymalną do analiz NPS w próbkach biologicznych. Charakteryzuje się niską granicą wykrywalności, ponadto jest to metoda, czuła, specyficzna, szybka, nie wymagająca procesu derywatyzacji co zdecydowanie przemawia za jej zastosowaniem w analizach rutynowych.

Opisane w tej pracy metody miały posłużyć jako wstęp do dalszych badań na matrycach biologicznych (krew, mocz i włosy). Przygotowany przegląd literaturowy pozwolił na podjęcie prac opisanych w kolejnych publikacjach stanowiących podstawę niniejszej rozprawy doktorskiej.

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REVIEW ARTICLE

Overview of analytical methods for determining novel psychoactive substances, drugs and their metabolites in biological samples

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ABSTRACT

Recent years have witnessed a growing in interest in psychoactive substances, particularly those available in e-commerce. These have led to an increase in the number of drug-related poisonings, deaths, and road accidents. Illegal drugs are available on an unprecedented scale and cause previously unknown adverse effects, which creates a challenge for analysts to find rapid methods for identifying these substances and taking appropriate action in the shortest possible time. New psychoactive substances (NPSs) can be lethal at very low concentrations, which give particularly serious cause for concern. These drugs are easily accessible and often regarded (or claimed) to be safe, which encourages many people, in particular young people, to try them. The widespread use of these substances is compounded by the awareness that they are difficult to detect with the existing rapid screening tests. Simple, fast, sensitive, and specific methods for determining the largest possible number of black-market psychoactive substances and their metabolites are therefore essential. Such methods will facilitate treatment and increase the effectiveness of measures aiming to reduce drug addiction. The objective of this review article was to critically compare the most commonly used analytical methods for determining NPS and their metabolites in biological material, with special emphasis on the sample preparation process, and to highlight the possibilities offered by the existing analytical methods.

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1. Introduction

Recent years have witnessed a growing interest in new psychoactive substances (NPSs), including synthetic cannabinoids, in Europe and the United States (Van Gorp et al 2017; Cohen and Weinstein 2018). According to the 2017 World Drug Report of the United Nations Office on Drugs and Crime (UNODC 2016), almost 900 novel NPS had been identified between 2009 and 2019 (UNODC 2019). These substances are monitored by the European Monitoring Center for Drugs and Drug Addiction. To improve the security of drug-related crime, the EU Drugs Agency in Lisbon has developed the EU4Monitoring Drugs (EU4MD) project which covers European Neighborhood Policy (ENP) countries. The purpose of this program is to support national and regional readiness to identify and respond to drug safety and health threats. The aim of the research conducted within this framework is to facilitate the identification of novel NPS and to curb the sale of these drugs not only at the national level, but also in the European Union or even around the world. Most NPS are modifications of the existing (illegal) substances. NPSs are legal because they are obtained by modifying well-known and popular compounds, but their effects are similar to those of prohibited narcotic drugs (UNODC 2014).

The consumption of NPS is on the rise because young people perceive such legal highs to be a safe alternative to illegal psychoactive substances. In addition, a wide range of illegal psychoactive substances is still available on the market. These substances as well as NPS contribute to crime, accidents, and increased mortality. However, research has

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shown that NPSs have numerous side effects, including psychosis, paranoia, agitation, convulsions, anxiety, cardiotoxic effects, acute renal failure, respiratory depression, rhabdomyolysis, withdrawal symptoms, coma and, in extreme cases, death (Cannaert et al. 2016). The fact that NPS are often taken in combination with other psychoactive substances or alcohol makes it difficult to attribute specific symptoms to a particular substance. NPSs are not identified during routine toxicological analyses of blood, urine, or hair samples due to structural modifications, and they require more detailed, sensitive, and specific methods. New modifications are being continuously introduced, which additionally impedes analysis of NPS (Debruyne and Le Boisselier 2015). Due to the problems associated with NPS detection in real-life samples, effective medical intervention protocols for dealing with toxic poisoning are not available, which increases mortality and prevents the determination of the cause of death. In the long-term perspective, these problems can impede legal actions aiming to curtail the trade in NPS and prohibit their sale. Therefore, new analytical techniques are needed to exclude or confirm the presence of known psychoactive substances, and to identify as many NPS as possible. The existing analytical methods should be expanded to meet the analytical challenges associated with the development of the black market and the ever-increasing availability of psychoactive substances. A sensitive and specific method for determining NPS would enable the authorities to take the appropriate legal steps and increase public safety by limiting the sale of these toxic substances.

NPSs include groups of compounds, such as tryptamines, synthetic cannabinoids, phenethylamines, and synthetic cathinones (Brandt et al. 2014; Hurst 2019). The metabolic processes associated with various psychoactive substances have been explored by numerous researchers (Fleckenstein et al. 2000; Meltzer et al. 2006; Cozzi et al. 2009; Halberstadt et al. 2011; Nichols 2012; Lõpez-Arnau et al. 2012; Baumann et al. 2013; Eshleman et al. 2013; Meyer et al. 2014; Marusich et al. 2014; Blough et al. 2014; Simmler et al. 2014, 2013, Michely et al. 2015; Welter-Luedeke and Maurer 2016; Tyrkko et al. 2016). Metabolic processes differ depending on the affected system and the subtypes of activated receptors. The ingested substance and its metabolites should be analyzed due to the wide range of metabolic processes and their rapidity. Tyrkko et al. (2016) demonstrated that in analyses of cathinones and phenethylamines, the parent compound is detected in most user samples; however, the results should be confirmed by the presence of metabolites.

The purpose of this article was to review the literature on the existing techniques for analyzing psychoactive substances and promote the development of analytical methods for rapid identification of NPS. The developed methods should be modifiable to support rapid and unambiguous detection of both known and novel NPS. The article reviews the most popular methods of preparing biological samples, identifying psychoactive substances, and their metabolites as well as novel substances which pose a considerable challenge for toxicological laboratories.

2. Mechanisms, reactions, and assessment of health hazards associated with exposure to toxic substances

Psychoactive substances can be delivered to the body in many different ways: by gastrointestinal absorption, serum protein binding, hepatic metabolism, renal excretion, and competition for receptor sites (Shen 1997), insufflation, intravenous injection, transdermal absorption, crossing the blood–brain barrier. Depending on the substance, these processes determine whether the dose is therapeutic or toxic (Shen 1997). Before they are eliminated from the body, most psychoactive drugs have to be metabolized to more polar compounds by cytochrome P450 (CYP)-dependent monooxygenases in the hepatic endoplasmic reticulum, which is a phase I biotransformation process. The resulting products usually undergo another transformation *via* conjugation with endogenous glucuronide, which is a phase II biotransformation process. Most conjugated products do not have psychoactive properties and can be easily excreted from the body through the kidneys (Shen 1997). NPSs includes groups of compounds, such as tryptamines, synthetic cannabinoids, phenethylamines, and synthetic cathinones (Brandt et al. 2014; Hurst 2019).

2.1. Metabolism of synthetic tryptamines

Synthetic tryptamines interact with the serotonergic system, activate 5-HT1A and 5-HT2A receptor subtypes (Meyer et al. 2014) and increase the release of serotonin (5-HT) (Cozzi et al. 2009; Halberstadt et al. 2011; Halberstadt and Geyer 2011; Nichols 2012; Blough et al. 2014). Michely et al. (2015) analyzed two psychoactive substances (N,N-Diallyltryptamine [DALT] and 5-Metoksy-N,N-diallilotryptamine [5-MeODALT]) and attempted to identify their metabolites in urine samples with the use of MS-MS spectra. DALT was metabolized by hydroxylation reactions, and metabolic products were rehydrolyzed to dihydroxy metabolites and then to trihydroxy metabolites. N-dealkylation and N-oxidation reactions were also observed. Arylhydroxy metabolites were glucuronidated and sulfated. A similar pathway was observed in 5-MeODALT (Michely et al. 2015). Welter-Luedeke and Maurer (2016) investigated new amphetamine and methamphetamine derivatives with modified ring systems, including camfetamine (CFA), 3-methyl (phenyl) amphetamines (2-MA, 3-MA, and 4-MA), 2-metiopropamine (2-MPA) and 5-(2-aminopropyl) benzofuran (5-APB), 6-(2-aminopropyl) benzofuran (6 APB, also known as benzofuras), as well as their N-methyl derivatives: N-methyl 5-(2-aminopropyl) benzofuran (5-MAPB) and N-methyl-6-(2-aminopropyl) benzofuran (6-MAPB). CFA is an analog of N-ethyl analog fencamfamine (N-ethyl-3-phenylnorbornan-2-amine [FCF]), which is widely used as an appetite suppressant. Due to the effects of CFA (stimulation and increased alertness) and its structural similarity to FCF, Welter-Luedeke and Maurer assumed that CFA stimulates the nervous system because it can inhibit dopamine (DA) reuptake and promote the release of DA and noradrenaline (NA). Reactions, such as N-demethylation, aromatic and aliphatic hydroxylation, aromatic di-hydroxylation followed by

O-methylation, and combinations of these steps were observed in a study of CFA metabolism. CYP as well as isoenzymes that participate in aromatic hydroxylation (CYP2C19 and CYP2D6), N-demethylation (CYP2B6, CYP2C19, CYP2D6, and CYP3A4), and aliphatic hydroxylation (CYP1A2 and CYP246) were involved in metabolic processes. Glucuronidation of nearly all hydroxylated metabolites and several sulfates was also observed. CFA was extensively metabolized, and in addition to CFA, hydroxyaryl, and normetabolites were the most abundant compounds in urine (Welter-Luedeke and Maurer 2016). 2-MA, 3-MA, and 4-MA triggered the secretion of DA and NA at a similar level to amphetamine, but 5-HT secretion was higher (Welter-Luedeke and Maurer 2016). In the reported cases, 4-MA induced similar effects to amphetamine, including mydriasis, hyperthermia, hypertension, tachycardia, insomnia, and anxiety. Research has demonstrated that each of these isomers had different metabolites, probably due to differences in the position of the methyl group, which led to differences in enzyme affinity. 2-MA, 3-MA, and 4-MA were characterized by the highest number of metabolites in the group of the studied NPS. Aromatic hydroxylation was the most important metabolic step in each isomer. Aliphatic hydroxylation and hydroxylation in the benzyl group, followed by oxidation to the corresponding carboxylic acid, were also observed. Two ring hydroxylations followed by O-methylation were noted in 2-MA and 3-MA, but not in 4-MA. Glucuronidation and sulfation were not very important in the metabolic process of these compounds, but at least one glucuronide was detected for each isomer, and sulfates were identified only in 2-MA. CYP2D6 is the only human CYP isoenzyme involved in aromatic hydroxylation (the main stage for all three isomers), and it also catalyzes the aromatic hydroxylation of amphetamines. The cited authors also analyzed 2-methipropamine which has similar pharmacological properties to methamphetamine and acts as an NA and DA reuptake inhibitor. This psychoactive agent causes stimulation and mild euphoria, and the observed side effects include tachycardia, hypertension, and increased sweating. The main stages of biotransformation were N-demethylation, side chain hydroxylation followed by oxidation to the corresponding ketone compound or mono- and di-hydroxylation on the thiophene ring followed by O-methylation. Combinations of these steps as well as further glucuronidation and sulfation of hydroxymetabolites were also noted. The following isoenzymes were involved in the metabolic process: CYP1A2, CYP2B6, CYP2C19, CYP2D6, CYP2E1, and CYP3A4 in N-demethylation; CYP1A2 CYP2C19, CYP2D6, CYP2E1, and CYP3A4 in ring hydroxylation, and CYP2A2. The last compound had a furan ring added to the benzene ring. The resulting 5-APB and 6-APB and their 5-MAPB and 6-MAPB derivatives are associated not only with stimulants, such as amphetamine and methamphetamine, but also with entactogenic designer drugs, such as 3,4-methylenedioxyamphetamine (MDA) and 3,4-methylenedioxymethamphetamine (MDMA, ecstasy) which produce similar symptoms to MDA and MDMA. These drugs have euphoric and empathogenic effects, and side effects include tachycardia, hypertension, hyperthermia, insomnia, and anxiety. The effects of 5-APB and 6-APB and their ability to bind to various transporters and receptors were tested. Similarly to amphetamine, these compounds inhibited the DA transporter, NA transporter, and 5-HT transporter, but had greater affinity for the 5-HT transporter, especially 5-APB. 5-APB and 6-APB have high binding affinity for 5-HT2A and 5-HT2B receptors. In addition, 6-APB had high affinity for the a2C adrenergic receptor. N-demethylation was the main metabolic stage for 5- and 6-MAPB. In addition, ring cleavage initiated by hydroxylation in the furan ring system produced unsaturated aldehyde which was reduced to the corresponding aldehyde and, subsequently, to the appropriate alcohol or was oxidized to the corresponding carboxylic acid. These metabolites were observed in all four compounds. The following human CYP isoenzymes were involved in N-demethylation of 5-MAPB: CYP1A2, CYP2B6, CYP2C19, and CYP2D6; and in N-demethylation of 6-MAPB: CYP1A2, CYP2D6, and CYP3A4.

2.2. Metabolism of cathinones and phenylethylamines

Tyrkko et al. (2016) examined a group of cathinones and phenethylamines. Synthetic cathinones, such as amphetamines and cocaine, affect the levels of catecholamines: DA, NA, and 5-HT, in the central nervous system, exerting stimulatory effects. Cathinones integrate with monoamine transporters in two different ways: as transporter reuptake blockers and as transporter substrates. Both mechanisms of action increase extracellular concentrations of monoamines. Transporter substrates induce transport from the intracellular to extracellular, while blockers inhibit the uptake of neurotransmitters from synapses. Several studies have shown that MDPV, mephedrone, and α-pyrrolidinovalerophenone (α-PVP) interact and enhance DA, NA, and 5-HT neurotransmission by binding to monoamine transporters (DAT, NET, and SERT) on neurons, thus increasing catecholamine levels. Mephedrone and other ring-substituted cathinones are nonselective transporting substrates in DAT, NET, and SERT, while MDPV and α-PVP act as selective DAT and NET blockers (Fleckenstein et al. 2000; Meltzer et al. 2006; Lõpez-Arnau et al. 2012; Baumann et al. 2013; Eshleman et al. 2013; Simmler et al. 2013, 2014; Marusich et al. 2014). Marusich et al. (2014) have shown that α-PVP pyrrolidinophenones and α-PBP α-pyrrolidinobutyrophenone (α-PPP) are potent DAT and NET reuptake blockers, but do not exert any effects on SERT. All cathinones with pyrrolidinone structure, i.e. MDPV, α-PVP, αPBP, and α-PPP, stimulate motor activity, and their potency is consistent with their DAT-blocking power. Mephedrone affects the dopaminergic system rather than the serotoninergic system (Eshleman et al. 2013; Simmler et al. 2014). Metabolic profile of mephedrone is shown in Figure 1. Tyrkko et al. (2016) demonstrated that in both cathinones and phenethylamines, the parent compound is generally detected in user samples; however, their detection should be confirmed by the presence of specific metabolites. Many cathinones and phenylethylamines are metabolized by CYP2D6 enzymes.

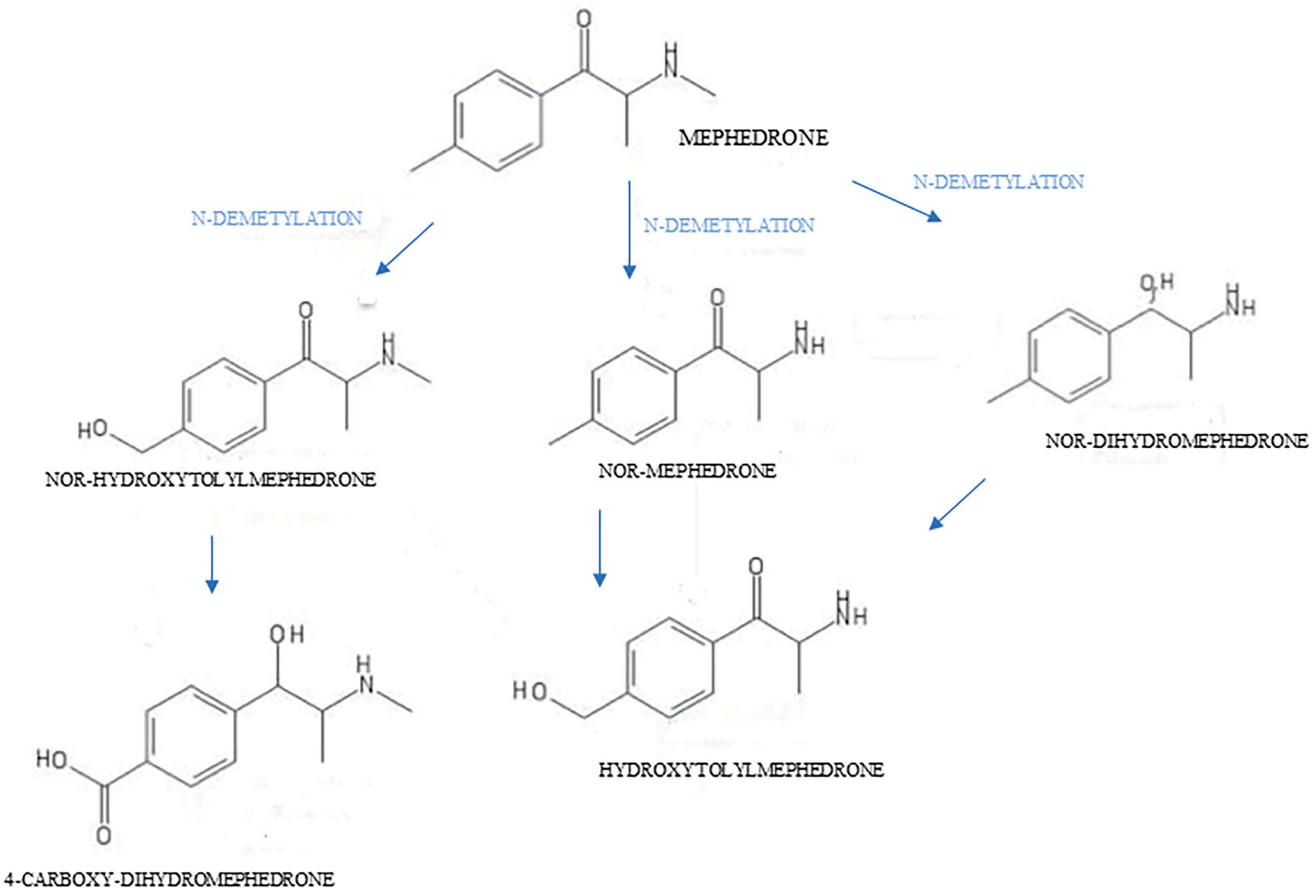

Figure 1. The metabolic profile of mephedrone.

3. Sample preparation methods

Samples for instrumental analysis require the appropriate treatment (sample preparation). The purpose of this process is to isolate the analytes from the examined material and to remove interference components that can disrupt the determination of the investigated substances. In the final step, the resulting extract is concentrated, enriched, or diluted according to analytical needs. The existing analytical methods are modified and new requirements are imposed on laboratories to address the growing number of tested substances. The most popular methods for preparing biological samples, including their limitations and potential for further modification, are discussed in this section. Biological materials are highly complex matrices, and components such as proteins, phospholipids, and salts have to be removed from the sample before analysis. Protein particles have to be removed from blood samples, whereas urine samples are subjected to hydrolysis. Acetonitrile is most commonly used to precipitate proteins from blood samples, and it has been applied by several researchers to analyze psychoactive compounds. Urine samples are usually hydrolyzed with β-glucuronidase which supports the determination of free metabolites of psychoactive substances (Yanes and Lovett 2012). Samples prepared with this enzyme can be subjected to further processes that facilitate effective determination of the analyzed substances.

3.1. Solid-phase extraction

Solid-phase extraction (SPE) is one of the most popular extraction techniques for pretreating samples in analyses of psychoactive substances. Analytes are extracted into solvent, and the sample is applied onto a SPE cartridge packed with the sorbent. Samples are washed with the appropriate solvent to remove interference components, and the desired analytes are eluted with solvents (Buszewski et al. 2012; Buszewski 2012).

The use of SPE for identifying psychoactive substances and drugs is presented in Table 1. The following SPE cartridges have been used in the literature: oasis HLB (60 mg) (Yeter 2017), Resprep Drug Prep I (200 mg) (Swortwood et al. 2013), Waters Oasis MCX (3 ml, 60 mg) (Barroso et al. 2010; Tang et al. 2014; Imbert et al. 2014), SOLA SCX (10 mg) (Concheiro et al. 2013), Chromabond Drug (200 mg) (Wohlfarth et al. 2010), PlyCrom Clin II (3 mL, 35 mg) (Kerrigan, Banuelos, et al. 2011; Kerrigan, Mellon, et al. 2011), Chromabond Drug (200 mg) (Mueller et al. 2005), and Strata X-C (Lendoiro et al. 2017).

Yeter (2017) relied on the SPE method to isolate 162 psychoactive substances and drugs from the blood with a recovery rate of 4.2–122%. Higher recovery rates were reported for benzodiazepines. The lowest recovery rates were noted for chlordiazepoxide, methylecgonine, metronidazole,

Table 1. List of solid-phase extraction (SPE) methods used to extract psychoactive substances from biological samples.

Group of analytes (number of analytes)	Matrix	Sample amount	Extraction solvent	SPE cartridge	SPE conditions			Recovery (%)	LOD	LOQ	References
					Precondition	Wash	Elution				
Opiates and opioids, benzodiazepines, amphetamines, barbiturates, cannabinoids, cathinones (162[a,*])	Blood	0.5 mL	Water	Oasis HLB, 60 mg	Water	Water	1 mL MeOH, 1 mL ethyl acetate	4.2–122	No data	No data	Yeter (2017)
Amphetamines, phenethylamines, cathinones (32[b,*])	Serum	1 mL	Sodium phosphate buffer (100 mM, pH 6.0)	Resprep Drug Prep I, 200 mg	3 mL MeOH, 3 mL water, 1 mL phosphate buffer	1 mL water, 1 mL 0.1 M acetic acid, 1 mL MeOH	1.5 mL dichloromethane, IPA, ammonium hydroxide (80:20:2 v/v/v/)	67.3–128.5	10–100 pg/mL	1-10 ng/mL	Swortwood et al. (2013)
Amphetamines, phenethylamines, opiates and opioids, benzodiazepines, Z-drugs, cathinones, cannabinoids, barbiturates (93[c,*])	Urine	1 mL	Sodium phosphate buffer (100 mM, pH 6.0)	Waters Oasis MCX, 3 cc, 60 mg	2 mL MeOH, 2 mL distilled water, 1 mL 100mM phosphate buffer (pH 6.0)	2 mL destilated water, 2 mL phosphate buffer	1 mL MeOH, ethyl acetate/isopropanol/ 20% ammonium hydroxide (84:14:2 v/v)	2–97	1–250 ng/mL	no data	Tang et al. (2014)
Cathinones (28[d,*])	Urine	250 µl	Sodium phosphate buffer (100 mM, pH 6.0)	SOLA SCX, 10 mg	1 mL MeOH, 1 mL 0.1 M phosphate buffer pH 6	1 mL 1M acetic acid, 1 mL MeOH, 1 mL hexane:ethyl acetate (50:50, v/v)	2 × 1 mL 2% NH4OH in dichloromethane/2-propanol (85:5 v/v)	78.9–116.7	0.25–1 µg/L	0.5–1 µg/L	Concheiro et al. (2013)
Cathinones, phenethylamines, piperazines, anesthetics (35[e,*])	Plasma	1 mL	Sodium phosphate buffer (100 mM, pH 6.0)	Chromabond Drug, 200 mg	1 mL MeOH, phosphate buffer (pH 6)	1 mL water, 1 mL acetic acid, 1 mL MeOH	1.5 mL dichloromethane/ isopropanol/25% ammonia (80:20:2; v/v/v)	72–90	1.0-5.0 ng/mL	No data	Wohlfarth et al. (2010)
Phenethylamines (10[f,*])	Urine	2 mL	Sodium phosphate buffer (100 mM, pH 6.0)	PlyCrom Clin II, 3 cc, 35 mg	1 mL deionized water, 1 mL 1M acetic acid	1 mL hexane, 1 mL ethyl acetate, 1 mL MeOH	1 mL 2% ammonium hydroxide in 95:5 (v/v) methylene chloride/isopropyl alcohol	63–94	2–10 ng/mL	2–10 ng/mL	Kerrigan, Banuelos, et al. (2011); Kerrigan, Mellon, et al. (2011)
Opiates and opioids, benzodiazepines, Z-drugs, phenethylamines, cannabinoids, antidepressants, cathinones (301[g,*])	Plasma	1 mL	Sodium phosphate buffer (100 mM, pH 6.0)	Chromabond Drug, 200 mg	–	–	Rapid trace; for the acidic/neutral fraction: 1.5 mL acetone/ dichloromethane (1:1; v/v), for the basic fraction: 1.5 mL dichloromethane/ isopropanol/25% aqueous ammonium (80:20:2; v/v/v)	–	–	–	Mueller et al. (2005)

*List of analytes available in the supplementary.

[a]6-Acetylmorphne, 7-Aminiclonazepam, Alprazolam, Amisulpride, Amitriptyline, Amlodipin, Amphetamine, Atenolol, Atropin, Benzoylecgonine, Biperiden, Bromazepam, Buprenorphine, Carbamazepine, Chlordiazepoxide, Chlorpheniramine, Chlotpromazine,, Citalopram, Clobazam, Clomipramine, Clonazepam, Clozapine, Cocaine, Codeine, Desipramine, Dextromethorphan, Diazepam, Diclofenac, Diltiazem, Diphenhydramine, Doxepin, Doxylamine, Etodolac, Famotidine, Fentanyl, Fluclonazole, Flunitrazepam, Fluoxetine, Flurazepam, Fluvoxamine, Haloperidol, Hydroxyzine, Imipramine, Ketamine, Lansoprazole, Lidocaine, Loperamide, Lorazepam, MDA, MDEA, MDMA, Metformin, Methadone, Methamphetamine, Methylecgonine, Metoclopramide, Metoprolol, Metronidazole, Mianserin, Midazolam, Mirtazapine, Moclobemide, Morphine, Naproxen, Nifedipine, Nordiazepam, Nortriptiline, Opipramol, Ornidazole, Oxazepam, Oxcarbazepine, Pantoprazole, Paracetamol, Paroxetine, Pentobarbital, Pentoxifylline, Pethidine, Pheniramine, Phenobarbital, Phenytoin, Prilocaine, Propafenone, , Propranolol, Propyphenazone, Pseudoephedrine, Quetiapine, Risperidone, Sertraline, Sildenafil, Tadalafil, THC, THC-COOH, Thiopental, Thioridazine, Tramadol, Verdenafil, Venlafaxine, Verapamil, CP 47,497 C8, CP 47,497, WIN 55,212-2,CP 55,940, 5-F-AKB-48-4-hydroxypentyl, 5-F-PB-22-3-carboxy-indole, 5-F-AB-Pinaca, 5-F-AKB-48, 5 F-ADB, AB-Chminaca, AB-Fubinaca-M2, AB-Pinaca-5-hydroxylpentyl, AB-Pinaca-pentanoic acid, AB-Chminaca-M1, AB-Chminaca-M2, ADB-Pinaca-pentanoic acod, ADB-Pinaca, AKB-48-N-5-hydroxypentyl, AKB-48-N-pentanoic acid, AM 2201, AM2201-6-hydroxyindole, AM 2201-N-4-hydroxypentyl, HU 210, JWH 0814-hydroxynaphtyl, JWH 081 N-5-hydroxypentyl, JWH 122 N-4-hydroxypentyl, JWH 122 N-5-hydroxypentyl, JWH 203 N -pentanoic acid, JWH 203, JWH 210 5-hydroxyindole, JWH 210 N-4-hydroxypentyl, JWH 210 N-5-hydroxypentyl, JWH 210 N-pentanoic acid, JWH 210, JWH 250 N-4-hydroxypentyl, JWH250 N-pentanoic acid, JWH 398 N-5- hydroxypentyl, JWH 398 N-pentanoic acid, JWH 018 N-pentanoic acid, JWH 018, JWH 018 N-5-hydroxypentyl, JWH 019, JWH 073, JWH 073 4-hydroxybutyl, JWH 073 N-butanoic acid, JWH 081, JWH 200, JWH 201, JWH 250 N-5-hydroxypentyl, JWH 250, MAM 2201 4-hydroxypentyl, MAM 2201 N-pentanoic acid, MAM 2201, PB-22-3-carboxyindole, RCS-4, RCS-4-N-5-carboxypentyl, RCS-4-N-5-hydroxypentyl, RCS-8, UR-144 N-5-hydroxypentyl, UR-144 N-pentanoic acid, UR-144, XLR- 11 6-hydroxyindle, XLR-11 N-4-hydroxypentyl, XLR-11.

[b]DOB, DOET, DOM, TMA, 2 C-B, 2 C-E, 2 C-I, 2 C-T-4, 2 C-T-7, MDA, MDEA, MDMA, Amphetamine, Methamphetamine, Ethylamphetamine, MDPV, Mephedrone, Cathinone, Methcathinone, Methedrone, 4-MEC, Flephedrone, Methylone, Butylone, BZP, DBZP, mCPP, TFMPP, AMT, DMT, 5-MeO-DMT, 5-MeO-DiPT.

[c]4-FA, 4-Methylthioamphetamine, Amphetamine, Bromo-dragonfly, Chloroamphetamine, DOB, DOET, DOM, HMMA, MBDB, MDA, MDEA, MDMA, Methamphetamine, N-ethylamphetamine, PMA, PMMA, Codeine, Norcodeine, Heroin, 6-MAM, Morphine, Normorphine, Cocaine, Benzoylecgonine, Cocaethylene, Norcocaine, Ketamine, Norketamine, Methoxetamine, Tiletamine, Chlordiazepoxide, Diazepam, Nordiazepam, Edtazolam, Flunitrazepam, 7-aminoflunitrazepam, Midazoam, 1-OH-Midazolam, 4-OH-

Midazolam, Nimetazepam, Oxazepam, Temazepam, Triazolam, 1-OH-triazolam, Carboxy-THC, THC-OH, JWH-018, JWH-018 4-OH- indole, JWH-018 N-5-OH-pentyl, JWH-073, CP-47,497, CP-47,497 C8 homolog, 2 C-B, 2 C-H, 2 C-I, 2 C-T-2, 2 C-T-4, 2 C-T-7, Mescaline, BZP, mCPP, MDBP, pFPP, pMeOPP, TFMPP, Cathinone, Ethylone, Mephedrone, Methcathinone, Methedrone, MethyIone, 5-MeO-DIPT, Alpha-methyltryptamine,Dimethyltryptamine, Psilocin, MDPV, Mitragynine, Salvinorin A, Dextromethorphan, Dextrorphan, Methadone, EDDP, Methaqualone, Phentermine, Zolpidem, Zopicolne, Amobarbital, Butarbital, Secobarbital.

[d]Cathinone, Methcathinone, 4-Fluoromethacathinone, Methylone, Ethylcathinone, alpha-PPP, Bupgedrone ephedrine, Ethylone, 4-Methoxymethcathinone, Buphedrone, Normephedrone, Diethylcathinone, MDPPP, 4- Methylephedrine, Butylone, Mephedrone, 4-MEC, 4-MEC metabolite, MDPBP, Pentedrone, Pentylone, 3,4-DMMC, alpha-PVP, 4-MPBP, MDPV, Pyrvalerone, Benzedrone, Naphyrone.

[e]Cathinone, Ethylamphetamine, Methcathinone, PMA, AMT, BZP, PMMa, 2C-H, 4-MTA, DMT, MeOPP, 2,5-DMA, 2C-D, 3,4-DMA, mCPP, MDDMA, DOM, MiPT, 5MeO-DMT, MDBP, 2C-P, DOET,3,4,5-TMA, TMA-6, TFMPP, Ketamine, 2C-T-2, Phencyclidine, DiPT, DPT, 2C-T-4, 2C-T-7, 2C-B, DOB, 2C-I, dimethylphenylpiperazine.

[f]2C-H, 4-MTA, DOM, DOET, 2 C-B, DOB, 2 C-I, DOI, 2 C-T-2, 2 C-T-7.

[g]6-O-monoacetylmorphine, Acebutolol, Aceprometazine, Acrivastine, Ajmaline, Alprazolam, Alprenolol, Amantadine, Amiloride, Aminophenazone, Aminopromazine, Amiodarone, Amitriptyline, Amodipine, Amphetamine, Apomorphine, Airidine, Astemizole, Atenolo, Atropine, Befunolol, Benazepril, Benzatripine, Benzocaine, Benzoctamine, Benzoylecgonine, Betaxolol, Biperiden, Bisoprolol, Bromazepam, Bromipheniramine, Bromocriptine, Brotizolam, Bunitrolol, Bupivacine, Bupranolol, Buprenorpnine, Buspirone, Butaperazine, Caffeine, Candesartan, Captopril, Carazolol Carbamazepine, Carbimazole, Carbinoxamine, Carbuterol, Carisoprodol, Carteolol, Carvedilol, Celiprolol, Cetrizine, Chlorcyclizine, Chlordiazepoxide, Chloroquine, Chlorphenethiazine, Chlorpheniramine, Chlorpromazine, Chlorprothixene, cinnarizine, Cisapride, Citalopram, Clemastine, Clenbuterol, Clobazam, Malathion, MDA, MDE, MDMA, Meclozine, Medazepam, Meloxicam, Meperone, Mepindolol, Meprobamate, Mescaline, Mesoridazine, Metaclazepam, Methamphetamine, Metformin, Methadone, Normethadone, Methylphenidate, Methylscopolamine, Metipranol, Metoclomipramide, Metoprolol, Metrinodazole, Mexiletine, Mianserin, Miconazole, Midazolam, Mirtazapine, Mizolastine, Moclobemide, Molindone, Molsidomine, Morphine, Morphine-3-β-D-glucuronide, Naloxone, Naltrexone, Nateglinide, Niciridipine, Nicotine, Nifedipine, Nilvadipine, Nimodipine, Nisoldipine, Nitrazepam, Nitrendipine, Nizatidine, Norbuprenorphine, Normorphine, Nortriptiline, Noscapine, Obidoxime, OH-THC, Olanzapine, Ondansetron, Opipramol, Orphenadrine, Oxazepam, Oxacarbazepine, Oxitropium, Oxprenolol, Oxycodone, Papaveerine, Paracetamol, Paroxetine, Penbutolol, Norclobazam, Clobutinol, Clomethiazole, Clomipramine, Desmethylclomipramine, Clonazepam, Clonidine, Clozapine, Cocaine, Codeine, Coumatetralyl, Cyclizine, Demoxepam, Dextropropoxyphene, Diazepam, Dibenzepin, Dihydrocodeine, Dihydroergotamine, Dilazep, Dilitiazem, Diphenhydramine, Dipyridamole, Disopyramide, Dixyrazine, Doxapram, Doxepin, Ebastine, Ecgonine methylester, Embutramide, Enalapril, Eprosartan, Ergotamine, Esmolol, Ethenzamide, Ethylmorphine, Ethylparathion, GFelodipine, Fenazepam, Fendilline, Fenetylline, Fenfluramine, Fentanyl, Fexofenadine, Flecainide, Fluconazole, Flunitrazepam, Fluoxetine, Flupetixol, Fluphenazine, Flurazepam, Fluvoxamine, Gallopamil, Glibenclamide, Glibornuride, Glicazide, Glimepiride, Glipizide, Gliquidone, Haloperidol, Heroin, Hydrcodone, Hydroxychloroquine, Hydroxyzine, Pentoxyvprazosin, Prilocaine, Primidone, Procainamide, Procaine, Promazine, Promethazine, Prometryn, Propafenone, Propionylpromazine, Propranolol, Pindolol, Pioglitazon, Pirbuterol, Piroxycam, Practolol, Prajmalium, Prazepam, Prazosin, Prilocaine, Primidone, Procainamide, Procaine, Promazine, Promethazine, Prometryn, Propafenone, Propionylpromazine, Propranolol, Propyphenazone, Prothipendyl, Protriptyline, Pseudoephedrine, Quetiapine, Quinapril, Quinine, Ramipril, Rantidine, Repaglinide, Reproterol, Risperidone, Rocuronium, Ropivacine, Rosiglizatone, Scopolamine, Sertindole, Sertraline, Sildenafil, Sotalol, Sulindac, Sulpride, Talinolol, Telmisartan, Temazepam, Terfanadine, Tertalolol, Tetracaine, Tetrahydrocannabinol, THC-COOH, Theobromine, Theophylline, Thioridazine, Tilidazine, Tilidine, Timolol, Thiothixene, Tizandine, Tocainide, Imipramine, Indomethacin, Irbesartan, Isoniazid, Isradipine, Ketamine, Ketoprofen, Ketorolac, Labetalol, Lacidipine, Lamotrigine, Lercarnidipine, Levobunolol, Levocabastine, Levomepromazine, Lidocaine, Lisinopril, Loratadine, Lorazepam, Losartan, Lysergic acid diethylamide, Tolbutamide, Toliprolol, Tolbuterol, Tramadol, Trazodone, Triamterene, Traizolam, Trifluorperazine, trifluperidol, Trimethoprim, Trimipramine, Valsartan, Vardenafil, Venlafaxine, Verapamil, Warfaine, Zolpidem, Zpiclone, Zuclopenthixol, Vincamine, Zimeldne.

paracetamol, CP 47.497, HU 210, and JWH 018 N-5-hydroxypentyl at 5.4%, 7.4%, 4.2%, 5.9%, 5.8%, 6.7%, and 5.4%, respectively. The highest recovery rates were obtained for Δ9-THC (122%), 5-F-AKB-48-4-hydroxypenttyl (118.6%), ADB-Pinaca (118.3%), Metoprolol (112.2%), and Imipramine (114%). Swortwood et al. (2013) analyzed a significantly smaller number of cathinones and other designer drugs in the blood with recovery rates in the range of 67.3–128.5%. These results suggest that extraction losses can be significantly reduced by focusing on a specific group of compounds. The lowest recovery rates were reported for 2 C-T-4 (69.5%) and 2 C-T-7 (67.3%), which was attributed to the presence of sulfur in the structure of these compounds. Recovery rates in excess of 100% were attributed to possible losses during the drying and enrichment phase.

Tang et al. (2014) extracted 93 analytes from urine with the use of Oasis columns. Recovery rates were determined within a wide range of values (2–97%), and similar results were reported by Yeter (2017). Normorphine, benzoylecgonine, and 4-OH-midazolam were characterized by relatively low extraction efficiency (41–46%), and significantly lower recovery rates were noted in cannabinoid compounds. JWH-018 and its 4-OH-indole metabolite, JWH-073, and the C8 homolog of CP-47,497 had an extraction efficiency $<10\%$. Such low recovery values were attributed to the use of glucuronidase because cannabinoids were more effectively extracted when this compound was not applied in the sample preparation process.

Tang et al. (2014) and Barroso et al. (2010) used Oasis columns to extract psychoactive substances from hair. Imbert et al. (2014) observed that heroin is rarely detected in blood or urine samples, but can be effectively extracted from hair. The IDA values for the analyzed substances were determined in the range of 10–20 pg/mg, and the limit of quantification (LOQ) was 50 pg/mg. However, the average recovery rate was 91.3–101.3%. In a study by Barroso et al. (2010), piperazine was extracted from hair with the use of Oasis columns, and the LOQ was determined at 50 pg/mg. Lendoiro et al. (2017) relied on modified SPE methods to extract piperazine and cathinones from hair samples. The average recovery rates ranged from 47.8% to 85.0%, whereas IDA and LOQ values were determined at 0.2–5 and 2–10 pg/mg, respectively. The authors discussed the difficulties associated with extracting numerous substances from a limited number of samples.

Concheiro et al. (2013) analyzed 28 synthetic cannabinoids and their metabolites in urine samples. Recovery rates were determined within a relatively narrow range (78.9–116.7%), and similar results were reported by Swortwood et al. (2013) who examined a smaller number of compounds. Wohlfarth et al. (2010) isolated amphetamines, tryptamines, and piperazines from blood samples and analyzed 35 substances belonging to these groups of substances. Extraction efficiency ranged from 72% to 90%. Kerrigan, Banuelos, et al. (2011) and Kerrigan, Mellon, et al. (2011) extracted phenylethylamine compounds with a recovery rate of 63–94%. The lowest recoveries were obtained for DO group drugs, and the polarity of the elution solvent had to be increased to optimize the recovery rate. Mueller et al. (2005) analyzed 301 substances based on the existing database of substance

spectra. However, the effectiveness of blood extraction or the detection limit of the examined substances was not determined in the cited study. The same method was applied by Rojek et al. (2017), which indicates that despite its disadvantages, this approach is still used in laboratories.

SPE generates large amounts of waste during sample preparation, which increases analytical costs (Yanes and Lovett 2012). However, one of the greatest advantages of SPE is that the process can be easily automated, thus reducing run times and waste generation. These observations suggest that the columns used by the cited researchers are not suitable for all groups of compounds. The smaller the range of the analytes, the higher the recovery values. However, run time is prolonged, more materials are used, and analytical costs increase when several types of columns are used to analyze a single blood or urine sample.

3.2. Liquid–liquid extraction

Liquid–liquid extraction (LLE) is the second most popular method for extracting psychoactive substances. An immiscible organic solvent is added to the sample, the contact between liquid phases is increased, and the organic solvent is removed/diluted. When the phases come into contact, analytes are transferred from the sample to an organic solvent (Aldlgan and Torrance 2016).

The results of LLE are summarized in Table 2. Organic solvents such as butyl acetate (Mueller et al. 2005), acetonitrile (Adamowicz and Tokarczyk 2016), chloroform (Papoutsis et al. 2010), or solvent mixtures of acetonitrile with ammonium formate (Cannaert et al. 2016), n-hexane with ethyl acetate (Kneisel and Auwärter 2012; Salomone et al. 2012; Salomone et al. 2014; Gottardo et al. 2014), 1-chlorobutane with a mixture of dichloromethane and ethyl acetate (Wicka et al. 2014), diethyl ether with ethyl acetate (Montenarh et al. 2015), and a mixture of hexane with chloroform, ethanol and diethyl ether (Shah et al. 2012) were successfully used to prepare samples for LLE. Mueller et al. (2005) extracted 301 substances from blood by LLE, but did not specify the recovery values or detection limits. However, they concluded that the developed method could be successfully used to analyze real-world samples. When a single solvent was used for extraction, recovery rates were determined in a wide range of 1.8–133% (Adamowicz and Tokarczyk 2016) and 74–119% (Papoutsis et al. 2010). Similarly to SPE, the range of recovery values was narrowed down when a smaller number of analytes were examined.

Adamowicz and Tokarczyk (2016) examined 143 analytes and determined LOD values for 104 compounds in the range 0.01–3.09 ng/mL. Much higher LOD values were obtained (0.52–58.47 ng/mL) when ACN was replaced with chloroform in the extraction process (Papoutsis et al. 2010). However, these results were noted in a different group of analytes; therefore, reliable conclusions about the influence of the above solvents on extraction efficiency cannot be drawn. Cannaert et al. (2016) used ACN with 10 M ammonium formate to extract analytes from urine samples. The LOQ was 0.01 ng/mL for each of the seven tested analytes. This result could suggest that these mixtures can be used in the extraction process to lower the detection limit while maintaining satisfactory process efficiency. The mixture of n-hexane and ethyl acetate (99:1 v/v) used by Kneisel and Auwärter (2012) produced low recovery values (5.70–56.2%). Despite low LOD values (0.01–2.00 ng/mL), this is a considerable disadvantage in analyses of biological samples when the concentrations of the examined substances are low and when analytes are lost in the extraction stage. In the work of Wicka et al. (2014), a mixture of 1-chlorobutane and dichloromethane with ethyl acetate (70:30 v/v) produced significantly lower detection limits (0.1 ng/mL for benzodiazepines; (up to 5 ng/mL for other substances) than chloroform (0.52–58.47 ng/mL). Salomone et al. (2014), Gottardo et al. (2014), and Salomone et al. (2012) used the above mixture to analyze hair samples. In the work of Salomone et al. (2014), the recovery range was 84–114%, but it was not specified by the remaining researchers. In the cited study, the values of LOD and LOQ were determined at 0.2–24.0 and 0.7–80.0 pg/mg, respectively. The LOQ values were determined at 0.02–3.0 pg/mg by Gottardo et al. (2014) and at 0.07–9.9 mg by Salomone et al. (2012). Montenarh et al. (2015) also analyzed cannabinoids and reported LOQ values in the range of 10–20 pg/mg. The average recovery rate was 72–130%, and LOD was in the range of 10–500 pg/mg. Shah et al. (2012) investigated a different extraction mixture which was characterized by high average recovery (90.4–110.4%) and LOD and LOQ values of 2.5–5 and 5–10 pg/mg, respectively. However, the extraction efficiency of the above solvents cannot be compared because recovery was not specified by Shah et al. (2012). The LLE method was also successfully used in recent years (Alexandridou et al. 2020; Fels et al. 2020; Institóris et al. 2022), which suggests that LLE is a highly promising extraction technique.

LLE is a fast, versatile, and simple technique that can be applied in analyses of contaminated samples. However, reagent costs can be high, and the method can generate large amounts of harmful waste. Miniaturized approaches to LLE and droplet-based LLE can significantly reduce costs and waste generation. Despite the fact that recovery values are similar in LLE and SPE, LOD values tend to be lower in LLE, and analytical costs and run times can be reduced. Analytes should be isolated with the use of solvents that guarantee the highest extraction efficiency for a large group of compounds. LLE also has considerable potential for hair tests which are widely used to combat drug crime.

3.3. Molecularly imprinted polymers

Methods that rely on molecularly imprinted polymers (MIPs) are also used to detect psychoactive substances. MIPs combined with micro-SPE (μ-SPE) can be effectively applied to analyze the ever-growing number of novel drugs. New psychoactive substances are being developed and placed on the black market to replace drugs that are known and controlled by the existing laws. The miniaturization of the extraction process is particularly useful for pre-concentrating low-volume samples because it prevents analyte loss in successive

Table 2. List of liquid-liquid extraction (LLE) methods used to extract psychoactive substances from biological samples.

Group of analytes (number of analytes)	Matrix	Analytical method	Sample amount	Extraction solvent	Recovery (%)	LOD	LOQ	References
Cannabinoids (7[a]*)	Urine	LC-MS/MS	0.5 mL	1.5 mL ACN with 0.5 mL 10M ammonium formate	No data	No data	0.01 ng/mL	Cannaert et al. (2016)
Amphetamines, benzodiazepines, opiates, phenethylamines, cathinones, cannabinoids, Z-drugs, other (301[b]*)	Plasma	HPLC-MS/MS	1 mL	Butyl acetate	–	–	–	Mueller et al. (2005)
Cathinones, cannabinoids, phenethylamines, amphetamines (143[c]*)	Blood	LC-MS	200 µL	ACN	1.8–133	0.01–3.09 [ng/mL]	No data	Adamowicz and Tokarczyk (2016)
Benzodiazepines (23[d]*)	Blood	EI-GC-MS	1 mL	Chloroform	74–119	0.52–58.47 ng/mL	1.58–177.2 ng/mL	Papoutsis et al. (2010)
Cannabinoids (30[e]*)	Serum	LC-MS/MS	1 mL	n-Hexane : ethyl acetate (99:1 v/v)	3.5–56.2	0.01–2.00 ng/mL	No data	Kneisel and Auwärter (2012)
Opiates and opioids, benzodiazepines, Z-drugs, amphetamines (30[f]*)	Blood	LC-MS/MS	1 mL	1-Chlorobutane: mixture of dichloromethane and ethyl acetate (70: 30 v/v)	No data	100 pg/mL- 5 ng.mL	No data	Wicka et al. (2014)

*List of analytes available in the supplementary.

[a]JWH-018, JWH-122, MAM-2201, JWH-210, EAM-2201. PB-22, 5F-PB-22.

[b]6-O-monoacetylmorphine, Acebutolol, Acepromethazine, Acrivastine, Ajmaline, Alprazolam, Alprenolol, Amantadine, Amiloride, Aminophenazone, Aminopromazine, Amiodarone, Amitriptyline, Amodipine, Amphetamine, Apomorphine, Airidine, Astemizole, Atenolo, Atropine, Befunolol, Benazepril, Benzatripine, Benzocaine, Benzoctamine, Benzoylecgonine, Betaxolol, Biperiden, Bisoprolol, Bromazepam, Bromipheniramine, Bromocriptine, Brotizolam, Bunitrolol, Bupivacine, Bupranolol, Buprenorpnine, Buspirone, Butaperazine, Caffeine, Candesartan, Captopril, Carazolol Carbamazepine, Carbimazole, Carbinoxamine, Carbuterol, Carisoprodol, Carteolol, Carvedilol, Celiprolol, Cetrizine, Chlorcyclizine, Chlordiazepoxide, Chloroquine, Chlorphenethiazine, Chlorpheniramine, Chlorpromazine, Chlorprothixene, cinnarizine, Cisapride, Citalopram, Clemastine, Clenbuterol, Clobazam, Malathion, MDA, MDE, MDMA, Meclozine, Medazepam, Meloxicam, Meperone, Mepindolol, Meprobamate, Mescaline, Mesoridazine, Metaclazepam, Methamphetamine, Metformin, Methadone, Normethadone, Methylphenidate, Methylscopolamine, Metipranol, Metoclomipramide, Metoprolol, Metrinodazole, Mexiletine, Mianserin, Miconazole, Midazolam, Mirtazapine, Mizolastine, Moclobemide, Molindone, Molsidomine, Morphine, Morphine-3-β-D-glucuronide, Naloxone, Naltrexone, Nateglinide, Nicirdipine, Nicotine, Nifedipine, Nilvadipine, Nimodipine, Nisoldipine, Nitrazepam, Nitrendipine, Nizatidine, Norbuprenorphine, Normorphine, Nortriptiline, Noscapine, Obidoxime, OH-THC, Olanzapine, Ondansetron, Opipramol, Orphenadrine, Oxazepam, Oxacarbazepine, Oxitropium, Oxprenolol, Oxycodone, Papaveerine, Paracetamol, Paroxetine, Penbutolol, Norclobazam, Clobutinol, Clomethiazole, Clomipramine, Desmethylclomipramine, Clonazepam, Clonidine, Clozapine, Cocaine, Codeine, Coumatetralyl, Cyclizine, Demoxepam, Dextropropoxyphene, Diazepam, Dibenzepin, Dihydrocodeine, Dihydroergotamine, Dilazep, Dilitiazem, Diphenhydramine, Dipyridamole, Disopyramide, Dixyrazine, Doxapram, Doxepin, Ebastine, Ecgonine methylester, Embutramide, Enalapril, Eprosartan, Ergotamine, Esmolol, Ethenzamide, Ethylmorphine, Ethylparathion, GFelodipine, Fenazepam, Fendilline, Fenetylline, Fenfluramine, Fentanyl, Fexofenadine, Flecainide, Fluconazole, Flunitrazepam, Fluoxetine, Flupetixol, Fluphenazine, Flurazepam, Fluvoxamine, Gallopamil, Glibenclamide, Glibornuride, Glicazide, Glimepiride, Glipizide, Gliquidone, Haloperidol, Heroin, Hydrcodone, Hydroxychloroquine, Hydroxyzine, Pentoxyvprazosin, Prilocaine, Primidone, Procainamide, Procaine, Promazine, Promethazine, Prometryn, Propafenone, Propionylpromazine, Perazine, Perphenazine, Pethidine, henazone, Phenylbutazone, Phenylpropanolamine, Phenyltoloxamine, Phenytoin, Pilocarpine, Pindolol, Pioglitazon, Pirbuterol, Piroxycam, Practolol, Prajmalium, Prazepam, Prazosin, Prilocaine, Primidone, Procainamide, Procaine, Promazine, Promethazine, Prometryn, Propafenone, Propionylpromazine, Propranolol, Propyphenazone, Prothipendyl, Protriptyline, Pseudoephedrine, Quetiapine, Quinapril, Quinine, Ramipril, Rantidine, Repaglinide, Reproterol, Risperidone, Rocuronium, Ropivacine, Rosiglizatone, Scopolamine, Sertindole, Sertraline, Sildenafil, Sotalol, Sulindac, Sulpride, Talinolol, Telmisartan, Temazepam, Terfanadine, Tertalolol, Tetracaine, Tetrahydrocannabinol, THC-COOH, Theobromine, Theophylline, Thioridazine, Tilidazine, Tilidine, Timolol, Thiothixene, Tizandine, Tocainide, Imipramine, Indomethacin, Irbesartan, Isoniazid, Isradipine, Ketamine, Ketoprofen, Ketorolac, Labetalol, Lacidipine, Lamotrigine, Lercarnidipine, Levobunolol, Levocabastine, Levomepromazine, Lidocaine, Lisinopril, Loratadine, Lorazepam, Losartan, Lysergic acid diethylamide, Tolbutamide, Toliprolol, Tolbuterol, Tramadol, Trazodone, Triamterene, Traizolam, Trifluorperazine, trifluperidol, Trimethoprim, Trimipramine, Valsartan, Vardenafil, Venlafaxine, Verapamil, Warfaine, Zolpidem, Zpiclone, Zuclopenthixol, Vincamine, Zimeldne.

[c]25B-NBOMe, 25 C-NBOMe, 25H-NBOMe, 25I-NBOMe, 2-AI, 2 C-B, 2 C-C, 2 C-D, 2 C-E, 2C-H, 2 C-I, 2C-N, 2 C-T-2, 2C-T-2, 2C-T-7, 2-DPMP, 2-FA, 2-MMC, 3,4-DMMC, 3 C-P, 3-FMC, 3-MeO-PCP, 3-MMC, 4-acetoxy-DiPT,4-BMC, 4-CMC, 4-EMC, 4-FA, 4-FMA, 4-FMC, 4-hydroxy-DET, 4-hydroxy-DiPT, 4-hydroxy-MET, 4-hydroxy-MiPT, 4-MBC, 4-MEC, 4-MeO-DMT, 4-MTA, 5-APB, 5-APDB, 5-CI-UR-144, 5-HTP, 5-IT, 5-MAPB, 5-MeO-AMT, 5-MeO-DALT, 5-mEO-DiPT, 5-MeO-DMT, 5-MeO-MiPT, 6-APB, 6-IT, alpha-MT, alpha-PBP, alpha-PPP, alpha-PVP, APINACA, AM-679, AM-679, AM-694, AM-1220, AM-2201, AM-2233, BDB, BMDP, Buphedrone, Bupropion, Butylone, BZP, CP 80633, D2PM, DCPP, DET, Dibutylone, Diethylpropion, DiPT, DMC, Dimethylone, DMA, DMT, DOET, DOI, DOM, DPT, EAM-2201, Ephedrone, Ethcathinone, Ethylone, Ethylphenidate, Eutylone, HU-308, JWH-0007, JWH-018, JWH-018-D9, JWH-019, JWH-073, JWH-081, JWH-098, JWH-122, JWH-122-7-methylnaphtyisomer, JWH-182, JWH-200, JWH-203, JWH-210, JWH-250, JWH-251, JWH-307, JWH-398, JWH-412, M-Alpha, mCPP, MDAI, MDPBP, MDPPP, MDPV, MeBP, MeOPP, MeP, 4-MMC, 4-MMC D3, MET, Metamfepramone, Methedrone, Methoxetamine, Methylone, MPA, MPBP, MPPP, Naphyrone, NEB, NMT, PCP, pCPP, Pnetedrone, Pentylone, pMeOPP, PPA, RCS-4, SDB-001, STS-135, TFMPP, THJ-2201, TMA, TMA-2, UR-144, URB-597, XLR-11.

[d]Alprazolam, Bromazepam, Camazepam, Chlordiazepoxide, Clobazam, Clonazepam, Diazepam, Fludiazepam, Flinitrazepam, 7-aminoflunitrazepam, Flurazepam, Lorazepam, Lormetazepam, Medazepam, Midazolam, Nimetazepam, Nitrazepam, Nordiazepam, Ozaxepam, Prazepam, Temazepam, Tetrazepam, Triazolam.

[e]JWH-007, JWH-015, JWH-018, JWH-018 adamantyl derivative, JWH-019, JWH-020, JWH-073, JWH-081, JWH-122, JWH-122 5-fluoropentyl derivative, JWH-200, JWH-203, JWH-210, JWH-250, JWH-251, JWH-307, JWH-387, JWH-398, JWH-412, AM-694, AM-1220, AM-2201, AM-2233, CRA-13, Methanandamide, RCS-4, RCS-4 ortho isomer, RCS-8, WIN 48,098, WIN 55,212-2.

[f]Alprazolam, Bromazepam, Chloridiazepoxide, Clobazam, Clonazepam, Diazepam, Estazolam, Lorazepam, Lormetazepam, Nitrazepam, Temazepam, Oxazepam, Midazolam, Medazepam, Clorazepam, Zolpidem, Zaleplon, Zopiclone, Nordiazepam, MDMA, MDEA, MDA, Amhetamine, methamphetamine, OH- amhetapmine, Cocaine, Benzoylecgonine, Morphine Codeine, LSD.

Table 3. Methods with high uncertainty and unsuitable for routine analysis.

Analytes	Concentration	Test type	Cross-reactivity [%]	LOD	Reference
Amphetamine, Pseudoephedrine, Phentermine, MDA, MDMA, MDEA, PMA, 4-MTA,2CB, MBDB, Phenylethylamine, Putrescine, Tryptamine, Tyramine, Methamphetamine, Ephedrine	50 ng/mL	Bio-Quant Methamphetamine	2–73	1 ng/mL (methamphetamine)	Maher et al. (2007)
Amphetamine, Methamphetamine, Ephedrine, PMA, 4-MTA, MBDB, Phenthylamine, Pseudoephedrine, Phentermine, MDA, MDMA,MDEA, 2C-B, Putrescine, Trytamine, Tyramine	50 ng/mL	Bio-Quant Amphetamine	2–282	1 ng/mL (for amphetamine)	
Amphetamine, MDMA, Methamphetamine,4-MTA, DOB, DOI, DOM, 2C-B, 2C-H, 2C-I, 2C-T-2, 2C-T-4, 2C-T-7	200 ng/mL	Immunalysis Methamphetamine	<0.4–100	200 ng/mL (for methamphetamine)	Kerrigan et al. (2011)
Amphetamine, MDMA, Methamphetamine, 4-MTA,DOB, DOI, DOM, 2C-B, 2C-H, 2C-I, 2C-T-2, 2C-T-4, 2C-T-7	200 ng/mL	Venture Labs Methamphetamine	<0.4–350	200 ng/mL (for methamphetamine)	
Amphetamine, MDMA, Methamphetamine, 4-MTA, DOB, DOI, DOM, 2C-B, 2C-H, 2C-I, 2C-T-2, 2C-T-4, 2C-T-7	200 ng/mL	IDS Methamphetamine/ MDMA	<0.4–100	200 ng/mL (for methamphetamine)	
Amphetamine, MDMA, Methamphetamine, 4-MTA, DOB, DOI, DOM, 2C-B, 2C-H, 2C-I, 2C-T-2, 2C-T-4, 2C-T-7	200 ng/mL	OraSure Methamphetamine	<0.4–100	200 ng/mL (for methamphetamine)	
Amphetamine, MDMA, Methamphetamine, 4-MTA, DOB, DOI, DOM, 2C-B, 2C-H, 2C-I, 2C-T-2, 2C-T-4, 2C-T-7	200 ng/mL	Venture Labs MDMA	<0.4–100	200 ng/mL (for MDMA)	
Amphetamine, MDMA, Methamphetamine, 4-MTA, DOB, DOI, DOM, 2C-B, 2C-H, 2C-I, 2C-T-2, 2C-T-4, 2C-T-7	200 ng/mL	Neogen Methamphetamine/ MDMA	<0.4–100	200 ng/mL (for methamphetamine)	
Amphetamine, Methaphetamine, MDMA, 4-MTA,DOI, 2C-B, 2C-H, 2C-I, 2C-T-2, 2C-T-4, 2C-T-7, DOB, DOM	200 ng/mL	Neogen Amphetamine	<0.4–100	200 ng/mL (for amphetamine)	
Amphetamine, Methamphetamine, MDMA, 4-MTA, DOB, DOM, 2C-H, 2C-I, 2C-T-2, 2C-T-4, 2C-T-7, DOI, 2C-B	200 ng/mL	Immunalysis Amphetamine	<0.4–200	200 ng/mL (for amphetamine)	
Amphetamine, Methamphetamine, MDMA, 4-MTA, DOB, DOI, DOM, 2C-B, 2C-H, 2C-I, 2C-T-2, 2C-T-4, 2C-T-7	200 ng/mL	OraSure Amphetamine	<0.4–200	200 ng/mL (for amphetamine)	
Phenazepam, Etizolam, Pyrazolam, Flubramazepam, Diclazepam, Delorazepam	5 ng/mL in PBS buffer	Immunalysis Benzodiazepine ELISA Kit	89–111	–	O'Connor et al. (2016)
Phenazepam, Etizolam, Pyrazolam, Flubramazepam, Diclazepam, Delorazepam	10 ng/mL in PBS buffer	Immunalysis Benzodiazepine ELISA Kit	75–110	–	
Phenazepam, Etizolam, Pyrazolam, Flubramazepam, Diclazepam, Delorazepam	100 ng/mL in PBS buffer	Immunalysis Benzodiazepine ELISA Kit	72–143	–	
Phenazepam, Etizolam, Pyrazolam, Flubramazepam, Diclazepam, Delorazepam	300 ng/mL in PBS buffer	Immunalysis Benzodiazepine ELISA Kit	93–143	–	
Phenazepam, Etizolam, Pyrazolam, Flubramazepam, Diclazepam, Delorazepam	5 ng/mL in blank blood	Immunalysis Benzodiazepine ELISA Kit	85–100	–	
Phenazepam, Etizolam, Pyrazolam, Flubramazepam, Diclazepam, Delorazepam	10 ng/mL in blank blood	Immunalysis Benzodiazepine ELISA Kit	88–109	–	
Phenazepam, Etizolam, Pyrazolam, Flubramazepam, Diclazepam, Delorazepam	100 ng/mL in blank blood	Immunalysis Benzodiazepine ELISA Kit	70–126	–	
Phenazepam, Etizolam, Pyrazolam, Flubramazepam, Diclazepam, Delorazepam	300 ng/mL in blank blood	Immunalysis Benzodiazepine ELISA Kit	62–107	–	
4-FMA, MDEA, PMMA, 5-APDB, Pentylone, 5-IT, beta-keto-EBDB,2C-T-7, MDPV, beta-keto-MDDMA, N-Ethylcathinone, 2-AI, beta-keto-MBDB, 4-FA, 4-MTA, 5-APB, DOB, AMT, BZP, 5-APDI, DOEt, DMA, DOI, DPT, MDPPP, beta-keto-MDEA, MAPB, Pentedrone, MPA, PMA, DOM, DMT, 5-MeO-AMT, MDPBP, MOPPP, beta-keto-MDMA, Methedrone, 5-IAI, DOC, 4-CAB, 6-APB, 2C-B, 2C-I, DMMA, 4-EEC, 1-(3-TFMPP), mCPP, Naphyrone, MDAI, 4-MA, 2C-C, 4-MEC, 4-MMC, 1-(4-TFMPP),25-I-NBOMe, 25C-NBOMe, 25B-NBOMe, 2C-E, 2C-T-2, 2C-T-4, 2C-T, 4-OH-DET,5-MeO-MiPT, 5-methoxy-DALT, 5-MeO-DMT, MPHP, 4-MPBP, MPPP, Pyrovalerone, D2PM, alpha-PBP, alpha-PVP, alpha-PPP, 4-MBC, 3,4-DMMC, 4-FMC, Cathinone, Diethylcathinone, Methcathinone, N,N-	100 μg/mL	CEDIA Amohetamine/ Ecstasy	0.25–100	–	Regester et al. (2015)

(*continued*)

Table 3. Continued.

Analytes	Concentration	Test type	Cross-reactivity [%]	LOD	Reference
Dimethylcathinone, MT-45, DBZP, BDF, TMA, Escaline, Mescaline, 2-DPMP, 4-MeO-PCP, BCP, MXE, CFT					
AMT, 4-FMA, DOEt, DOM, 6-APB, 4-FA, 5-APDB, BDF, MPA, DOC, DMA, PMMA, beta-keto-MDEA, N-Ethylcathinone,2C-T, 2C-I, 5-APB, DOB, 2C-B, 5-APDI, 5-IT,2C-T-2, 4-MEC, DOI, 5-IAI, 5-MeO-MiPT, TMA, MDAI, 2C-E, 2C-T-4, 2C-C, 4-MTA, MDEA, DMMA, 5-MeO-AMT, 4-MA, PMA, 4-MBC, DBZP, 2C-T-7, 4-CAB, 25-I-NBOMe,25C-NBOMe, 25B-NBOMe, 4-OH-DET, 5-methoxy-DALT, 5-MeO-DiPT, DiPT, 5-MeO-DMT, DMT, DPT, Naphyrone, MDPBP, MDPV, MDPPP, MPHP, MOPPP,4-MPBP, MPPP, Pyrovalerone, D2PM, alpha-PBP, alpha-PVP, alpha-PPP, Pentylone, beta-keto-MDMA, 3,4-DMMC, beta-keto-MBDB, 4-EEC, 4-FMC, Methedrone, 4-MMC, Cathinone, Diethylcathinone, beta-keto-MDDMA, Methcathinone, N,N- Dimethylcathinone, MAPB, Pentedrone, beta-keto-EBDB, MT-45, 1-(3-TFMPP), 1-(4-TFMPP), BZP, mCPP, 2-AI, Escaline, Mescaline, 2-DPMP, 4-MeO-PCP, BCP, MXE, CFT	100 μg/mL	Syva EMIT II Plus Amphetamine	0.20–100	–	
mCPP, 4-FMA, 5-IT, 1-(3-TFMPP), MPA, PMMA, 5-APB, MAPB, MDEA, 4-MA, beta-keto-MBDB, 4-MTA, beta-keto-MDMA, 4-MMC, 5-APDB, DMT, beta-keto-MDDMA, BZP, Methcathinone, PMA, 5-APDI, Pentedrone, 4-EEC, Methedorne, 4-MEC, N,N-Dimethylcathinone, 4-FA, 4-MPBP, beta-keto-MDEA, 3,4-DMMC, beta-keto-EBDB, N-Ethylcathinone, 6-APB, MDPBP, MPPP, alpha-PBP, 4-CAB, DOEt, DOM, DMA, DOB, DOC, DOI, 25-I-NBOMe, 25C-NBOMe, 25B-NBOMe, 2C-B, 2C-C, 2C-E, 2C-T-2, 2C-I, 2C-T-4, 2C-T, 2C-T-7, AMT, 4-OH-DET, 5-MeO-MiPT, 5-methoxy-DALT, 5-MeO-DiPT, DiPT, 5-MeO-DMT, DPT, 5-MeO-AMT, Naphyrone, MDPV, MDPPP, MPHP, MOPPP, Pyrovalerone, D2PM, alpha-PVP, alpha-PPP, Pentylone, 4-MBC, 4-FMC, Cathinone, Diethylcathinone, MT-45, 1-(4-TFMPP), DBZP, BDF, 2-AI, TMA, MDAI, 5-IAI, Escaline, Mescaline, DMMA, 2-DPMP, 4-MeO-PCP, BCP, MXE, CFT	100 μg/mL	LIN-ZHI Methamphetamine	0.70–90	–	
5-APDB, MDEA, Methedrone, 4-MA, 4-FMA, 6-APB, 4-MTA, 5-APB, PMMA, 4-CAB, 5-APDI, 4-FA, PMA, beta-keto-EBDB, beta-keto-MBDB, beta-keto-MDMA, MDPBP, beta-keto-MDEA, DOEt, DOM, DMA, DOB, DOC, DOI, 25-I-NBOMe, 25C-NBOMe, 25B-NBOMe, 2C-B, 2C-C, 2C-E, 2C-T-2, 2C-I, 2C-T-4, 2C-T, 2C-T-7, AMT, 4-OH-DET, 5-MeO-MiPT, 5-methoxy-DALT, 5-MeO-DiPT, DiPT, 5-MeO-DMT, DMT, DPT, 5-MeO-AMT, Naphyrone, MDPBP, MDPV, MDPPP, MPHP, MOPPP, 4-MPBP, MPPP, Pyrovaleron, D2PM, Alpha-PBP, alpha-PVP, alpha-PPP, Pentylone, 4-MBC, 3,4-DMMC, 4-EEC, 4-FMC, 4-MEC, 4-MMC, Cathinone, Diethylcathinone, beta-keto-MDDMA, Methcathinone, N,N-Dimethylcathinone, N-Ethylcathinone, MAPB, Pentedrone, MT-45, 1-(3-TFMPP), 1-(4-TFMPP), DBZP, BZP, mCPP, BDF, 2-AI, TMA,5-IT, MDAI, 5-IAI, Escaline, Mescaline, MPA, DMMA, 2-DPMP, 4-MeO-PCP, BCP, MXE, CET	100 μg/mL	Microgenics DRI MDMA	0.20–100	–	
alpha-PVP, 4-MeO-PCP, MDPV, alpha-PBP, MPHP, BCP,alpha-PVP, Naphyrone, MPPP, Pyrovalerone, 2-DPMP, MDPBP, MOPPP, MDPPP, D2PM, alpha-PPP, 5-methoxy-DALT, 4-MPBP, MXE, DOEt, DOM, DMA, DOB, DOC, DOI, 25-I-NBOMe, 25C-NBOMe, 25B-NBOMe, 2C-B, 2C-C, 2C-E, 2C-T-2,2C-I, 2C-T-4, 2C-T, 2C-T-7, AMT, 4-OH-DET, 5-MeO-MiPT, 5-MeO-DiPT, DIPT, 5-MeO-DMT, DMT, DPT, 5-MeO-AMT, Pentylone, 4-MBC, beta-keto-MDEA, beta-keto-MDMA, 3,4-DMMC, beta-keto-MBDB, 4-EEC, 4-FMC, Methedrone, 4-MEC, 4-MMC, Cathinone, Diethylcathinone, beta-keto-MDDMA, Methcathinone, N,N-Dimethylcathinone, N-Ethylcathinonne, MAPB, Petedrone, beta-keto-EBDB, MT-45, 1-(3-TFMPP), 1-(4-TFMPP), DBZP, BZP, mCPP, BDF, 2-AI, TMA, 4-CAB, 4-FMA, 4-MA, 4-MTA, 5-APDI, 5-APDB, 5-APB, 5-IT, MDAI, 5-IAI, 6-APB, Escaline, Mescaline, MPA, MDEA, DMMA,4-FA, PMA, PMMA, DFT	100 μg/mL	Microgenics DRI PCP	0.40–90	–	
2,5-DMA, DOC, DOET, DON, DOPR, 2C-N, 2C-T, 2C-T-2, 2C-T-5, 2C-T-7, 2C-T-13, 2C-T-17, ALEPH, ALEPH-2, ALEPH-5, ALEPH-7, TMA, TMA-2, TMA-3, TMA-6, MDIP, MDBZ, MDCPM, BOH, BOB, BOD, BOHD, DOI, ALEPH-13, ALEPH-17	10 ng/mL	Neogen Amphetamine Specific Kit (from blood)	<0.1–0.20	–	
2,5-DMA, DOC, DOET, DOI, DON, DOPR, 2C-N, 2C-T, 2C-T-2, 2C-T-5, 2C-T-7, 2C-T-13, 2C-T-17, ALEPH, ALEPH-2, ALEPH-5, ALEPH-7, ALEPH-13, ALEPH-17, TMA, TMA-2, TMA-3,TMA-6, MDIP, MDBZ, MDCPM, BOH, BOB, BOD, BOHD	10 ng/mL	Neogen Amphetamine Specific Kit (from urine)	<0.1	–	
2,5-DMA, DOC, DOET, DOI, DON, DOPR, 2C-N, 2C-T, 2C-T-2, 2C-T-5, 2C-T-7, 2C-T-13, 2C-T-17, ALEPH-2, ALEPH-5, ALEPH-7, ALEPH-13, TMA, TMA-2, TMA-3,TMA-6, MDIP, MDBZ, MDCPM, BOH, BOB, BOD, BOHD,ALEPH, ALPEH-17	10 ng/mL	Neogen Amphetamine Specific Kit (from oral fluid)	<0.1–0.10	–	

(*continued*)

Table 3. Continued.

Analytes	Concentration	Test type	Cross-reactivity [%]	LOD	Reference
2,5-DMA, DOC, DOET, DOI, DON, DOPR, 2C-N, 2C-T, 2C-T-2, 2C-T-5, 2C-T-7, 2C-T-13, 2C-T-17, ALEPH, ALEPH-2, ALEPH-5, ALEPH-7, ALEPH-13, ALEPH-17, TMA, TMA-2, TMA-3,TMA-6, MDBZ, BOH, BOB, BOD, BOHD, MDCPM, MDIP	10 ng/mL	Neogen Methamphetamine/ MDMA Kit (from blood)	<0.7–0.10	–	
2,5-DMA, DOC, DOET, DOI, DON, DOPR, 2C-N, 2C-T, 2C-T-2, 2C-T-5, 2C-T-7, 2C-T-13, 2C-T-17, ALPEH, ALEPH-2, ALEPH-5, ALEPH-7, ALEPH-13, ALEPH-17, TMA, TMA-2, TMA-3, TMA-6, MDIP, MDBZ, MDCPM, BOH, BOB, BOD, BOHD	10 ng/mL	Neogen Methamphetamine/ MDMA Kit (from urine)	<0.7	–	
2,5-DMA, DOC, DOET, DOI, DON, DOPR, 2C-N, 2C-T, 2C-T-2, 2C-T-5, 2C-T-7, 2C-T-13, 2C-T-17, ALPEH, ALEPH-2, ALEPH-5, ALEPH-7, ALEPH-13, ALEPH-17, TMA, TMA-2, TMA-3, TMA-6, MDBZ, MDCPM, BOH, BOB, BOD, BOHD, MDIP	10 ng/mL	Neogen Methamphetamine/ MDMA Kit (from oral fluid)	<0.7	–	
PMMA, PMA, TMA-6, MDIP, MDBZ, MDCPM, 2,5-DMA, DOB, DOC, DOET, DOI, DOM, DON, DOPR, 2C-B, 2C-C, 2C-I, 2C-N, 2C-M, 2C-T, 2C-T-2, 2C-T-4, 2C-T-5, 2C-T-7, 2C-T-8, 2C-T-13, 2C-T-17, APLEPH, ALPEH-2, ALEPH-4, ALEPH-5, ALEPH-7, ALEPH-8, ALEPH-13, ALEPH-17, TMA, TMA-2, TMA-3, BOH, BOB, BOD	500 ng/mL	Emit II Plus Amphetamines assay	<5–50	–	Nieddu et al. (2013)
PMA, PMMA, BOH, MDIP, MDBZ, MDCPM, 2,5-DMA, DOB, DOC, DOET, DOI, DOM, DON, DOPR, 2C-B, 2C-C, 2C-I, 2C-N, 2C-M, 2C-T, 2C-T-2, 2C-T-4, 2C-T-5, 2C-T-7, 2C-T-8, 2C-T-13, 2C-T-17, APLEPH, ALPEH-2, ALEPH-4, ALEPH-5, ALEPH-7, ALEPH-8, ALEPH-13, ALEPH-17, TMA, TMA-2, TMA-3, TMA-6, BOB, BOD	500 ng/mL	Emit II Plus Ecstasy assay	<5–100	–	
DOB, PMMA, DOC, TMA-3; 2,5-DMA, PMA, DOET, DOI, DOM, DON, DOPR, 2C-B, 2C-I, 2C-N, 2C-M, 2C-T, 2C-T-2, 2C-T-4, 2C-T-5, 2C-T-7, 2C-T-13, 2C-T-17, ALEPH, ALPEH-2, ALEPH-5, ALEPH-7, ALEPH-8, ALEPH-13, ALEPH-17, TMA, TMA-2, TMA-6, MDIP, MDBZ, MDCPM, BOH, BOB, BOD, BOHD	500 ng/mL	Screen 7 test for amphetamine	<5–100	–	Nieddu et al. (2014a)
TMA-3, PMMA, PMA, 2,5-DMA, DOB, DOC, DOET, DOI, DOM, DON, DOPR, 2C-B, 2C-I, 2C-N, 2C-M, 2C-T, 2C-T-2, 2C-T-4, 2C-T-5, 2C-T-7, 2C-T-13, 2C-T-17, ALEPH, ALEPH-2, ALEPH-5, ALEPH-7, ALEPH-8, ALEPH-13, ALEPH-17, TMA, TMA-2, TMA-6, MDIP, MDBZ, MDCPM, BOH, BOB, BOD, BOHD	500 ng/mL	Screen 7 test for methamphetamine	<5–100	–	
PMMA, MDIP, MDBZ, TMA-3, MDCPM, PMA, 2,5-DMA, DOB, DOC, DOET, DOI, DOM, DON, DOPR, 2C-B, 2C-I, 2C-N, 2C-M, 2C-T, 2C-T-2, 2C-T-4, 2C-T-5, 2C-T-7, 2C-T-13, 2C-T-17, ALEPH, ALEPH-2, ALEPH-5, ALEPH-7, ALEPH-8, ALEPH-13, ALEPH-17, TMA, TMA-2, TMA-6, BOH, BOB, BOD, BOHD	500 ng/mL	Screen 7 test for MDMA	<5–250	–	
DOB, PMMA, DOC, TMA-3; 2,5-DMA, PMA, DOET, DOI, DOM, DON, DOPR, 2C-B, 2C-I, 2C-N, 2C-M, 2C-T, 2C-T-2, 2C-T-4, 2C-T-5, 2C-T-7, 2C-T-13, 2C-T-17, ALEPH, ALPEH-2, ALEPH-5, ALEPH-7, ALEPH-8, ALEPH-13, ALEPH-17, TMA, TMA-2, TMA-6, MDIP, MDBZ, MDCPM, BOH, BOB, BOD, BOHD	500 ng/mL	SureStep test for amphetamine	<5–100	–	
PMMA, PMA, 2,5-DMA, DOB, DOC, DOET, DOI, DOM, DON, DOPR, 2C-B, 2C-I, 2C-N, 2C-M, 2C-T, 2C-T-2, 2C-T-4, 2C-T-5, 2C-T-7, 2C-T-13, 2C-T-17, ALEPH, ALEPH-2, ALEPH-5, ALEPH-7, ALEPH-8, ALEPH-13, ALEPH-17, TMA, TMA-2, TMA-3, TMA-6, MDIP, MDBZ, MDCPM, BOH, BOB, BOD, BOHD	500 ng/mL	SureStep test for methamphetamine	<5–200	–	
PMMA, MDIP, MDBZ, MDCPM, PMA, 2,5-DMA, DOB, DOC, DOET, DOI, DOM, DON, DOPR, 2C-B, 2C-I, 2C-N, 2C-M, 2C-T, 2C-T-2, 2C-T-4, 2C-T-5, 2C-T-7, 2C-T-13, 2C-T-17, ALEPH, ALEPH-2, ALEPH-5, ALEPH-7, ALEPH-8, ALEPH-13, ALEPH-17, TMA, TMA-2, TMA-3, TMA-6, BOH, BOB, BOD, BOHD	500 ng/mL	SureStep test for MDMA	<5–500	–	
DOET, DOI, DOM, DON, DOPR, 2C-B, 2C-I, 2C-N, 2C-M, 2C-T, 2C-T-2, 2C-T-4, 2C-T-5, 2C-T-7, 2C-T-13, 2C-T-17, ALEPH, ALPEH-2, ALEPH-5, ALEPH-7, ALEPH-8, ALEPH-13, ALEPH-17, TMA, TMA-2, TMA-6, MDIP, MDBZ, MDCPM, BOH, BOB, BOD, BOHD	500 ng/mL	InstAlert test for amphetamine	<5–100	–	
PMMA,PMA, 2,5-DMA, DOB, DOC, DOET, DOI, DOM, DON, DOPR, 2C-B, 2C-I, 2C-N, 2C-M, 2C-T, 2C-T-2, 2C-T-4, 2C-T-5, 2C-T-7, 2C-T-13, 2C-T-17, ALEPH, ALEPH-2, ALEPH-5, ALEPH-7, ALEPH-8, ALEPH-13, ALEPH-17, TMA, TMA-2, TMA-3, TMA-6, MDIP, MDBZ, MDCPM, BOH, BOB, BOD, BOHD	500 ng/mL	InstAlert test for methamphetamine	<5–200	–	
PMMA, MDIP, MDBZ, MDCPM, PMA, 2,5-DMA, DOB, DOC, DOET, DOI, DOM, DON, DOPR, 2C-B, 2C-I, 2C-N, 2C-M, 2C-T, 2C-T-2, 2C-T-4, 2C-T-5, 2C-T-7, 2C-T-13, 2C-T-17, ALEPH, ALEPH-2, ALEPH-5, ALEPH-7, ALEPH-8, ALEPH-13, ALEPH-17, TMA, TMA-2, TMA-3, TMA-6, BOH, BOB, BOD, BOHD	500 ng/mL	InstAlert test for MDMA	<5–500	–	
AMT, Amphetamine, MDA, DOM, MDEA, TMA, MDMA, Methamphetamine, 2C-E, DOET, Ethylamphetamine, MDPV, Mephedrone, Cathinone, Methcathinone, Methylone, 4-MEC, Flephedrone, Butylone, mCPP, Methedrone, 5-MeO-DiPT, DOB, 2C-B, DMT, BZP, 2C-I, 2C-T-7, TFMPP, 2C-T-4	100 µg/mL	Immunalysis Amphetamine	<0.25– >250	25 ng/mL	Swortwood et al. (2014)

(*continued*)

Table 3. Continued.

Analytes	Concentration	Test type	Cross-reactivity [%]	LOD	Reference
DMT, BZP, Cathinone, TFMPP, MDA, Methacathinone, Flephedrone, AMT, MDEA, MDMA, mCPP, Amphetamine, 2C-E, DOET, DOM, TMA, MDPV, Mephedrone, Methylone, Butylone, 5-MeO-DiPT, 2C-B, 2C-I, 2C-T-7, 2C-T-4, Methamphetamine, Ethylamphetamine, 4-MEC, Methedrone, DOB	100 μg/mL	Neogen Amphetamine	<0.50– >500	50 ng/mL	
DOET, DOM, TMA, MDA, Amphetamine, AMT, Methamphetamine, 2C-E, MDEA, MDMA, Ethylamhetamine, MDPV, Mephedrone, Cathinone, Methcathinone, Methylone, 4-MEC, Flephedrone, Butylone, mCPP, Methedrone, 5-MeO-DiPT, DOB, 2C-B, DMT, BZP, 2C-I, 2C-T-7,TFMPP,2C-T-4	100 μg/mL	Neogen Amphetamine Specific	<0.5–100	50 ng/mL	
Methcathinone, DMT, MDA, TFMPP, AMT, MDMA,MDEA, mCPP, Amphetamine, BZP, 2C-E, DOET, DOM, TMA, MDPV, Mephedrone, Methylone, 4-MEC, Butylone, Methedrone, 5-MeO-DiPT, 2C-B, 2C-I, 2C-T-7, 2C-T-4, Methamphetamine, Ethylamphetamine, Cathinone, Flephedrone, DOB	100 μg/mL	Neogen Amphetamine Ultra	<0.5–>500	50 ng/mL	
MDA, Amphetamine, AMT, Methamphetamine, 2C-E, DOET, DOM, TMA, MDEA, MDMA, Ethylamphetamine, MDPV, Mephedrone, Cathinone, Methcathinone, Methylone, 4-MEC, Flephedrone, Butylone, mCPP, Methedrone, 5-MeO-DiPT, DOB, 2C-B, DMT, BZP, 2C-I, 2C-T-7, TFMPP, 2C-T-4	100 μg/mL	OraSure Amphetamine Specific	<0.5–116	50 ng/mL	
Methylone, Mephedrone ,4-MEC, Ethylamphetamine, MDEA, Methamphetamine, Amphetamine, 2C-E, DOET, DOM, TMA, MDPV, Cathinone, mCPP, 5-MeO-DiPT, DOB, 2C-B, DMT, BZP, AMT, 2C-I, 2C-T-7, TFMPP, 2C-T-4, MDMA, Flephedrone, Butylone, MDA, Methcathinone, Methedrone	100 μg/mL	Imunalysis Methamphetamine	<0.25 – >250	25 ng/mL	
Mephedrone, 4-MEC, Flephedrone, MDA, Methedrone, MDEA, Ethylamphetamine, Methamphetamine, MDMA, 2C-E, DOET, DOM, TMA, MDPV, Cathinone, mCPP, 5-MeO-DiPT, DOB, 2C-B, DMT, BZP, 2C-I, 2C-T-7, TFMPP, 2C-T-4, Methcathinone, Methylone, Butylone, AMT, Amphetamine	100 μg/mL	Neogen Methaphetamine/MDMA	<0.25–167	25 ng/mL	
MDA, Butylone, Mephedrone, 4-MEC, Ethylamphetamine, Methamphetamine, MDEA, Methcathinone, Methylone, Methedrone, Flephedrone, MDMA, Amphetamine, AMT, 2C-E, DOET, DOM, TMA, MDPV, Cathinone, mCPP, 5-MeO-DiPT, DOB, 2C-B, DMT, BZP, 2C-I, 2C-T-7, TFMPP, 2C-T-4	100 μg/mL	OraSure Methamphetamine	<0.1–>100	10 ng/mL	
BZP, Amphetamine, 2C-E, DOET, DOM, TMA, MDA, Ethylamphetamine, MDPV, Mephedrone, Cathinone, Methcathinone, Methylone,4-MEC, Flephedrone, Butylone, mCPP, Methedrone, 5-MeO-DiPT, DOB, 2C-B, AMT, 2C-I, 2C-T-7, TFMPP, 2C-T-4, Methamphetamine, MDEA, MDMA, DMT	100 μg/mL	Neogen Benzylpiperazine	<0.25–100	25 ng/mL	
Amphetamine, Methamphetammine, 2C-E, DOET, DOM, TMA, MDA, MDEA, MDMA, Ethylamphetamine, MDPV, Mephedrone, Cathinone, Methcathinone, Methylone, 4-MEC, Flephedrone, Butylone, mCPP, Methedrone, 5-MeO-DiPT, DOB, 2C-B, DMT, BZP, AMT, 2C-I, 2C-T-7, TFMPP, 2C-T-4	100 μg/mL	Neogen Ketamine	<0.5	50 ng/mL	
Amphetamine, Methamphetammine, 2C-E, DOET, DOM, TMA, MDA, MDEA, MDMA, Ethylamphetamine, MDPV, Mephedrone, Cathinone, Methcathinone, Methylone, 4-MEC, Flephedrone, Butylone, mCPP, Methedrone, 5-MeO-DiPT, DOB, 2C-B, DMT, BZP, AMT, 2C-I, 2C-T-7, TFMPP, 2C-T-4	100 μg/mL	Neogen Methylphenidate	<0.1	10 ng/mL	
Methamphetamine, MDMA, MDA, Ethylamphetamine, MDEA, Amphetamine, 2C-E, DOET, DOM, TMA, MDPV, Mephedrone, Cathinone, Methcathinone, Methylone, 4-MEC, Flephedrone, Butylone, mCPP, Methedrone, 5-MeO-DiPT, DOB, 2C-B, DMT, BZP, AMT, 2C-I, 2C-T-7, TFMPP, 2C-T-4	100 μg/mL	Neogen Mephentermine	<0.1–5	10 ng/mL	
MDPV, Butylone, 4-MEC, Methylone, Amphetamine, Methamphetamine, 2C-E, DOET, DOM, TMA, MDA, MDEA, Ethylamphetamine, Mephedrone, Cathinone, Methcathinone, Flephedrone, Butylone, mCPP, Methedrone, 5-MeO-DiPT, DOB, 2C-B, DMT, BZP, AMT, 2C-I, 2C-T-7, TFMPP, 2C-T-4	100 μg/mL	RANDOX MDPV	<0.1–100	10 ng/mL	
Mephedrone	100 μg/mL	RANDOX Mephedrone/ Methcathinone	<0.0125–100	1.25 ng/mL	
Amphetamine, 2C-3, DOET, DOM, TMA, MDA, Ethylamphetamine, MDPV, mCPP, DOB, 2C-B, DMT, BZP, AMT, 2C-I, 2C-T-7, TFMPP, 2C-T-4, Methcathinone, Methylone, 4-MEC, Flephedrone, Butylone, Methedrone, MDEA, 5-MeO-DiPT, Methamphetamine, MDMA, Cathinone					
Amphetamine, Methamphetamine, 2C-E, DOET, DOM, TMA, MDA, MDEA, MDMA, Ethylamphetamine, MDPV, Mephedrone, Cathinone, Methcathinone, Methylone, 4-MEC, Flephedrone, Butylone, mCPP, Methedrone, 5-MeO-DiPT, DOB, 2C-B, DMT, BZP, AMT, 2C-I, 2C-T-7, TFMPP, 2C-T-4	100 μg/mL	OraSure PCP	<0.2	20 ng/mL	
Amphetamine, Methamphetamine, 2C-E, DOET, DOM, TMA, MDA, MDEA, MDMA, Ethylamphetamine, MDPV, Mephedrone, Cathinone, Methcathinone,	100 μg/mL	OraSure Cotinine	<1	100 ng/mL	

(*continued*)

Table 3. Continued.

Analytes	Concentration	Test type	Cross-reactivity [%]	LOD	Reference
Methylone, 4-MEC, Flephedrone, Butylone, mCPP, Methedrone, 5-MeO-DiPT, DOB, 2C-B, DMT, BZP, AMT, 2C-I, 2C-T-7, TFMPP, 2C-T-4					
PMA,PMMA, 2,5-DMA, DOB, DOC, DOET, DOI, DOM, DON, DOPR, 2C-B, 2C-I, 2C-N, 2C-M, 2C-T, 2C-T-2, 2C-T-4, 2C-T-5, 2C-T-7, 2C-T-13, 2C-T-17, ALEPH, ALEPH-2, ALEPH-5, ALEPH-7, ALEPH-8, ALEPH-13, ALEPH-17, TMA, TMA-2, TMA-3, TMA-6, MDIP, MDBZ, MDCPM, BOH, BOB, BOD, BOHD	5000 ng/mL	Screen test for AMP	<0.1–25	50 ng/mL	Nieddu et al. (2014b)
PMA, DOB, DOC, DOET, DOI, DOM, DON, DOPR, 2C-B, 2C-I, 2C-N, 2C-M, 2C-T, 2C-T-2, 2C-T-4, 2C-T-5, 2C-T-7, 2C-T-13, 2C-T-17, ALEPH, ALEPH-2, ALEPH-5, ALEPH-7, ALEPH-8, ALEPH-13, ALEPH-17, TMA, TMA-2, TMA-3, TMA-6, MDIP, MDBZ, MDCPM, BOH, BOB, BOD, BOHD	5000 ng/mL	Screen test for MET	<1–250	50 ng/mL	
PMA, PMMA, 2,5-DMA, DOB, DOC, DOET, DOI, DOM, DON, DOPR, 2C-B, 2C-I, 2C-N, 2C-M, 2C-T, 2C-T-2, 2C-T-4, 2C-T-5, 2C-T-7, 2C-T-13, 2C-T-17, ALEPH, ALEPH-2, ALEPH-5, ALEPH-7, ALEPH-8, ALEPH-13, ALEPH-17, TMA, TMA-2, TMA-3, TMA-6, MDIP, MDBZ, MDCPM, BOH, BOB, BOD, BOHD, PMMA, 2,5-DMA	5000 ng/mL	GIMA test for AMP	<0.1–50	50 ng/mL	
PMMA, 2,5-DMMA, PMA, DOB, DOC, DOET, DOI, DOM, DON, DOPR, 2C-B, 2C-I, 2C-N, 2C-M, 2C-T, 2C-T-2, 2C-T-4, 2C-T-5, 2C-T-7, 2C-T-13, 2C-T-17, ALEPH, ALEPH-2, ALEPH-5, ALEPH-7, ALEPH-8, ALEPH-13, ALEPH-17, TMA, TMA-2, TMA-3, TMA-6, MDIP, MDBZ, MDCPM, BOH, BOB, BOD, BOHD	5000 ng/mL	GIMA test for MET	<1–25	50 ng/mL	

steps of the extraction process, including filtration, centrifugation, or elution (Sánchez-González et al. 2019).

Micro-SPE with MIPs (MIMSPE) has been used to detect cocaine and its metabolites in urine (Sánchez-González et al. 2015) and plasma (Sánchez-González et al. 2016). This method was also applied to screen urine and plasma samples for cannabinoids and their metabolites (Sánchez-González et al. 2017). Sánchez-González et al. (2019) developed MIPs for identifying synthetic cathinones in urine samples. They analyzed 10 substances belonging to the cathinone group. Intra-day and inter-day recoveries ranged from 92 ± 6% to 102 ± 4% and from 87 ± 4% to 100 ± 8%, respectively. LOD and LOQ values range were determined at 0.14–1.51 and 0.48–5.03 μg/L, respectively. Lowdon et al. (2018) relied on MIPs to detect methoxphenidine (MXP) and its isomers. The developed method supported simultaneous identification of three MXP isomers with high recovery (>90%). These results indicate that MIPs have considerable potential for toxicological analyses.

Lowdon et al. (2019) used MIPs to detect 2-MXP. They developed a sensor platform by grafting MIP layers onto aluminum substrates, which increased the sensitivity, selectivity, and efficiency of the analysis relative to conventional deposition. The proposed method enables mass production and analysis at very low concentration levels, which is a considerable advantage. Despite the fact that MIPs are widely applied for analytical purposes, there are few reports on their use in NPS identification. Synthetic MIPs are characterized by high sensitivity because the created recognition sites are capable of binding to the target analyte instead of molecules that are closely related to it. Another advantage of MIPs is that the obtained extracts are pure, which improves the reliability of mass spectrometry results. The matrix effect is reduced, and the method's precision and accuracy are improved (Meyer and Maurer 2016). MIPs offer a promising solution for identifying the emerging NPS. However, the preparation process is time consuming, and MIPs target only a single substance. In toxicological analyses aiming to determine the cause of poisoning or death, a wide range of psychoactive substances have to be examined in a short time, which is difficult to accomplish with MIPs. In standard laboratory practice, many samples have to be tested for numerous substances in a single day, and the application of MIPs significantly increases run time and cost of the analysis. However, MIPs can be used to detect isomers that cannot be unambiguously identified during routine analyses.

4. Separation and detection methods

Depending on the applied method, the sample preparation process is followed by the separation of analytes, detection and identification of substances in the sample. The method of analysis is selected depending on the available options, costs, applicable guidelines, and the purpose of the analysis – screening or confirmation. The most frequently used procedures are discussed in this section, with special emphasis on approaches that enable the development of new analytical techniques.

Table 4. List of chromatographic methods used to detect psychoactive substances.

Group of analytes (number of analytes)	Matrix	Analytical method	Extraction method	Sample amount	Extraction solvent	Recovery (%)	LOD	LOQ	Reference
Cannabinoids (7[a*])	Urine	LC-MS/MS	LLE	0.5 mL	1.5 mL ACN with 0.5 mL10M ammonium formate	No data	No data	0.01 ng/mL	Cannaert et al. (2016)
Opiates and opioids, Benzodiazepines, Antipsychotics, Amphetamines, Cannabinoids, Barbiturates, Cathinones (162[b])	Blood	LC-MS/MS	SPE	0.5 mL	water	4.2–122	No data	No data	Yeter (2017)
Phenethylamines, Piperazines, Amphetamines, Cathinones (32[c*])	Serum	LC-QQQ-MS/MS	SPE	1 mL	sodium phosphate buffer (100 mM, pH 6.0)	67.3–128.5	10–100 pg/mL	1–10 ng/mL	Swortwood et al. (2013)
Opiates and opioids, Benzodiazepines, Amphetamines, Phenethylamines, Cannabinoids, Cathinones, Z-drugs, Piperazines, Barbiturates (93[d*])	Urine	UHPLC-MS/MS	SPE	1 mL	–	2–97	1–250 ng/mL	No data	Tang et al. (2014)
Cathinones (28[e*])	Urine	LC-HRMS	SPE	250 µL	–	78.9–116.7	0.25–1 µg/L	0.5–1 µg/L	Concheiro et al. (2013)
Cathinones, Anesthetics (35[f*])	Plasma	LC-MS/MS	SPE	1 mL	–	72–90	1.0–5.0 ng/mL	No data	Wohlfarth et al. (2010)
Phenethylamines (10[g*])	Urine	GC-MS	SPE	2 mL	–	63–94	2–10 ng/mL	2–10 ng/mL	Kerrigan, Mellon, et al. (2011); Kerrigan, Banuelos, et al. (2011)
Amphetamines, Benzodiazepines, Opiates, Phenethylamines, Cathinones, Cannabinoids, Z-drugs, Other (301[h*])	Plasma	HPLC-MS/MS	LLE SPE	1 mL	butyl acetate	–	–	–	Mueller et al. (2005)
Cathinones, Cannabinoids, Phenethylamines, Amphetamines (143[i*])	Blood	LC-MS	LLE	200 µL	ACN	1.8–133	0.01–3.09 ng/mL	No data	Adamowicz and Tokarczyk (2016)
Benzodiazepines (23[j*])	Blood	EI-GC-MS	LLE	1 mL	Chloroform	74–119	0.52–58.47 ng/mL	1.58–177.2 ng/mL	Papoutsis et al. (2010)
Cannabinoids (30[k*])	Serum	LC-MS/MS	LLE	1 mL	n-hexane: ethyl acetate (99:1 v/v)	3.5–56.2	0.01–2.00 ng/mL	No data	Kneisel and Auwärter (2012)
Opiates and opioids, Benzodiazepines, Z-drugs, Amphetamines (30[l*])	Blood	LC-MS/MS	LLE	1 mL	1-chlorobutane: mixture of dichloromethane and ethyl acetate (70: 30 v/v)	No data	100 pg/mL– 5 ng/mL	No data	Wicka et al. (2014)
Antidepresants, Benzodiazepines, Amphetamines, Phenethylamines, Opiates and opioids, Z-drugs, Cathinones (175[m*])	Blood	UPLC-TOF-MS	SPE	200 µL	–	–	–	–	Dalsgaard et al. (2012)

*List of analytes available in the supplementary.

[a]JWH-018, JWH-122, MAM-2201, JWH-210, EAM-2201. PB-22, 5 F-PB-22.

[b]6-Acetylmorphne, 7-Aminiclonazepam, Alprazolam, Amisulpride, Amitriptyline, AmLodipin, Amphetamine, Atenolol, Atropin, Benzoylecgonine, Biperiden, Bromazepam, Buprenorphine, Carbamazepine, Chlordiazepoxide, Chlorpheniramine, Chlotpromazine,, Citalopram, Clobazam, Clomipramine, Clonazepam, Clozapine, Cocaine, Codeine, Desipramine, Dextromethorphan, Diazepam, Diclofenac, Diltiazem, Diphenhydramine, Doxepin, Doxylamine, Etodolac, Famotidine, Fentanyl, Fluclonazole, Flunitrazepam, Fluoxetine, Flurazepam, Fluvoxamine, Haloperidol, Hydroxyzine, Imipramine, Ketamine, Lansoprazole, Lidocaine, Loperamide, Lorazepam, MDA, MDEA, MDMA, Metformin, Methadone, Methamphetamine, Methylecgonine, Metoclopramide, Metoprolol, Metronidazole, Mianserin, Midazolam, Mirtazapine, Moclobemide, Morphine, Naproxen, Nifedipine, Nordiazepam, Nortriptiline, Opipramol, Ornidazole, Oxazepam, Oxcarbazepine, Pantoprazole, Paracetamol, Paroxetine, Pentobarbital, Pentoxifylline, Pethidine, Pheniramine, Phenobarbital, Phenytoin, Prilocaine, Propafenone, Propranolol, Propyphenazone, Pseudoephedrine, Quetiapine, Risperidone, Sertraline, Sildenafil, Tadalafil, THC, THC-COOH, Thiopental, Thioridazine, Tramadol, Verdenafil, Venlafaxine, Verapamil, CP 47,497 C8, CP 47,497, WIN 55,212-2,CP 55,940, 5-F-AKB-48-4-hydroxypentyl, 5-F-PB-22-3-carboxy-indole, 5-F-AB-Pinaca, 5-F-AKB-48, 5 F-ADB, AB-Chminaca, AB-Fubinaca-M2, AB-Pinaca-5-hydroxylpentyl, AB-Pinaca-pentanoic acid, AB-Chminaca-M1, AB-Chminaca-M2, ADB-Pinaca-pentanoic acod, ADB-Pinaca, AKB-48-N-5-hydroxypentyl, AKB-48-N-pentanoic acid, AM 2201, AM2201-6-hydroxyindole, AM 2201-N-4-hydroxypentyl, HU 210, JWH 0814-hydroxynaphtyl, JWH 081 N-5-hydroxypentyl, JWH 122 N-4-hydroxypentyl, JWH 122 N-5-hydroxypentyl, JWH 203 N -pentanoic acid, JWH 203, JWH 210 5-hydroxyindole, JWH 210 N-4-hydroxypentyl, JWH 210 N-5-hydroxypentyl, JWH 210 N-pentanoic acid, JWH 210, JWH 250 N-4-hydroxypentyl, JWH250 N-pentanoic acid, JWH 398 N-5- hydroxypentyl, JWH 398 N-pentanoic acid, JWH 018 N-pentanoic acid, JWH 018, JWH 018 N-5-hydroxypentyl, JWH 019, JWH 073, JWH 073 4-hydroxybutyl, JWH 073 N-butanoic acid, JWH 081, JWH 200, JWH 201, JWH 250 N-5-hydroxypentyl, JWH 250, MAM 2201 4-hydroxypentyl, MAM 2201 N-pentanoic acid, MAM 2201, PB-22-3-carboxyindole, RCS-4, RCS-4-N-5-carboxypentyl, RCS-4-N-5-hydroxypentyl, RCS-8, UR-144 N-5-hydroxypentyl, UR-144 N-pentanoic acid, UR-144, XLR- 11 6-hydroxyindle, XLR-11 N-4-hydroxypentyl, XLR-11.

[c]DOB, DOET, DOM, TMA, 2 C-B, 2 C-E, 2 C-I, 2 C-T-4, 2 C-T-7, MDA, MDEA, MDMA, Amphetamine, Methamphetamine, Ethylamphetamine, MDPV, Mephedrone, Cathinone, Methcathinone, Methedrone, 4-MEC, Flephedrone, Methylone, Butylone, BZP, DBZP, mCPP, TFMPP, AMT, DMT, 5-MeO-DMT, 5-MeO-DiPT.

[d]4-FA, 4-Methylthioamphetamine, Amphetamine, Bromo-dragonfly, Chloroamphetamine, DOB, DOET, DOM, HMMA, MBDB, MDA, MDEA, MDMA, Methamphetamine, N-ethylamphetamine, PMA, PMMA, Codeine, Norcodeine, Heroin, 6-MAM, Morphine, Normorphine, Cocaine, Benzoylecgonine, Cocaethylene, Norcocaine, Ketamine, Norketamine, Methoxetamine, Tiletamine, Chlordiazepoxide, Diazepam, Nordiazepam, Edtazolam, Flunitrazepam, 7-aminoflunitrazepam, Midazoam, 1-OH-Midazolam, 4-OH-Midazolam, Nimetazepam, Oxazepam, Temazepam, Triazolam, 1-OH-triazolam, Carboxy-THC, THC-OH, JWH-018, JWH-018 4-OH- indole, JWH-018 N-5-OH-pentyl, JWH-073, CP-47,497, CP-47,497 C8 homolog, 2 C-B, 2 C-H, 2 C-I, 2 C-T-2, 2 C-T-4, 2 C-T-7, Mescaline, BZP, mCPP, MDBP, pFPP, pMeOPP, TFMPP, Cathinone, Ethylone, Mephedrone, Methcathinone,

Methedrone, Methylone, 5-MeO-DIPT, Alpha-methyltryptamine,Dimethyltryptamine, Psilocin, MDPV, Mitragynine, Salvinorin A, Dextromethorphan, Dextrorphan, Methadone, EDDP, Methaqualone, Phentermine, Zolpidem, Zopicolne, Amobarbital, Butarbital, Secobarbital.

[e]Cathinone, Methcathinone, 4-Fluoromethacathinone, Methylone, Ethylcathinone, alpha-PPP, Bupgedrone ephedrine, Ethylone, 4-Methoxymethcathinone, Buphedrone, Normephedrone, Diethylcathinone, MDPPP, 4-Methylephedrine, Butylone, Mephedrone, 4-MEC, 4-MEC metabolite, MDPBP, Pentedrone, Pentylone, 3,4-DMMC, alpha-PVP, 4-MPBP, MDPV, Pyrvalerone, Benzedrone, Naphyrone.

[f]Cathinone, Ethylamphetamine, Methcathinone, PMA, AMT, BZP, PMMa, 2 C-H, 4-MTA, DMT, MeOPP, 2,5-DMA, 2 C-D, 3,4-DMA, mCPP, MDDMA, DOM, MiPT, 5MeO-DMT, MDBP, 2 C-P, DOET,3,4,5-TMA, TMA-6, TFMPP, Ketamine, 2 C-T-2, Phencyclidine, DiPT, DPT, 2 C-T-4, 2 C-T-7, 2 C-B, DOB, 2 C-I, dimethylphenylpiperazine.

[g]2 C-H, 4-MTA, DOM, DOET, 2 C-B, DOB, 2 C-I, DOI, 2 C-T-2, 2 C-T-7.

[h]6-O-monoacetylmorphine, Acebutolol, Aceprometazine, Acrivastine, Ajmaline, Alprazolam, Alprenolol, Amantadine, Amiloride, Aminophenazone, Aminopromazine, Amiodarone, Amitriptyline, Amodipine, Amphetamine, Apomorphine, Airidine, Astemizole, Atenolo, Atropine, Befunolol, Benazepril, Benzatripine, Benzocaine, Benzoctamine, Benzoylecgonine, Betaxolol, Biperiden, Bisoprolol, Bromazepam, Bromipheniramine, Bromocriptine, Brotizolam, Bunitrolol, Bupivacine, Bupranolol, Buprenorpnine, Buspirone, Butaperazine, Caffeine, Candesartan, Captopril, Carazolol Carbamazepine, Carbimazole, Carbinoxamine, Carbuterol, Carisoprodol, Carteolol, Carvedilol, Celiprolol, Cetrizine, Chlorcyclizine, Chlordiazepoxide, Chloroquine, Chlorphenethiazine, Chlorpheniramine, Chlorpromazine, Chlorprothixene, cinnarizine, Cisapride, Citalopram, Clemastine, Clenbuterol, Clobazam, Malathion, MDA, MDE, MDMA, Meclozine, Medazepam, Meloxicam, Meperone, Mepindolol, Meprobamate, Mescaline, Mesoridazine, Metaclazepam, Methamphetamine, Metformin, Methadone, Normethadone, Methylphenidate, Methylscopolamine, Metipranol, Metoclomipramide, Metoprolol, Metrinodazole, Mexiletine, Mianserin, Miconazole, Midazolam, Mirtazapine, Mizolastine, Moclobemide, Molindone, Molsidomine, Morphine, Morphine-3-β-D-glucuronide, Naloxone, Naltrexone, Nateglinide, Nicirdipine, Nicotine, Nifedipine, Nilvadipine, Nimodipine, Nisoldipine, Nitrazepam, Nitrendipine, Nizatidine, Norbuprenorphine, Normorphine, Nortriptiline, Noscapine, Obidoxime, OH-THC, Olanzapine, Ondansetron, Opipramol, Orphenadrine, Oxazepam, Oxacarbazepine, Oxitropium, Oxprenolol, Oxycodone, Papaveerine, Paracetamol, Paroxetine, Penbutolol, Norclobazam, Clobutinol, Clomethiazole, Clomipramine, Desmethylclomipramine, Clonazepam, Clonidine, Clozapine, Cocaine, Codeine, Coumatetralyl, Cyclizine, Demoxepam, Dextropropoxyphene, Diazepam, Dibenzepin, Dihydrocodeine, Dihydroergotamine, Dilazep, Dilitiazem, Diphenhydramine, Dipyridamole, Disopyramide, Dixyrazine, Doxapram, Doxepin, Ebastine, Ecgonine methylester, Embutramide, Enalapril, Eprosartan, Ergotamine, Esmolol, Ethenzamide, Ethylmorphine, Ethylparathion, GFelodipine, Fenazepam, Fendilline, Fenetylline, Fenfluramine, Fentanyl, Fexofenadine, Flecainide, Fluconazole, Flunitrazepam, Fluoxetine, Flupetixol, Fluphenazine, Flurazepam, Fluvoxamine, Gallopamil, Glibenclamide, Glibornuride, Glicazide, Glimepiride, Glipizide, Gliquidone, Haloperidol, Heroin, Hydrcodone, Hydroxychloroquine, Hydroxyzine, Pentoxyvprazosin, Prilocaine, Primidone, Procainamide, Procaine, Promazine, Promethazine, Prometryn, Propafenone, Propionylpromazine, Perazine, Perphenazine, Pethidine, henazone, Phenylbutazone, Phenylpropanolamine, Phenyltoloxamine, Phenytoin, Pilocarpine, Pindolol, Pioglitazon, Pirbuterol, Piroxycam, Practolol, Prajmalium, Prazepam, Prazosin, Prilocaine, Primidone, Procainamide, Procaine, Promazine, Promethazine, Prometryn, Propafenone, Propionylpromazine, Propranolol, Propyphenazone, Prothipendyl, Protriptyline, Pseudoephedrine, Quetiapine, Quinapril, Quinine, Ramipril, Rantidine, Repaglinide, Reproterol, Risperidone, Rocuronium, Ropivacine, Rosiglizatone, Scopolamine, Sertindole, Sertraline, Sildenafil, Sotalol, Sulindac, Sulpride, Talinolol, Telmisartan, Temazepam, Terfanadine, Tertalolol, Tetracaine, Tetrahydrocannabinol, THC-COOH, Theobromine, Theophylline, Thioridazine, Tilidazine, Tilidine, Timolol, Thiothixene, Tizandine, Tocainide, Imipramine, Indomethacin, Irbesartan, Isoniazid, Isradipine, Ketamine, Ketoprofen, Ketorolac, Labetalol, Lacidipine, Lamotrigine, Lercarnidipine, Levobunolol, Levocabastine, Levomepromazine, Lidocaine, Lisinopril, Loratadine, Lorazepam, Losartan, Lysergic acid diethylamide, Tolbutamide, Toliprolol, Tolbuterol, Tramadol, Trazodone, Triamterene, Traizolam, Trifluorperazine, trifluperidol, Trimethoprim, Trimipramine, Valsartan, Vardenafil, Venlafaxine, Verapamil, Warfaine, Zolpidem, Zopiclone, Zuclopenthixol, Vincamine, Zimeldne.

[i]25B-NBOMe, 25 C-NBOMe, 25H-NBOMe, 25I-NBOMe, 2-AI, 2 C-B, 2 C-C, 2 C-D, 2 C-E, 2 C-H, 2 C-I, 2 C-N, 2 C-T-2, 2 C-T-2, 2 C-T-7, 2-DPMP, 2-FA, 2-MMC, 3,4-DMMC, 3 C-P, 3-FMC, 3-MeO-PCP, 3-MMC, 4-acetoxy-DiPT,4-BMC, 4-CMC, 4-EMC, 4-FA, 4-FMA, 4-FMC, 4-hydroxy-DET, 4-hydroxy-DiPT, 4-hydroxy-MET, 4-hydroxy-MiPT, 4-MBC, 4-MEC, 4-MeO-DMT, 4-MTA, 5-APB, 5-APDB, 5-CI-UR-144, 5-HTP, 5-IT, 5-MAPB, 5-MeO-AMT, 5-MeO-DALT, 5-mEO-DiPT, 5-MeO-DMT, 5-MeO-MiPT, 6-APB, 6-IT, alpha-MT, alpha-PBP, alpha-PPP, alpha-PVP, APINACA, AM-679, AM-679, AM-694, AM-1220, AM-2201, AM-2233, BDB, BMDP, Buphedrone, Bupropion, Butylone, BZP, CP 80633, D2PM, DCPP, DET, Dibutylone, Diethylpropion, DiPT, DMC, Dimethylone, DMA, DMT, DOET, DOI, DOM, DPT, EAM-2201, Ephedrone, Ethcathinone, Ethylone, Ethylphenidate, Eutylone, HU-308, JWH-0007, JWH-018, JWH-018-D9, JWH-019, JWH-073, JWH-081, JWH-098, JWH-122, JWH-122-7-methylnaphtyisomer, JWH-182, JWH-200, JWH-203, JWH-210, JWH-250, JWH-251, JWH-307, JWH-398, JWH-412, M-Alpha, mCPP, MDAI, MDPBP, MDPPP, MDPV, MeBP, MeOPP, MeP, 4-MMC, 4-MMC D3, MET, Metamfepramone, Methedrone, Methoxetamine, Methylone, MPA, MPBP, MPPP, Naphyrone, NEB, NMT, PCP, pCPP, Pnetedrone, Pentylone, pMeOPP, PPA, RCS-4, SDB-001, STS-135, TFMPP, THJ-2201, TMA, TMA-2, UR-144, URB-597, XLR-11.

[j]Alprazolam, Bromazepam, Camazepam, Chlordiazepoxide, Clobazam, Clonazepam, Diazepam, Fludiazepam, Flinitrazepam, 7-aminoflunitrazepam, Flurazepam, Lorazepam, Lormetazepam, Medazepam, Midazolam, Nimetazepam, Nitrazepam, Nordiazepam, Ozaxepam, Prazepam, Temazepam, Tetrazepam, Triazolam.

[k]JWH-007, JWH-015, JWH-018, JWH-018 adamantyl derivative, JWH-019, JWH-020, JWH-073, JWH-081, JWH-122, JWH-122 5-fluoropentyl derivative, JWH-200, JWH-203, JWH-210, JWH-250, JWH-251, JWH-307, JWH-387, JWH-398, JWH-412, AM-694, AM-1220, AM-2201, AM-2233, CRA-13, Methanandamide, RCS-4, RCS-4 ortho isomer, RCS-8, WIN 48,098, WIN 55,212-2.

[l]Alprazolam, Bromazepam, Chloridiazepoxide, Clobazam, Clonazepam, Diazepam, Estazolam, Lorazepam, Lormetazepam, Nitrazepam, Temazepam, Oxazepam, Midazolam, Medazepam, Clorazepam, Zolpidem, Zaleplon, Zopiclone, Nordiazepam, MDMA, MDEA, MDA, Amhetamine, methamphetamine, OH- amhetapmine, Cocaine, Benzoylecgonine, Morphine Codeine, LSD.

[m]2 C-B, 2 C-I, A29, Acebuterol, Acepromazine, Acrivastine, Alfentanil, Alprazolam, Amfepramone, Amisulpride, Amitriptyline, AmLodipine, Amphetamine, Aripiprazole, Atenolol, Atrovastatin, Atropine, Bambuterol, Benzphentermine, Benzocaine, Benzoylecgonine, Biperiden, Bisoprolol, Bromazepam, Brotizolam, Bupivacine, Buprenorphine, Buspirone, Carvedilol, Cathine, Cetirizine, Chlordiazepoxide, demethylchlordiazepoxide, Chlorpromazine, Chlorprothixene, Cinnarizine, Citalopram, demethyl-citalopram, Clobazam, Norclobazam, Clomipramine, Clonazeppam, 7-aminoclonazepam, Clonidine, Clozapine, Cocaine, Codeine, Cyclizine, Demoxepam, Dextromethotphan, Dextropropoxyphene, Dextrorphan, Diazepam, Demethyldiazepam, Diltiazem, Diphenoxylate, DMA, DMT, Doxazosin, Doxepine, Eletriptan, Enalapril, Ephedrine, Estazolam, Felodipine, Fentanyl, Fexofenadine, Flecainide, Flumazenil, Flunitrazepam, 7-aminoflunitrazepam, Fluoxetine, Norfluoxetine, Flurazepam, N-dealkylflurazepam, Fluvoxamine, Formoterol, Gabapentin, Halazepam, Haloperidol, Hydrocone, Hydromorphone, Hydroxizine, Ibogaine, Imipramine, Ndapamid, Isradipine, Ketamine, Ketobemidone, Labetalol, Lamotrigine, Lercanidipine, Levomepromazine, Levorphanol Loperamide, Loratadine, Lorazepam, Lormetazepam, Losartan, LSD, MBDB, mCPP, MDA, MDMA, Medazepam, MeOPP, Mepivacine, Mepyramine, Mescaline, Methamphetamine, Methadone, Methaqualone, Methylphenidate, Metoclopramide, Mianserine, Midazolam, Mirtazapine, Moclobemide, Morphine, Naloxone, Naltrexone, Nifedipine, Nimodipine, Nitrazepam, 7-aminonitrazepam, Nortriptiline, Noscapine, Orphenadrine, Oxazepam, Oxcarbamazepine, Oxycodone, Oxymorphone, Paroxetine, Pethidine, Phenazepam, Phencyclidine, Phentermin, Pimozide, Pindolol, PMA, PMMA, Prazepam, Procyclidine, Promethazine, Propafenone, Propranolol, Pseudoephedrine, Quazepam, Quetiapine, Reboxetine, Remifentanil, Salmeterol, Scopolamine, Selegiline, Sertinol, Sertraline, Sildenafil, Sotalol, STP, Sulpride, Temazepam, Terbutaline, TFMPP, Tolbutamide, Tramadol, Triazolam, Trimipramine, Vardenafil, Venlafaxine, Verapamil, Zaleplon, Zolmitriptan, Zolpidem, Zopiclone.

Immunochemical methods are most commonly used to identify psychoactive substances. Many tests target different groups of analytes or specific substances (Szukalski 2001; Maher et al. 2007; Kerrigan, Banuelos, et al. 2011; Kerrigan, Mellon, et al. 2011; Nieddu et al. 2013; Nieddu et al. 2014a, 2014b; Swortwood et al. 2014; Nieddu et al. 2016; Scheidweiler et al. 2015; Regester et al. 2015; O'Connor et al. 2016. The enzyme-linked immunosorbent assay (ELISA) is one of the most commonly used immunochemical tests for screening drugs. In this approach, an enzyme-labeled antigen competes for primary antibody binding sites with the sample antigen, and enzymatic activity increases proportionally to the concentration of the target substance. The immunofluorescence method is equally often used for screening. In this method, the antigen is labeled with a fluorescent dye which is displaced by the analyzed substance, and the resulting change in fluorescence polarization is measured with a detector (Szukalski 2001).

Methods that are burdened by high uncertainty and are unsuitable for routine analyses can be eliminated based on the data presented in Table 3. The specificity of tests targeting a given analyte or group of analytes has to be verified. In addition, only a small number of tests have a low detection limit, which is a further impediment because concentration levels in biological matrices are often low. The fact that new psychoactive substances cannot be identified with this approach poses a significant problem. However, according to Rojek et al. (2017), this method is appropriate for screening and selecting samples for quantitative analysis. The increasing volume and diversity of illegal drugs forces laboratories to develop new analytical methods to identify illicit substances (Scheidweiler et al. 2015). To meet analytical needs, further chromatographic methods are being developed to identify new psychoactive substances. These include mass spectrometry coupled with gas chromatography (GC–MS) (Papoutsis et al. 2010; Kerriga et al. 2011; Tomczak et al. 2018; Alexandridou et al. 2020; Institóris et al. 2022) and liquid chromatography (LC–MS) (Mueller et al. 2005; Wohlfarth et al. 2010; Dalsgaardet al. 2012; Kneisel and Auwärter 2012; Concheiro et al. 2013; Swortwood et al. 2013; Tang et al. 2014; Wicka et al. 2014; Adamowicz and Tokarczyk 2016; Cannaert et al. 2016; Yeter 2017). Chromatographic methods are presented in Table 4. GC–MS supports the detection of substances that cannot be identified with immunochemical methods (Kerrigan, Banuelos, et al. 2011; Kerrigan, Mellon, et al. 2011).

GC–MS is characterized by a lower detection limit than immunochemical tests (Papoutsis et al. 2010; Kerrigan, Banuelos, et al. 2011; Kerrigan, Mellon, et al. 2011). However, GC–MS requires a derivatization step to identify a higher number of psychoactive substances (Papoutsis et al. 2010). Derivatization prolongs run time and increases analytical costs, which poses an additional problem for toxicology laboratories. Due to these shortcomings, LC–MS methods are more widely used than GC–MS (Mueller et al. 2005; Wohlfarthet al. 2010; Dalsgaard et al. 2012; Kneisel and Auwärter 2012; Swortwood et al. 2013; Tang et al. 2014; Wicka et al. 2014; Adamowicz and Tokarczyk 2016; Cannaert et al. 2016; Rojek et al. 2017; Salomone et al. 2017; Yeter 2017; Fels et al. 2020). LC–MS supports the determination of numerous compounds (Mueller et al. 2005; Delsgaard et al. 2012; Tang et al. 2014; Adamowicz and Tokarczyk 2016; Yeter 2017). These methods are characterized by lower LOD values, shorter run time, and lower costs. The optimal method for detecting psychoactive substances should eliminate deuterated compounds which increase the cost of the analysis. Particular focus should be placed on chromatographic methods that enable the separation and subsequent determination of substances with the same m/z ratios. Such analytes cannot be identified by multiple reaction monitoring (MRM) alone without proper chromatographic separation of the analyzed substances.

In addition to traditional methods of analyzing psychoactive substances, high-resolution mass spectrometry (HRMS) has emerged as a popular approach in recent years. This method supports highly accurate measurements of the mass-to-charge ratio, and it operates in the data-independent acquisition (DIA) mode (Remane et al. 2016). The applicability of HRMS for forensics and clinical toxicology has been studied by several authors (Meyer and Maurer 2012; Ojanperä et al. 2012; Meyer and Maurer 2016). Pellegrini et al. (2020) compared the effectiveness of HRMS and GC–MS in an analysis of synthetic cannabinoids in urine samples. The obtained LOD and LOQ values were identical for both methods. Ultra-high-performance liquid chromatography–HRMS speeds up analysis and supports the identification of substances for which standards are not available. However, both methods have the same sensitivity and specificity, which indicates that cheaper and simpler methods can be used with satisfactory results. Salomone et al. (2021) relied on the UHPLC-QTOF-HRMS method to analyze fentanyl analogs and their metabolites in hair samples. The developed method has been successfully validated, and it supports retrospective analysis. This approach is characterized by low LOD and LOQ values, and it can be effectively applied to detect even trace amounts of toxic substances. The only drawback is that the method is based on spectra and requires software for generating empirical formulas of the examined substances. According to Maurer and Meyer (2016), the main advantages of HRMS are that it supports the differentiation of compounds with identical nominal weights, but different exact weights, and that other analytes can be easily incorporated into the method. High equipment costs and non-intuitive software requiring qualified personnel were listed as the main disadvantages of the discussed technique. HRMS is considered a gold standard for the analysis of suspected NPS samples. This method enables full MS and MS/MS scanning, and it can also be used for retrospective analysis. In the future, this technique can be further refined to detect the analogs of known psychoactive substances that often occur at very low concentrations (Pasin et al. 2017).

Liquid and gas chromatography coupled with mass spectrometry is also used to determine psychoactive substances in unconventional matrices such as hair (Barroso et al. 2010; Hutter et al. 2012; Salomone et al. 2012; Shah et al. 2012; Rust et al. 2012; Namera et al. 2013; Kim et al. 2013; Salomone et al. 2014; Gottardo et al. 2014; Imbert et al. 2014; Strano-Rossi et al. 2014; Wicka et al. 2014; Kim et al. 2015;

Montenarh et al. 2015; Salomone et al. 2016; Frison et al. 2016; Franz et al. 2016). Hair is an analytical matrix that carries important information, but hair samples are difficult to prepare because they have to be divided into fragments and weighed, segments have to be identified, and individual hair sections have to be analyzed. Hair samples can be used in retrospective analysis, and they support the identification of substances that are rapidly decomposed in the body and cannot be detected in blood or urine samples. Unconventional matrices contribute important information in NPS analyses, which is why effective methods for identifying these compounds are needed.

5. Electrochemical methods

Electrochemical methods offer new possibilities in NPS analyses and pose an alternative to chromatographic methods. An approach based on electrochemical methods was described by Smith, Metters, Irving, et al. (2014) and Smith, Metters, Khreit, et al. (2014). The cited authors proposed a methodology for reducing cathinone, mephedrone, and 4-MEC substitutes. The developed method supports the identification of illegal substances in seized drug samples with the use of cyclic voltammetry. Detection limits were determined in the range of 11.60–11.60 μg/mL (Smith, Metters, Irving, et al. 2014; Smith, Metters, Khreit, et al. 2014). A graphite screen-printed electrode (GSPE) for detecting NRG-2 in street samples was also discussed, and the obtained results were validated by liquid chromatography (Smith, Metters, Irving, et al. 2014; Smith, Metters, Khreit, et al. 2014). Effective methods for the rapid identification of piperazines in street samples have not been developed to date. However, Philp et al. (2013) proposed a novel method for analyzing benzylpiperazine (BZP) using a specific color test. Sodium 1,2-naphthoquinone-4-sulphonate (NQS) formed a red-colored complex with BZP which clearly differed from other color reactions occurring in the sample with potential cross-reagents. Elie et al. (2012) analyzed BZP together with MDAI and mephedrone. They used a microcrystalline identification method involving mercury chloride as a microcrystalline agent. The resulting crystals were analyzed and compared with other illegal substances to identify MDAI in samples containing different compounds. Crystal methamphetamine has been used recreationally since the 1960s, and electrochemical methods can be effectively deployed to detect this compound in street tests. However, these methods involve mercury, which is a harmful substance, and additional modifications are needed to improve the safety of the analysis. Unconventional NPS detection methods, described in the above studies, offer new opportunities for developing new screening techniques that can be applied in the field. The absence of such methods poses a considerable problem for toxicologists and law enforcement agencies.

6. Conclusions

The emergence of new psychoactive substances gives serious cause for concern. Acute poisonings and fatalities linked with NPS are on the rise, and this problem needs to be addressed in the fight against drug-related crime. Analytical methods that support the identification of NPS at low concentrations and in the shortest possible time is needed, which poses an immense challenge for toxicology laboratories. LC–MS should be further refined to create rapid, sensitive, and specific methods for the determination of new psychoactive substances. The sample preparation stage should be simplified to isolate as many analytes as possible in the shortest possible time, to minimize waste generation and reduce analytical costs. The resulting approaches will decrease the number of drug-related deaths, promote the development of new treatment methods and the initiation of legal measures to limit the availability of new psychoactive substances.

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Declaration of interest

The authors' affiliations are shown above. All experts who have contributed to the study are listed as coauthors or are mentioned in the acknowledgments. The authors assume full responsibility for the content of the article. The content was not influenced by the organization funding the study. The authors have no conflict of interest to declare. None of the authors have participated in any legal, regulatory, or advocacy proceedings related to the contents of the article in the last 5 years.

References

Adamowicz P, Tokarczyk B. 2016. Simple and rapid screening procedure for 143 new psychoactive substances by liquid chromatography-tandem mass spectrometry. Drug Test Anal. 8(7):652–667.

Aldlgan AA, Torrance HJ. 2016. Bioanalytical methods for the determination of synthetic cannabinoids and metabolites in biological specimens. TrAC - Trends Anal Chem. 80:444–457.

Alexandridou A, Mouskeftara T, Raikos N, Gika HG. 2020. GC-MS anaysis of underivatised new psychoactivesubstances in whole blood and urine. J Chromatogr B Analyt Technol Biomed Life Sci. 1156:122308.

Barroso M, Costa S, Dias M, Vieira DN, Queiroz JA, Lopez-Rivadulla M. 2010. Analysis of phenylpiperazine-like stimulants in human hair as trimethylsilyl derivatives by gas chromatographymass spectrometry. J Chromatogr A. 1217(40):6274–6280.

Baumann MH, Partilla JS, Lehner KR, Thorndike EB, Hoffman AF, Holy M, Rothman RB, Goldberg SR, Lupica CR, Sitte HH, et al. 2013. Powerful cocaine-like actions of 3,4-methylenedioxypyrovalerone (MDPV), a principal constituent of psychoactive "bath salts" products. Neuropsychopharmacology. 38(4):552–562.

Blough BE, Landavazo A, Decker AM, Partilla JS, Baumann MH, Rothman RB. 2014. Interaction of psychoactive tryptamines with biogenic amine transporters and serotonin receptor subtypes. Psychopharmacology (Berl). 231(21):4135–4144.

Buszewski B, Szultka M, Gadzała-Kopciuch R. 2012. Sorbent chemistry, evolution, in: Comprehensive Sampling and Sample Preparation. Analytical Techniques for Scientists. Ed J Pawliszyn. Elsevier. 2: 243–256.

Buszewski B, Szultka M 2012. Past, Present, and Future of Solid Phase Extraction: A Review. Crit Rev Anal Chem. 42(3):198–213.

Brandt SD, King LA, Evans-Brown M. 2014. Evans-Brown M. The new drug phenomenon. Drug Test Anal. 6(7–8):587–597.

Cannaert A, Storme J, Franz F, Auwarter V, Stove CP. 2016. Detection and activity profiling of synthetic cannabinoids and metabolites with a newly developed bio-assay. Anal Chem. 88(23):11476–11485.

Cohen K, Weinstein A. 2018. The effects of cannabinoids on executive functions: evidence from cannabis and synthetic cannabinoids—a systematic review. Brain Sci. 8(3):40.

Concheiro M, Anizan S, Ellefsen K, Huestis MA. 2013. Simultaneous quantification of 28 synthetic cathinones and metabolites in urine by liquid chromatography-high resolution mass spectrometry. Anal Bioanal Chem. 405(29):9437–9448.

Cozzi NV, Gopalakrishnan A, Anderson LL, Feih JT, Shulgin AT, Daley PF, Ruoho AE. 2009. Dimethyltryptamine and other hallucinogenic tryptamines exhibit substrate behavior at the serotonin uptake transporter and the vesicle monoamine transporter. J Neural Transm (Vienna). 116(12):1591–1599.

Dalsgaard PW, Rasmussen BS, Muller IB, Linnet K. 2012. Toxicological screening of basic drugs in whole blood using UPLC-TOF-MS. Drug Test Analysis. 4(5):313–319.

Debruyne D, Le Boisselier R. 2015. Emerging drugs of abuse: current perspectives on synthetic cannabinoids. Subst Abuse Rehabil. 6(6): 113–129.

Elie L, Baron M, Croxton R, Elie M. 2012. Microcrystalline identification of selected designer drugs. Forensic Sci Int. 214(1–3):182–188.

Eshleman AJ, Wolfrum EK, Hatfield MG, Johnson RA, Murphy KV, Janowsky A. 2013. Substituted methcathinones differ in transporter and receptor interactions. Biochem Pharmacol. 85(12):1803–1815.

Fels H, Herzog J, Skopp G, Holzer A, Paul LD, Graw M, Musshoff F. 2020. Retrospective analysis of new psychoactive substances in blood samples of German drivers suspected of driving under the influence of drugs. Drug Test Anal. 12(10):1470–1476.

Fleckenstein AE, Gibb JW, Hanson GR. 2000. Differential effects of stimulants on monoaminergic transporters: pharmacological consequences and implications for neurotoxicity. Eur J Pharmacol. 406(1):1–13.

Franz F, Angerer V, Hermanns-Clausen M, Auwarter V, Moosmann B. 2016. Metabolites of synthetic cannabinoids in hair-proof of consumption or false friends for interpretation? Anal Bioanal Chem. 408(13): 3445–3452.

Frison G, Frasson S, Zancanaro F, Tedeschi G, Zamengo L. 2016. Detection of 3-methylmethcathinone and its metabolites 3-methylephedrine and 3-methylnorephedrine in pubic hair samples by liquid chromatography-high resolution/high accuracy Orbitrap mass spectrometry. Forensic Sci Int. 265:131–137.

Gottardo R, Sorio D, Musile G, Trapani E, Seri C, Serpelloni G, Tagliaro F. 2014. Screening for synthetic cannabinoids in hair by using LC-QTOF MS: a new and powerful approach to study the penetration of these new psychoactive substances in the population. Med Sci Law. 54(1): 22–27.

Halberstadt AL, Geyer MA. 2011. Multiple receptors contribute to the behavioral effects of indoleamine hallucinogens. Neuropharmacology. 61(3):364–381.

Halberstadt AL, Koedood L, Powell SB, Geyer MA. 2011. Differential contributions of serotonin receptors to the behavioral effects of indoleamine hallucinogens in mice. J Psychopharmacol. 25(11):1548–1561.

Hurst T. 2019. World drug report. https://doi.org/10.1002/9781118929803.ewac0543.

Hutter M, Kneisel S, Auwarter V, Neukamm MA. 2012. Determination of 22 synthetic cannabinoids in human hair by liquid chromatography-tandem mass spectrometry. J Chromatogr B Analyt Technol Biomed Life Sci. 903:95–101.

Imbert L, Dulaurent S, Mercerolle M, Morichon J, Lachatre G, Gaulier JM. 2014. Development and validation of a single LCMS/MS assay following SPE for simultaneous hair analysis ofamphetamines, opiates, cocaine and metabolites. Forensic Sci Int. 234:132–138.

Institóris L, Kovacs K, Sija E, Berkecz R, Körmöczi T, Nemeth I, Elek I, Bakos A, Urban I, Pap C, et al. 2022. Clinical symptoms and blood concentration of new psychoactive substances (NPS) in intoxicated and hospitalized patients in the Budapest region of Hungary (2018–19). Clin Toxicol. 60(1):18–24.

Kerrigan S, Banuelos S, Perrella L, Hardy B. 2011. Simultaneous detection of ten psychedelic phenethylamines in urine by gas chromatography-mass spectrometry. J Anal Toxicol. 35(7):459–469.

Kerrigan S, Mellon MB, Banuelos S, Arndt C. 2011. Evaluation of commercial enzyme-linked immunosorbent assays to identify psychedelic phenethylamines. J Anal Toxicol. 35(7):444–451.

Kim J, In S, Park Y, Park M, Kim E, Lee S. 2013. Deposition of JWH-018, JWH-073 and their metabolites in hair and effect of hair pigmentation. Anal Bioanal Chem. 405(30):9769–9778.

Kim J, Park Y, Park M, Kim E, Yang W, Baeck S, Lee S, Han S. 2015. Simultaneous determination of five naphthoylindole-based synthetic cannabinoids and metabolites and their deposition in human and rat hair. J Pharm Biomed Anal. 102:162–175.

Kneisel S, Auwärter V. 2012. Analysis of 30 synthetic cannabinoids in serum by liquid chromatography-electrospray ionization tandem mass spectrometry after liquid-liquid extraction. J Mass Spectrom. 47(7): 825–835.

Lendoiro E, Jimenez-Morigosa C, Cruz A, Paramo M, Lopez-Rivadulla M, de Castro A. 2017. An LC-MS/MS methodological approach to the analysis of hair for amphetamine-type-stimulant (ATS) drugs, including selected synthetic cathinones and piperazines. Drug Test Analysis. 9(1):96–105.

Lõpez-Arnau R, Martínez-Clemente J, Pubill D, Escubedo E, Camarasa J. 2012. Comparative neuropharmacology of three psychostimulant cathinone derivatives: butylone, mephedrone and methylone. Br J Pharmacol. 167(2):407–420.

Lowdon JW, Alkirkit SMO, Mewis RE, Fulton D, Banks CE, Sutcliffe OB, Peeters M. 2018. Engineering molecularly imprinted polymers (MIPs) for the selective extraction and quantification of the Novel Psychoactive Substance (NPS) methoxphenidine and its regioisomers. Analyst. 143(9):2002–2007.

Lowdon JW, Eersels K, Rogosic R, Boonen T, Heidt B, Diliën H, van Grinsven B, Cleij TJ. 2019. Surface grafted molecularly imprinted polymeric receptor layers forthermal detection of the New Psychoactive substance2-methoxphenidine. Sens Actuat A. 295:586–595.

Maher WA, Pianca DJ, Apollonio LG, Whittall IR, Kyd JM. 2007. Matrix effect and cross-reactivity of select amphetamine-type substances, designer analogues, and putrefactive amines using the bio-quant direct ELISA presumptive assays for amphetamine and methamphetamine. J Anal Toxicol. 31(4):208–213.

Marusich JA, Antonazzo KR, Wiley JL, Blough BE, Partilla JS, Baumann MH. 2014. Pharmacology of novel synthetic stimulants structurally related to the "bath salts" constituent 3,4-methylenedioxypyrovalerone (MDPV). Neuropharmacology. 87:206–213.

Maurer HH, Meyer MR. 2016. High-resolution mass spectrometry in toxicology: current status and future perspectives. Arch Toxicol. 90(9): 2161–2172.

Meltzer PC, Butler D, Deschamps JR, Madras BK. 2006. 1-(4-Methylphenyl)-2-pyrrolidin-1-yl-pentan-1-one (pyrovalerone) analogues: a promising class of monoamine uptake inhibitors. J Med Chem. 49(4):1420–1432.

Meyer MR, Caspar A, Brandt SD, Maurer HH. 2014. A qualitative/quantitative approach for the detection of 37 tryptamine-derived designer drugs, 5 β-carbolines, ibogaine, and yohimbine in human urine and plasma using standard urine screening and multi-analyte approaches. Anal Bioanal Chem. 406(1):225–237.

Meyer MR, Maurer HH. 2012. Current applications of high-resolution mass spectrometry in drug metabolism studies. Anal Bioanal Chem. 403(5):1221–1231.

Meyer MR, Maurer HH. 2016. Review: LC coupled to low- and high-resolution mass spectrometry for new psychoactive substance screening in biological matrices - Where do we stand today? Anal Chim Acta. 927:13–20.

Michely JA, Helfer AG, Brandt SD, Meyer MR, Maurer HH. 2015. Metabolism of the new psychoactive substances N,N-diallyltryptamine (DALT) and 5-methoxy-DALT and their detectability in urine by GC–MS, LC–MS^n, and LC–HR–MS–MS. Anal Bioanal Chem. 407(25): 7831–7842.

Montenarh D, Hopf M, Warth S, Maurer HH, Schmidt P, Ewald AH. 2015. A simple extraction and LC-MS/MS approach for the screening and identification of over 100 analytes in eight different matrices. Drug Test Anal. 7(3):214–240.

Mueller CA, Weinmann W, Dresen S, Schreiber A, Gergov M. 2005. Development of a multi-target screening analysis for 301 drugs using a QTrap liquid chromatography/tandem mass spectrometry system and automated library searching. Rapid Commun Mass Spectrom. 19(10):1332–1338.

Namera A, Urabe S, Saito T, Torikoshi-Hatano A, Shiraishi H, Arima Y, Nagao M. 2013. A fatal case of 3,4-methylenedioxypyrovalerone poisoning: coexistence of α-pyrrolidinobutiophenone and α-pyrrolidinovalerophenone in blood and/or hair. Forensic Toxicol. 31(2):338–343.

Nichols DE. 2012. Structure-activity relationships of serotonin 5-HT2A agonists. WIREs Membr Transp Signal. 1(5):559–579.

Nieddu M, Burrai L, Trignano C, Boatto G. 2014a. Cross-reactivities of 39 new amphetamine designer drugs on three abuse drugs urinary screening tests. Forensic Toxicol. 32(1):132–138.

Nieddu M, Burrai L, Trignano C, Boatto G. 2014b. Evaluation of commercial multi-drug oral fluid devices to identify 39 new amphetamine-designer drugs. Leg Med. 16(2):106–109.

Nieddu M, Trignano C, Burrai L, Pirisi MA, Boatto G. 2013. Cross-reactivities of 41 new amphetamine designer drugs to EMIT®immunoassays. Forensic Toxicol. 31(1):133–137.

Nieddu M, Burrai L, Baralla E, Pasciu V, Varoni MV, Briguglio I, Demontis MP, Boatto G, et. al. 2016. ELISA detection of 30 new amphetamine designer drugs in whole blood, urine and oral fluid using neogen® "amphetamine" and "methamphetamine/MDMA" kits. J Anal Toxicol. 40(7):492–497.

O'Connor LC, Torrance HJ, McKeown DA. 2016. ELISA detection of phenazepam, etizolam, pyrazolam, flubromazepam, diclazepam and delorazepam in blood using Immunalysis® Benzodiazepine kit. J Anal Toxicol. 40(2):159–161.

Ojanperä I, Kolmonen M, Pelander A. 2012. Current use of highresolution mass spectrometry in drug screening relevant to clinical and forensic toxicology and doping control. Anal Bioanal Chem. 403(5):1203–1220.

Papoutsis II, Athanaselis SA, Nikolaou PD, Pistos CM, Spiliopoulou CA, Maravelias CP. 2010. Development and validation of an EI-GC-MS method for the determination of benzodiazepine drugs and their metabolites in blood: applications in clinical and forensic toxicology. J Pharm Biomed Anal. 52(4):609–614.

Pasin D, Cawley A, Bidny S, Fu S. 2017. Current applications of high-resolution mass spectrometry for the analysis of new psychoactive substances: a critical review. Anal Bioanal Chem. 409(25):5821–5836.

Pellegrini M, Marchei E, Papaseit E, Farré M, Zaami S. 2020. UHPLC-HRMS and GC-MS screening of a selection of synthetic cannabinoids and metabolites in urine of consumers. Medicina. 56(8):408.

Philp M, Shimmon R, Stojanovska N, Tahtouh M, Fu S. 2013. Development and validation of a presumptive colour spot test method for the detection of piperazine analogues in seized illicit materials. Anal Methods. 5(20):5402–5410.

Regester LE, Chmiel JD, Holler JM, Vorce SP, Levine B, Bosy TZ. 2015. Determination of designer drug cross-reactivity on five commercial immunoassay screening kits. J Anal Toxicol. 39(2):144–151.

Remane D, Wissenbach DK, Peters FT. 2016. Recent advances of liquid chromatography-(tandem) mass spectrometry in clinical and forensic toxicology – an update. Clin Biochem. 49(13–14):1051–1071.

Rojek S, Korczyńska-Albert M, Kulikowska J, Kłys M. 2017. Współczesne wyzwania w toksykologii związane z nowymi substancjami psychoaktywnymi ilustrowane przypadkami zgonów po zażyciu UR-144 oraz UR-144 z pentedronem oznaczonych w próbkach krwi metodą LC-ESI-MS (Contemporary challenges in toxicology related to new psychoactive substances illustrated by cases of deaths after taking UR-144 and UR-144 with pentedrone determined in blood samples using the LC-ESI-MS method) Arch Med. Arch Med Sadowej Kryminol. 67(2): 104–120.

Rust KY, Baumgartner MR, Dally AM, Kraemer T. 2012. Prevalence of new psychoactive substances: a retrospective study in hair. Drug Test Anal. 4(6):402–408.

Salomone A, Gerace E, D'Urso F, Di Corcia D, Vincenti M. 2012. Simultaneous analysis of several synthetic cannabinoids, THC, CBD and CBN, in hair by ultra-high performance liquid chromatography tandem mass spectrometry. Method validation and application to real samples. J Mass Spectrom. 47(5):604–610.

Salomone A, Luciano C, Di Corcia D, Gerace E, Vincenti M. 2014. Hair analysis as a tool to evaluate the prevalence of synthetic cannabinoids in different populations of drug consumers. Drug Test Anal. 6(1–2): 126–134.

Salomone A, Gazzilli G, Di Corcia D, Gerace E, Vincenti M. 2016. Determination of cathinones and other stimulant, psychedelic, and dissociative designer drugs in real hair samples. Anal Bioanal Chem. 408(8):2035–2042.

Salomone A, Palamar JJ, Gerace E, Di Corcia D, Vincenti M. 2017. Hair testing for drugs of abuse and new psychoactive substances in a high-risk population. J Anal Toxicol. 41:376–381.

Salomone A, Di Corcia D, Negri P, Kolia M, Amante E, Gerace E, Vincenti M. 2021. Targeted and untargeted detection of fentanyl analogues and their metabolites in hair by means of UHPLC-QTOF-HRMS. Anal Bioanal Chem. 413(1):225–233.

Sánchez-González J, Odoardi S, Bermejo AM, Bermejo-Barrera P, Romolo FS, Moreda-Piñeiro A, Strano-Rossi S. 2019. HPLC-MS/MS combined with membrane protected - molecularly imprinted polymer micro-solid-phase extraction for synthetic cathinones monitoring in urine. Drug Test Anal. 11(1):33–44.

Sánchez-González J, García-Carballal S, Cabarcos P, Tabernero MJ, Bermejo-Barrera P, Moreda PA. 2016. Determination of cocaine and its metabolites in plasma by porous membrane-protected molecularly imprinted polymer micro-solid-phase extraction and liquid chromatography—tandem mass spectrometry. J Chromatogr A. 1451:15–22.

Sánchez-González J, Salgueiro-Fernández R, Cabarcos P, Bermejo AM, Bermejo-Barrera P, Moreda-Pineiro A. 2017. Cannabinoids assessment in plasma and urine by high performance liquid chromatography–tandem mass spectrometry after molecularly imprinted polymer microsolid-phase extraction. Anal Bioanal Chem. 409(5):1207–1220.

Sánchez-González J, Tabernero MJ, Bermejo AM, Bermejo-Barrera P, Moreda-Piñeiro A. 2015. Porous membrane-protected molecularly imprinted polymer microsolid-phase extraction for analysis of urinary cocaine and its metabolites using liquid chromatography - tandem mass spectrometry. Anal Chim Acta. 898:50–59.

Scheidweiler KB, Jarvis MJY, Marilyn AH. 2015. Nontargeted SWATH acquisition for identifying 47 synthetic cannabinoid metabolites in human urine by liquid chromatography-high-resolution tandem mass spectrometry. Anal Bioanal Chem. 407(3):883–897.

Shah SA, Deshmukh NI, Barker J, Petroczi A, Cross P, Archer R, Naughton DP. 2012. Quantitative analysis of mephedrone using liquid chromatography tandem mass spectroscopy: application to human hair. J Pharm Biomed Anal. 61:64–69.

Shen WW. 1997. The metabolism of psychoactive drugs: a review of enzymatic biotransformation and inhibition. Biol Psychiatry. 41(7): 814–826.

Simmler LD, Buser TA, Donzelli M, Schramm Y, Dieu LH, Huwyler J, Chaboz S, Hoener MC, Liechti ME. 2013. Pharmacological characterization of designer cathinones in vitro. Br J Pharmacol. 168(2):458–470.

Simmler LD, Rickli A, Hoener MC, Liechti ME. 2014. Monoamine transporter and receptor interaction profiles of a new series of designer cathinones. Neuropharmacology. 79:152–160.

Smith JP, Metters JP, Irving C, Sutcliffe OB, Banks CE. 2014. Forensic electrochemistry: the electroanalytical sensing of synthetic cathinone-derivatives and their accompanying adulterants in "legal high" products. Analyst. 139(2):389–400.

Smith JP, Metters JP, Khreit OIG, Sutcliffe OB, Banks CE. 2014. Forensic electrochemistry applied to the sensing of new psychoactive substances: electroanalytical sensing of synthetic cathinones and analytical validation in the quantification of seized street samples. Anal Chem. 86(19):9985–9992.

Strano-Rossi S, Odoardi S, Fisichella M, Anzillotti L, Gottardo R, Tagliaro F. 2014. Screening for new psychoactive substances in hair by ultrahigh performance liquid chromatography-electrospray ionization tandem mass spectrometry. J Chromatogr A. 1372c:145–156.

Swortwood MJ, Hearn WL, Decaprio AP. 2014. Cross-reactivity of designer drugs, including cathinone derivatives, in commercial enzyme-linked immunosorbent assays. Drug Test Analysis. 6(7–8):716–727.

Swortwood MJ, Boland DM, Decaprio AP. 2013. Determination of 32 cathinone derivatives and other designer drugs in serum by comprehensive LC-QQQ-MS/MS Analysis. Anal Bioanal Chem. 405(4): 1383–1397.

Szukalski B. 2001. Analysis of psychoactive substances in biological material. Alcohol Drug Addict. 14(l):151–163.

Tang MHY, Ching CK, Lee CYW, Lam Y, Mak TWL. 2014. Simultaneous detection of 93 conventional and emerging drugs of abuse and their metabolites in urine by UHPLC-MS/MS. J Chromatogr B Analyt Technol Biomed Life Sci. 969:272–284.

Tomczak E, Woźniak MK, Kata M, Wiergowski M, Szpiech B, Biziuk M. 2018. Blood concentrations of a new psychoactive substance 4-chloromethcathinone (4-CMC) determined in 15 forensic cases. Forensic Toxicol. 36(2):476–485.

Tyrkko E, Andersson M, Kronstrand R. 2016. The toxicology of new psychoactive substances: Synthetic cathinones and phenylethylamines. Ther Drug Monit. 38(2):190–216.

United Nations Office on Drugs and Crime (UNODC). 2014. World drug report 2014. Vienna, Austria: United Nations Publication, Sales No. E.14.XI.7.

United Nations Office on Drugs and Crime (UNODC). 2016. World drug report 2017-market analysis of synthetic drugs Amphetamine-type stimulants, new psychoactive substances. Vienna, Austria: United Nations Office on Drugs and Crime

United Nations Office on Drugs and Crime (UNODC). 2019. World drug report 2019. Vienna, Austria: United Nations Publication, Sales No. E.19.XI.8.

van Gorp F, Wejden LC, Stienstra NA, Kuck EM, Haas LEM. 2017. Severe neurological symptoms following synthetic cannabinoid intoxication. Neth J Med. 75(4):158–160.

Welter-Luedeke J, Maurer HH. 2016. New psychoactive substances: chemistry, pharmacology, metabolism, and detectability of amphetamine derivatives with modified ring systems. Ther Drug Monit. 38(1):4–11.

Wicka M, Chołbiński P, Kwiatkowska D, Pokrywka A. 2014. Detection of psychotropic substances in the blood by LC/MS/MS method (in Polish). Problemy Kryminalistyki. 284(2):1–13.

Wohlfarth A, Weinmann W, Dresen S. 2010. LC-MS/MS screening method for designer amphetamines, tryptamines, and piperazines in serum. Anal Bioanal Chem. 396(7):2403–2414.

Yanes EG, Lovett DP. 2012. High-throughput bioanalytical method for analysis of synthetic cannabinoid metabolites in urine using salting-out sample preparation and LC–MS/MS. J Chromatogr B Analyt Technol Biomed Life Sci. 909:42–50.

Yeter O. 2017. Determination of drugs in human blood via bidirectional solid phase extraction. LC-Tech Application Note 1–16. https://www.johnmorrisgroup.com/Content/Attachments/227518/LCTech-Application-Note-Drugs-Blood-en.pdf.

[D2] Jadwiga Musiał, Jolanta Powierska-Czarny, Jakub Czarny, Michał Raczkowski, Natalia Galant, Bogusław Buszewski, Renata Gadzała-Kopciuch, *One-step extraction and determiantion of 513 psychoactive substances, drugs, and their metabolites from hair by LC-MS/MS*, Archives of Toxicology, 2022, 96:2927-2933, https://doi.org/10.1007/s00204-022-03343-w, IF=6,168

W związku z ciągle wzrastającą liczbą substancji psychoaktywnych dostępnych w sprzedaży ulicznej, a także z wzrastającym zainteresowaniem tego typu używkami wzrasta zainteresowanie badaniami włosów pod kątem tego typu substancji chociażby ze względu na fakt, iż jest to jedyna matryca, w której możemy wykryć anality po tak długim czasie od ich zażycia. Dlatego też, skupiono się na opracowaniu metody analitycznej umożliwiającej oznaczenie jak największej liczby analitów zaliczanych do substancji psychoaktywnych/leków/ich metabolitów w próbkach włosów. Ważne, aby opracowana metoda była nieskomplikowana i dawała możliwość łatwego dodania kolejnych analitów, których ciągle przybywa w handlu ulicznym, a także stosunkowo łatwego dostosowania jej do innej matrycy. Chcąc wykorzystać możliwości chromatografii cieczowej sprzężonej z tandemową spektrometrią mas oraz biorąc pod uwagę ilość analitów, ich podobieństwo strukturalne oraz potencjalnie niskie poziomy stężeń w próbkach biologicznych zdecydowałam się na właśnie tę technikę. Opracowując procedurę analityczną skupiono się na uwzględnieniu wpływu matrycy oraz ograniczeniu zanieczyszczeń pochodzących z próbki, dlatego też zdecydowano się na sporządzenie krzywej wzorcowej w matrycy oraz rozcieńczenie próbki.

W pierwszym etapie prac przeprowadzono dobór warunków pracy spektrometru mas dla poszczególnych analitów. W tym celu każdy z analitów poddano automatycznej optymalizacji par MRM oraz wartości DP (potencjał rozgrupowania klastrów), CE (energii zderzeń), EP (potencjał wejścia) i CXP (potencjał wyjściowy). Dla każdego z analitów wybrano po 2 pary MRM do dalszych badań. Następnie dobrano warunki chromatograficzne umożliwiające rozdzielenie izomerów, które po optymalizacji na spektrometrze mas charakteryzowały się takimi samymi parami MRM. W tym celu weryfikowałam trzy kolumny chromatograficzne: Kinetex C18 (Phenomenex, 3,0 x 100 mm; 2,6 µm), Kinetex Biphenyl (Phenomenex, 3,0 x 100 mm; 2,6 µm) i Kinetex Phenyl-Hexyl (Phenomenex, 3,0 x 100 mm; 2,6 µm), a także różne składy faz ruchomych (metanol i acetonitryl oraz mrówczan amonu w stężeniach od 2 do 5 mM). Najlepsze rezultaty uzyskano dla kolumny Kinetex C18 i fazie ruchomej składającej się z 2 mM mrówczanu amonu z 0.1% kwasem mrówkowym w wodzie (faza A) i w metanolu (faza B). Zastosowanie acetonitrylu nie wniosło znaczących zmian

w otrzymanych wynikach, więc ze względu na koszty i szkodliwość odpadów pozostałam przy fazie B składającej się z metanolu i 2 mM mrówczanu amonu z 0,1% kwasem mrówkowym. Chromatograficzne rozdzielenie analitów z wyjątkiem 3-MMC i 4-MMC uzyskano stosując poniższy profil elucji gradientowej: 0-1 min (95% A, 5% B), 1-15 min (gradient liniowy do 5% A), 15-21 min (5% A, 95% B), 21-27 min (gradient liniowy do 95% A), 27-30 min (95% A, 5% B).

Kolejnym etapem prac było dobranie warunków ekstrakcji analitów z próbek włosów. Modyfikowano wiele parametrów w metodzie przygotowania próbki. Począwszy od sposobu obmycia próbki uwzględniając zarówno rozpuszczalnik używany do mycia jak i jego objętość i krotność przemyć poprzez sposób suszenia próbki, metodę proszkowania próbki, naważkę używaną do ekstrakcji, rodzaju rozpuszczalnika użytego do ekstrakcji czy też wymrażania próbki w trakcie procesu jej przygotowania. Aby przygotować próbkę włosów do analizy 1 cm włosów umieszczono w strzykawce o objętości 5 ml i trzykrotnie przemywano przy użyciu dichlorometanu. Strzykawkę zabezpieczono filtrem nieprzepuszczalnym dla włosów, wymieszano i pozostawiono do wysuszenia. Wysuszoną próbkę sproszkowano (5 min, 15 000 rpm). Do próbówki Eppendorfa odważono 20 mg sproszkowanej próbki dodano 20µl wzorca wewnętrznego (atrazyny) o stężeniu 2500 ng/ml i 0,5 ml metanolu. Tak przygotowaną próbkę wytrząsano przez 1h w temperaturze 21°C i 12 000 rpm. Następnie próbkę umieszczono w zamrażarce na 10 min. Kolejnym krokiem było odwirowanie próbki (5 min, 2000 rpm). Z tak przygotowanego ekstraktu pobrano 50 µl i dodano 450 µl fazy ruchomej A:B (90:10, v/v), przeniesiono do koszyczka z filtrem i wymieszano. Próbkę ponownie umieszczono w zamrażarce na 10 min i odwirowano (3 min 10 000 rpm). Z tak przygotowanej próbki pobrano 200 µl do fiolki o zmniejszonej objętości i poddano analizie za pomocą LC-MS/MS.

Opracowaną metodę analityczną poddałam procesowi walidacji zgodnie z wytycznymi SWGTOX [78]. Linowość sprawdzono poprzez analizę 6 powtórzeń krzywej wzorcowej przygotowanej w matrycy w stężeniach w zakresie od 0,025 do 1,250 ng/mg dla kannabinoidów, od 0,125 do 5 ng/mg dla pozostałych grup analitów. Ponadto w każdej serii analizowano próbkę ślepą (matrycę) i matrycę z wzorcem wewnętrznym. Krzywe kalibracyjne były liniowe w zakresie od 0,025 do 1,25 ng/mg dla kannabinoidów i 0,125 do 5 ng/mg dla pozostałych analitów. Współczynniki korelacji obliczone dla każdego analitu wynosiły ≥0,99.Aby wyznaczyć precyzję i BIAS analizowano sześciokrotnie trzy poziomy stężeń analitów (0,025 ng/mg; 0,125 ng/mg i 1,25 ng/mg dla kannabinoidów i 0,,125 ng/mg; 1,25 ng/mg i 5 ng/mg dla pozostałych analitów). Dla powyższych parametrów przyjęto zgodnie

z wytycznymi granicę ±20%. Wyznaczono odzyski, które mieściły się w zakresie od 80 do 120%. Za LOQ przyjęto najniższy punkt na krzywej wzorcowej, odpowiadający stosunkowi S/N ≥10. Do weryfikacji powtarzalności metody przystąpiono do anlizy próbek z badań biegłości. Opracowaną metodykę poddano badaniom biegłości, co pozwoliło na zasosowanie jej w rutynowych analizach w Instytucie Genetyki Sądowej w Bydgoszczy.

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ANALYTICAL TOXICOLOGY

One-step extraction and determination of 513 psychoactive substances, drugs, and their metabolites from hair by LC–MS/MS

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Abstract
The emergence of new psychoactive substances on the market is a significant problem on a global scale. This type of substance in society is associated with many negative consequences, such as traffic accidents, accidents at work, rape, homicide, poisoning, or overdose deaths. The analysis of these substances in biological samples is very important for further legal action and saving lives. Therefore, laboratories face a tremendous challenge in tackling the evolving drug market. The paper describes the optimization of the analytical LC–MS/MS method to identify and determine 513 psychoactive substances in hair samples. A method of chromatographic separation was developed, and the working parameters of the mass spectrometer were selected for each analyte. The method has been validated, and the results are as follows: the limit of quantification of the developed method ranges from 0.025 to 1.25 ng/mg hair. The mean recovery of the tested analytes ranges from 80 to 120%. The achieved coefficient of variation in within-run precision ranged from 1.05 to 19.99%. The results achieved for BIAS are in the range of ± 20%.

Keywords New psychoactive substances (NPS) · Drugs · Metabolites · Hair analysis · Liquid chromatography-tandem mass spectrometry (LC–MS/MS)

Introduction

Every year we observe an increase in interest in psychoactive substances, and new psychoactive substances (NPS) appear more and more often. They are considered a legal alternative to alcohol or popular illegal drugs such as amphetamines, cocaine, and MDMA. In the World Drug Report 2017 of the United Nations Office on Drugs and Crime (UNODC), 729 NPS were reported in 2009–2016 (World Drug Report 2017). Most of them belong to the group of synthetic cathinones or synthetic cannabinoids (World Drug Report 2017). These substances are chemically similar to the natural compounds corresponding to these groups; this makes them difficult to identify and they often remain undetected during routine analyses. The spread of these substances on the market is associated with health and life-threatening effects. Laboratories are constantly developing new methods of analyzing such substances in samples of saliva, urine, blood, or plasma of people suspected of taking drugs. However, such samples are not always collected in good time after the event. They are often given to another person for the purpose of committing a crime. These are difficult to detect because, by the time the person who has been given the illegal substance realizes it and reports for testing, it can no longer be detected even though it has been taken.

An alternative to these standard matrices are hair samples. Hair grows on average 0.35 mm/day or 1–1.5 cm/month, depending on anatomical location, race, sex, and age (Rivier 2000), so the portion of a hair located 3 cm from the scalp was formed by cells in a hair follicle about three months earlier. Thus it is likely that the substance introduced into the hair will appear 3 cm from the scalp three months after the substance was taken (Rivier 2000). There are two known ways to incorporate a substance/

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drug into the hair. These are (1) adsorption from the external environment to and into the developed hair shaft, and (2) transport to the growing hair shaft through the blood supply to the hair follicle (Rivier 2000). Both drugs and psychoactive substances accumulate in the hair, making it possible to detect them long after the event. Depending on the length of the hair, a retrospective analysis up to several months back from the date of sample collection can be carried out. It is also possible to determine whether the substance has been taken once or repeatedly/regularly, which is essential particularly if the use of psychoactive substances was related to crime or criminal behavior. The advantages of this matrix also include non-invasive sampling. Moreover, both non-metabolized substances and metabolites produced in the organism are accumulated (Moffat et al. 2011). Testing hair is often the only way to determine metabolites derived from synthetic cannabinoids. Studies (Sobolevsky et al. 2010; Grigoryev et al. 2011, 2013; Adamowicz et al. 2013; Kavanagh et al. 2013) observed that some substances in this group are metabolized at a high rate, which results in the absence of a parent analyte in the urine.

Despite the enormous potential of this matrix, there are few studies on NPS analysis in hair samples (Gottardo et al. 2014; Salomone et al. 2014; Hutter et al. 2012; Rust et al. 2012; Martin et al. 2012, 2015; Wyman et al. 2013; Strano-Rossi et al. 2014; Lee et al. 2011; Marsh et al. 2014). Two of these studies attempted to determine synthetic cannabinoids by incubating a hair sample in concentrated sodium hydroxide to remove keratin (Gottardo et al. 2014; Salomone et al. 2014). For the extraction, the authors used hexane/ethyl acetate 90:10 (v/v), and the obtained organic phase was evaporated to dryness under a stream of nitrogen. The sample was then reconstituted in methanol and analyzed by liquid chromatography coupled to mass spectrometry. The downside of this method is the need for additional extraction, which extends the analysis time and increases the risk of analyte loss. Hutter et al. (2012) also determined synthetic cannabinoids in the hair by liquid chromatography coupled with mass spectrometry (LC–MS/MS). However, they used ethanol for the extraction. The sample was then evaporated to dryness and reconstituted in mobile phase 50:50 (v/v). A two-step extraction method was presented by Rust et al. (2012). In the first stage, they used methanol with ultrasonication, and in the second, methanol was acidified with hydrochloric acid. Then, as in the previous work, the sample was evaporated to dryness and analyzed by LC–MS/MS. Another study (Lee et al. 2011) analyzed benzodiazepines with solid-phase extraction (SPE); gas chromatography with mass spectrometry (GC–MS) was used for the determination. Gas chromatography was also applied in the study on the analysis of mephedrone in hair samples (Martin et al. 2012). SPE was also used to extract psilocin, bufetenine and LSD (Martin et al. 2015).

This variety of extraction methods emphasizes how complex matrix the hair is. The analysis of hair samples is an enormous challenge and, at the same time, great hope for the work of toxicologists. This study aimed to develop an analytical method that allows quick yet sensitive and specific hair sample analysis for drugs and psychoactive substances, including NPS and their metabolites. The developed method is characterized by a rapid, single-step extraction of a wide range (513) of analytes, which are determined by LC–MS/MS operating in the MRM mode. This method was developed to enable the fight against drug crime and addictions and aid research on detecting this type of substance in specific social groups such as drivers or students.

Reagents and materials

The certified analytical standards of analyzed substances were purchased from Cayman Chemical, CHIRON, Lipomed Services to Health, and LGC Standards. To prepare samples and standard stock solutions, acetonitrile (ACN) for LC–MS, methanol (MeOH) for LC–MS, and formic acid for LC–MS, and dichloromethane were purchased from S. WITKO CHS, and ammonium formate for LC–MS was purchased from Sigma Aldrich. Working solutions were prepared by dilution of stock solution.

Calibration curve in matrix procedure

A section of hair (2 × 1 cm) without test analytes was collected into two 5 mL syringes. The hair was washed three times with 3 mL of dichloromethane. A syringe protected with a hair-impermeable filter was shaken, and the hair was then allowed to dry. The dried hair was pulverized (5 min; 15,000 rpm). 20 mg of the powdered hair was weighed into an Eppendorf tube; then 0.5 mL of methanol was added to it. The sample prepared in this way was shaken for 1 h at 21 °C and 12,000 rpm. During the next step, the sample was placed in the freezer for 10 min, followed by centrifugation at 5 min and 2000 rpm. Ten µL of the internal standard (atrazine) at a concentration of 500 ng/mL, 50 µL of the mix of standards at the appropriate concentration (at six different concentration levels in the range 0.025–5 ng/mg), 50 µL of hair extract, and 390 µL of mobile phase A: B (90:10, v/v) were transferred to the filter basket and mixed by hand. The mixed sample was placed back in the freezer for 10 min and centrifuged for 3 min and 10,000 rpm. 200 µL of thus obtained extract was withdrawn into a reduced volume vial.

Modification of the extraction method from hair samples

Many different parameters have been tested to develop a method of isolating psychoactive substances, drugs and their metabolites from hair samples. We were starting from the washing stage and ending with the filtration stage. The solvents used to wash the hair samples were verified, dichloromethane, dichloromethane and ethyl alcohol were checked. More favorable results are obtained when using only dichloromethane. In the next stage, the volume of this solvent used for washing and the number of repetitions was checked. In this case, washing was considered best three times with 3 ml of dichloromethane. The next stage that underwent modifications was drying the hair samples. Two options for drying the samples were tested. The first was sewing on tissue paper, and the second was drying with the use of an airtight dryer. In this case, lower losses of analytes were obtained for spontaneous drying on blotting paper. During the sample powdering stage, the amount of sample subjected to powdering and the number and size of the beads used for powdering were verified. The best results were obtained for a dose of about 20 mg and the use of one powdering ball with a diameter of 25 mm. In the next step, two extraction solvents were checked. It was methanol and acetonitrile. The use of acetonitrile did not contribute to the obtaining of better analysis results, and therefore, due to the harmfulness of the waste and the price of solvents, methanol was selected for further analysis. The tests also checked for re-freezing before the last centrifugation. However, the results showed that this freezing had no effect on the percent recovery of the analyte from the sample, so it was removed from the procedure.

Hair sample preparation procedure

A section of hair removed from a tested person (1 cm) was placed in a syringe with a volume of 5 mL. The hair was washed three times with 3 mL of dichloromethane. A syringe protected with a hair-impermeable filter was shaken, and the hair was then allowed to dry. The dried hair was pulverized (5 min; 15,000 rpm). 20 mg of the powdered hair was weighed into an Eppendorf tube. Then 20 µL of the internal standard (atrazine) at a concentration of 2500 ng/mL and 0.5 mL of methanol were added to the Eppendorf. The sample prepared in this way was shaken for 1 h at 21 °C and 12,000 rpm. The sample was placed in the freezer for 10 min, followed by centrifugation at 5 min and 2000 rpm in the next step. Fifty µL of hair extract and 450 µL of mobile phase A: B (90:10, v/v) were transferred to a filter basket and mixed by hand. The mixed sample was placed back in the freezer for 10 min and centrifuged for 3 min and 10,000 rpm. 200 µL of thus obtained extract was withdrawn into a reduced volume vial.

Chromatographic separation

Chromatographic separation was achieved by gradient elution on the liquid chromatography system consisted of an ExionLC AC Pump 2x, ExionLC Degaser, Exion AC Autosampler, and ExionLC Column Oven from AB SCIEX. Separation was carried out on a Kinetex C18 column (Phenomenex, 3.0 × 100 mm; 2.6 µm). A 20 µL sample was injected into the system at a flow rate of 0.5 mL/min. The gradient LC system was operated using ammonium formate 2 mM with 0.1% formic acid (mobile phase A) and 2 mM ammonium formate in MeOH with 0.1 formic acid (mobile phase B).

Optimum gradient elution for separation on chromatographic column was performed: 0–1 min (95% A, 5% B), 1–15 min (linear gradient to 5% A), 15–21 min (5% A, 95% B), 21–27 min (linear gradient to 95% A), 27–30 min (95% A, 5% B). Acetonitrile (ACN) was also checked in mobile phase B. The obtained results were not more favorable. The costs of the analyses were higher, and the waste generated during the analyses was more harmful. The influence of ammonium formate concentration on the results of the analyses was also checked. Values from 2 to 5 mM were checked. Increasing the ammonium formate concentration did not improve the separation of the analytes on the chromatography column. The optimized separation conditions of the analytes on the Kinetex C18 column (Phenomenex, 3.0 × 100 mm; 2.6 µm) were also checked on the other two columns Kinetex Biphenyl (Phenomenex, 3.0 × 100 mm; 2.6 µm) and Kinetex Phenyl-Hexyl (Phenomenex, 3.0 × 100 mm; 2.6 µm). The best results were obtained for the first column, and it was selected for further analysis. This gradient method allowed for the separation of all compounds except 3-MMC and 4-MMC in a 30 min run time. The retention times of all compounds were from 1.34 to 16.76 min and are presented in electronic supplementary material Table S1. The chromatogram obtained for the selected column and gradient is shown in electronic supplementary material Figure S1.

Mass spectrometric detection

The analysis was performed on the mass spectrometer AB SCIEX 5500 QTRAP with electrospray ionization in the positive mode. Data acquisition, data handling and instrument control were performed by Analyst 1.6.3 and

MultiQuant 3.0.3 software. Analytes were quantified in the double ion monitoring (MRM) mode. The spectrometric analysis parameters were optimized, and two MRM pairs were selected for each analyte according to the mass spectrometry standards. All results were based on the peak area ratio between the drug and the analytical standard. The MS conditions were set as followed: CUR: 30, CAD: medium, TEM: 400, GS1: 40, GS2: 70, dwell time ≥ 5 ms.

Analytical standards of all analyzed substances were subjected to individual optimization to select the best parameters of the mass spectrometer for each of them. Analyst 1.6.3 was used for this optimization. The conducted analyzes allowed for selecting parameters such as the ionization mode, Q1, Q3, declustering potential (DP), entrance potential (EP), collision energy (CE), collision cell exit potential (CXP). The positive ionization mode turned out to be better for the tested substances. The entrance potential (EP) for all analytes is 10. The MRM pairs and values DP, CE, CXP for each analyte have been collected in electronic supplementary material Table S1. In the developed method, MRM transitions for 517 analytes (two transitions for each analyte) were monitored only in specific detection windows that were defined on ± 0.5 min from the expected retention time.

Validation parameters

This presented analytical method was validated according to the SWGTOX validation guidelines (Scientific Working Group for Forensic Toxicology 2013). Fortification of hair samples was performed by adding 20 µL of the standard mix with a concentration of 200 ng/mL (corresponding to a concentration of 0.2 ng/mg hair to the matrix together with 0.5 mL of methanol. A blank sample was prepared by adding to the basket 10 µL of atrazine at a 500 ng/mL concentration, 50 µL of the obtained hair extract containing no test analytes, and 440 µL of the mixture of mobile phases A: B (90:10, v/v). The following steps were performed according to the hair sample preparation procedure.

Linearity validation was performed by analyzing six separate calibration curves in the matrix with concentrations ranging from 0.025 to 1.250 ng/mg for cannabinoids and from 0.125 to 5 ng/mg for other analytes. A blank matrix and blank matrix containing only internal standards were analyzed with each batch but not included in the calibration curves. Linearity was described using a weighted linear regression plot of peak area ratio (PAR) vs. spiked analyte concentration. Calibration curves in the matrix were linear in the range of 0.025–1.25 ng/mg for cannabinoids and 0.125–5 ng/mg for other analytes. Correlation coefficients (R^2) calculated for each analyte were ≥ 0.99. The calibration curve prepared in the matrix allowed eliminating the influence of the matrix effect in the actual samples.

To evaluate the precision and BIAS for our method, six replicates of calibration standards for three different concentrations from the calibration scale (0.025 ng/mg; 0.125 ng/mg, and 1.25 ng/mg for cannabinoids) and (0.125 ng/mg; 1.25 ng/mg and 5 ng/mg for other analytes) were used. For these parameters, an accuracy limit of ± 20% was used. The six repetitions were also used to determine the mean recovery. Accuracy was expressed as the average percentage recovery, and resulting values ranged from 80 to 120%.

According to the recommendations in the SWGTOX guideline (Scientific Working Group for Forensic Toxicology 2013), precision was evaluated by CV.

The determined CV for the tested analytes ranged from 1.05 to 19.99%, and BIAS ranged from − 20.00% to 20.00%. For precision and BIAS accuracy limit of ± 20% was used. The results of precision, BIAS, and recovery values for validated compounds are presented in electronic supplementary material Table S2.

The LOQ was determined to be the lowest calibration standard exhibited as S/N ratio ≥ 10. Proficiency tests were used to check the reproducibility of the analytical method. The estimated values of LOQ were from 0.025 to 1.25 ng/mg for 465 compounds, and the value was 0.5 ng/mL for other compounds. The LOQ values for each analyte are presented in electronic supplementary material Table S2.

Selectivity and specificity were assessed by spiking fortified samples with each analyte in a small mix to test for any interference. Hair without analytes was used to identify matrix interferences. It was possible to separate the isomers within the run time by gradient liquid chromatography. To verify the matrix effect, a standard curve in the matrix was used. The obtained points of the standard curve take into account the influence of the matrix on the analysis of actual samples. The mass spectrometer used enables the identification of the molecules of interest with high selectivity and specificity. Figure 1 shows the peaks obtained for several analytes (JWH-081, MN-18, 5F-APICA, JWH-182, 6-MAM, Codeine, Phenazepam, Lorazepam, Methadone, EDDP) included in the standard mixture. The gradient used ensures narrow peaks of the primary product ions for the defined retention time without any interference. The method was found to be selective for the tested compounds. The only exceptions are 3-MMC and 4-MMC, which do not separate on analysis. No interfering peaks were observed in the drug-free hair samples.

To check the stability, analyses of archival samples were performed. Four of the validated compounds did not meet the above criteria. The remaining 513 were included in the routine analysis of hair samples in our laboratory.

The developed method was verified by proficiency tests carried out by LGC Standards. During proficiency tests performed a quantitative analysis of two samples. In the first sample, the analyzed substances were Phenazepam,

Morphine, 6MAM, and Codeine. In the second sample, however, these were Methadone, EDDP, Methamphetamine, and Lorazepam. The obtained results met the criteria of proficiency tests.

Conclusions

The developed analytical method allowed us to introduce the analysis of hair samples to routine analyses in our laboratory. Use of methanol in the extraction process brought satisfactory results. With this procedure, we are able isolate as many as 513 psychoactive substances from hair samples. The performed validation has passed international proficiency tests. Due to the expected or required concentration levels in real samples, the method was developed with a division into one for synthetic cannabinoids with a lower LOQ and the other for analytes with a higher LOQ. Several of the analyzed substances did not meet the imposed validation requirements (FUB-PB-22, 2C-D, Oxymorphone, Stanozolol). This can be due to both the extraction process and the chromatographic separation method. Substances that did not meet the requirements were not included in the routine analyses, but the number

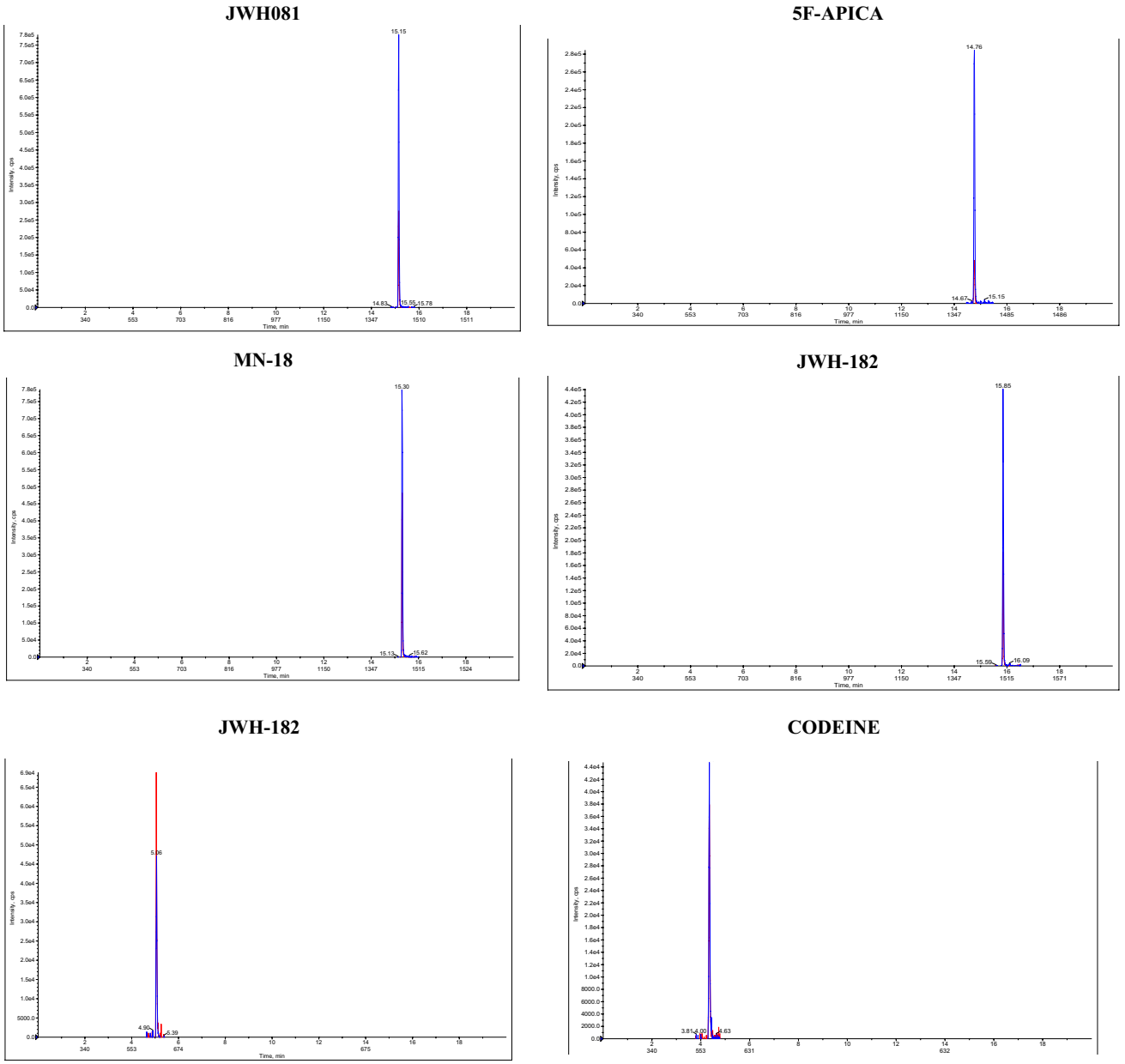

Fig. 1 Peaks obtained for several analytes included in the standard mixture

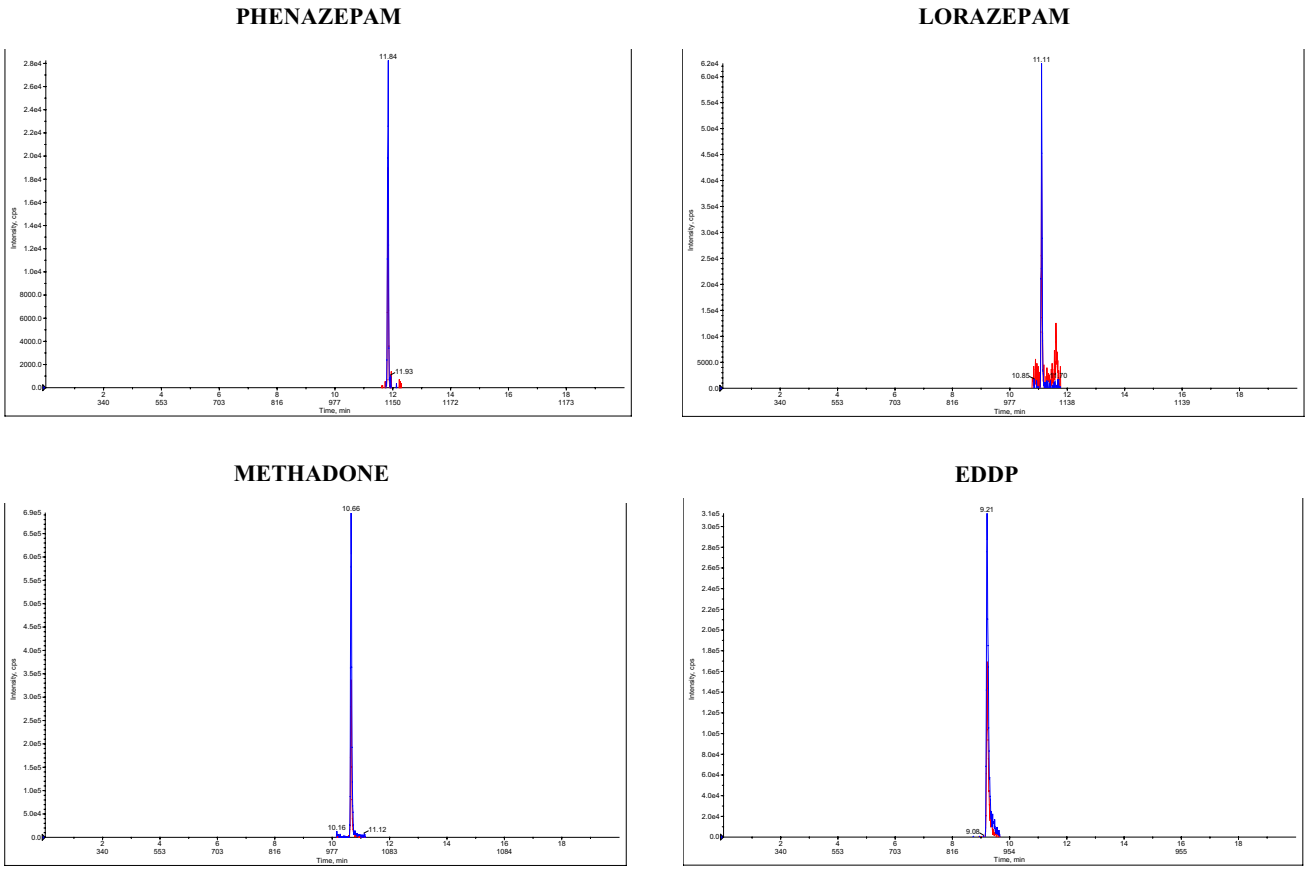

Fig. 1 (continued)

of substances that can be detected with the new method is large enough to meet the current needs. However, it is essential to refine the method so that substances that have not been validated can be determined with the modified method. The method can be developed further to cover new psychoactive substances as they appear on the market. Analyzing hair samples is an excellent alternative to the commonly used matrices such as blood or urine, particularly as it also enables retrospective analyses.

Supplementary Information The online version contains supplementary material available at https://doi.org/10.1007/s00204-022-03343-w.

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Data availability The data that support the findings of this study are available on request from the corresponding author.

Declarations

Conflict of interest All authors have given approval to the final version of the manuscript. The authors declare no competing interests.

References

Adamowicz P, Zuba D, Sekuła K (2013) Analysis of UR-144 and its pyrolysis product in blood and their metabolites in urine. Forensic Sci Int 233:320–327. https://doi.org/10.1016/j.forsciint.2013.10.005

Gottardo R, Sorio D, Musile G et al (2014) Screening for synthetic cannabinoids in hair by using LC-QTOFMS: a new and powerful approach to study the penetration of these new psychoactive substances in the population. Med Sci Law 54:22–27. https://doi.org/10.1177/0025802413477396

Grigoryev A, Melnik A, Savchuk S et al (2011) Gas and liquid chromatography-mass spectrometry studies on the metabolism of the synthetic phenylacetylindole cannabimimetic JWH-250, the psychoactive component of smoking mixtures. J Chromatogr B Anal Technol Biomed Life Sci 879:2519–2526. https://doi.org/10.1016/j.jchromb.2011.07.004

Grigoryev A, Kavanagh P, Melnik A (2013) The detection of the urinary metabolites of 1-[(5-fluoropentyl)-1H-indol-3-yl]-(2-iodophenyl) methanone (AM-694), a high affinity cannabimimetic, by gas chromatography - mass spectrometry. Drug Test Anal 5:110–115. https://doi.org/10.1002/dta.1336

Hutter M, Kneisel S, Auwärter V et al (2012) Determination of 22 synthetic cannabinoids in human hair by liquid chromatography-tandem mass spectrometry. J Chromatogr B Anal Technol Biomed Life Sci 903:95–101. https://doi.org/10.1016/j.jchromb.2012.07.002

Kavanagh P, Grigoryev A, Melnik A et al (2013) Detection and tentative identification of urinary phase I metabolites of phenylacetylindole cannabimimetics JWH-203 and JWH-251, by GC-MS and LC-MS/MS. J Chromatogr B Anal Technol Biomed Life Sci 934:102–108. https://doi.org/10.1016/j.jchromb.2013.07.005

Lee S, Han E, In S et al (2011) Determination of illegally abused sedative-hypnotics in hair samples from drug offenders. J Anal Toxicol 35:312–315. https://doi.org/10.1093/anatox/35.5.312

Marsh CM, Crawley LR, Himes SK et al (2014) Discovery of Syn-/Anti-cocaine-N-oxide diastereomers in unwashed postmortem hair via LC-MS-MS. J Anal Toxicol 38:360–367. https://doi.org/10.1093/jat/bku041

Martin M, Muller JF, Turner K et al (2012) Evidence of mephedrone chronic abuse through hair analysis using GC/MS. Forensic Sci Int 218:44–48. https://doi.org/10.1016/j.forsciint.2011.10.016

Martin R, Schürenkamp J, Gasse A et al (2015) Analysis of psilocin, bufotenine and LSD in hair. J Anal Toxicol 39:126–129. https://doi.org/10.1093/jat/bku141

Moffat A, Osselton D, Widdop B (2011) Clark's analysis of drugs and poisons in pharmaceuticals, body fluids and postmortem material. Pharmaceutical Press, London, pp 243–257

Rivier L (2000) Techniques for analytical testing of unconventional samples. Baillieres Clin Endocrinol Metab 14:147–165. https://doi.org/10.1053/beem.2000.0060

Rust KY, Baumgartner MR, Dally AM et al (2012) Prevalence of new psychoactive substances: a retrospective study in hair. Drug Test Anal 4:402–408. https://doi.org/10.1002/dta.1338

Salomone A, Luciano C, di Corcia D et al (2014) Hair analysis as a tool to evaluate the prevalence of synthetic cannabinoids in different populations of drug consumers. Drug Test Anal 6:126–134. https://doi.org/10.1002/dta.1556

Scientific Working Group for Forensic Toxicology (SWGTOX) (2013) Standard practices for method validation in forensic toxicology. J Anal Toxicol 37:452–474. https://doi.org/10.1093/jat/bkt054

Sobolevsky T, Prasolov I, Rodchenkov G (2010) Detection of JWH-018 metabolites in smoking mixture post-administration urine. Forensic Sci Int 200(1–3):141–147. https://doi.org/10.1016/j.forsciint.2010.04.003

Strano-Rossi S, Odoardi S, Fisichella M et al (2014) Screening for new psychoactive substances in hair by ultrahigh performance liquid chromatography-electrospray ionization tandem mass spectrometry. J Chromatogr A 1372:145–156. https://doi.org/10.1016/j.chroma.2014.10.106

United Nations Office on Drugs and Crime (2017) World Drug Report 2017 (ISBN:978-92-1-148291-1,eISBN: 078-92-1-0060623-3, United Nations publication, Sales No. E.17.XI.6)

Wyman JF, Lavins ES, Engelhart D et al (2013) Postmortem tissue distribution of MDPV following lethal intoxication by "bath salts." J Anal Toxicol 37:182–185. https://doi.org/10.1093/jat/bkt001

Electronic Supplementary Materials

for

One-step extraction and determination of 513 psychoactive substances, drugs, and their metabolites from hair by LC-MS/MS

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Table S1. Summary of operating parameters LC-MS/MS for identification of analytes, where: Q1 – precursor ion, Q3 – product ion, $\mathbf{t_R}$ - retention time, DP - declustering potential, CE – collision energy, CXP - collision cell exit potential**.**

Q1 $[M-H]^+$ (m/z)	**Q3 (m/z)**	**t_R (min)**	**Analyte**	**DP (V)**	**CE (V)**	**CXP (V)**
193.263	120.1	5.30	1-(2-METHOXYPHENYL)PIPERAZINE 1	106	43	8
193.263	150.1	5.30	1-(2-METHOXYPHENYL)PIPERAZINE 2	106	25	18
231.278	188	7.95	1-(3-TRIFLUOROMETHYLPHENYL)PIPERAZINE (TFMPP) 1	141	31	22
231.278	118	7.95	1-(3-TRIFLUOROMETHYLPHENYL)PIPERAZINE (TFMPP) 2	141	51	16
197.469	119.1	6.67	1-(4-CHLOROPHENYL)PIPERAZINE (pCPP) 1	121	33	14
197.469	118.1	6.67	1-(4-CHLOROPHENYL)PIPERAZINE (pCPP) 2	121	45	16
181.26	138.1	4.69	1-(4-FLUOROPHENYL)PIPERAZINE (FPP) 1	106	27	16
181.26	74	4.69	1-(4-FLUOROPHENYL)PIPERAZINE (FPP) 2	106	103	12
267.107	91	7.73	1.4-DIBENZYLPIPERAZINE (DBZP) 1	111	47	12
267.107	65.1	7.73	1.4-DIBENZYLPIPERAZINE (DBZP) 2	111	91	10
134.019	117.1	4.09	1-AMINOINDAN 1	56	15	14
134.019	115.1	4.09	1-AMINOINDAN 2	56	33	14
191.061	91	3.20	1-METHYL-4-BENZYLPIPERAZINE (MBZP) 1	86	31	12
191.061	65	3.20	1-METHYL-4-BENZYLPIPERAZINE (MBZP) 2	86	63	10
194.261	163	6.03	1-METHYLAMINO-1-(3.4-METHYLENEDIOXYPHENYL)PROPANE 1	61	13	22
194.261	105.1	6.03	1-METHYLAMINO-1-(3.4-METHYLENEDIOXYPHENYL)PROPANE 2	61	33	16
230.937	188	8.52	2.3-DICHLOROPHENYLPIPERAZINE (DCPP) 1	91	27	24
230.937	152	8.52	2.3-DICHLOROPHENYLPIPERAZINE (DCPP) 2	91	45	20
206.062	188.1	7.43	2.3-DIMETHYLETHCATHINONE (2.3-DMEC) 1	91	17	24
206.062	158.1	7.43	2.3-DIMETHYLETHCATHINONE (2.3-DMEC) 2	91	39	20
192.202	174	7.02	2.3-DIMETHYLMETHCATHINONE (2.3-DMMC) 1	66	17	20
192.202	159.1	7.02	2.3-DIMETHYLMETHCATHINONE (2.3-DMMC) 2	66	27	20
222.247	174.1	5.43	2.3-ETHYLONE ISOMER 1	86	23	8
222.247	146.1	5.43	2.3-ETHYLONE ISOMER 2	86	35	8
194.351	135	5.69	2.3-MDMA 1	91	25	18
194.351	77	5.69	2.3-MDMA 2	91	53	12
276.236	135	7.57	2.3-MDPV 1	91	31	16
276.236	126.1	7.57	2.3-MDPV 2	91	37	14
226.297	209.1	6.18	2.4.5-TRIMETHOXYAMPHETAMINE 1	76	15	10
226.297	179.1	6.18	2.4.5-TRIMETHOXYAMPHETAMINE 2	76	35	10
192.19	174.1	7.46	2.4-DIMETHYLMETHCATHINONE (2.4-DMMC) 1	76	17	20
192.19	159	7.46	2.4-DIMETHYLMETHCATHINONE (2.4-DMMC) 2	76	27	18
206.063	188.1	7.92	2.4-DMEC 1	41	17	12
206.063	158.1	7.92	2.4-DMEC 2	41	47	20
210.264	151.1	6.71	2.5-DMMA 1	56	23	20
210.264	121.1	6.71	2.5-DMMA 2	56	35	16
368.124	243	10.15	25B-NBF 1	106	27	12
370.116	245	10.15	25B-NBF 2	131	27	12
324.164	199	9.89	25C-NBF 1	111	25	10

324.164	184	9.89	25C-NBF 2	111	37	10
322.138	199	9.72	25C-NBOH 1	101	27	24
322.138	77	9.72	25C-NBOH 2	101	85	12
336.16	121.1	10.25	25C-NBOMe 1	96	25	14
336.16	91.1	10.25	25C-NBOMe 2	96	59	12
316.169	91	10.44	25D-NBOMe 1	81	57	12
316.169	121	10.44	25D-NBOMe 2	81	25	16
330.231	91	11.26	25E-NBOMe 1	106	61	12
330.231	121.1	11.26	25E-NBOMe 2	106	27	16
330.142	91	11.04	25G-NBOMe 1	81	61	12
330.142	121.1	11.04	25G-NBOMe 2	81	27	14
302.346	91	9.40	25H-NBOMe 1	81	55	12
302.346	121.1	9.40	25H-NBOMe 2	81	23	18
428.183	91	10.88	25-I-NB2OMe 1	121	75	12
428.183	121	10.88	25-I-NB2OMe 2	121	27	16
428.176	121.1	10.82	25I-NB3OMe 1	131	33	14
428.176	91.1	10.82	25I-NB3OMe 2	131	75	12
428.177	121.1	10.75	25I-NB4OMe 1	91	21	16
428.177	78	10.75	25I-NB4OMe 2	91	113	10
416.016	290.8	10.58	25I-NBF 1	121	29	12
416.016	276	10.58	25I-NBF 2	121	43	14
442.154	135.1	10.71	25I-NBMD 1	116	31	16
442.154	77	10.71	25I-NBMD 2	116	93	12
414.121	291	10.42	25I-NBOH 1	101	31	12
414.121	307.9	10.42	25I-NBOH 2	101	23	14
347.2	91	9.05	25N-NBOMe 1	86	59	12
347.2	121.1	9.05	25N-NBOMe 2	86	23	16
362.264	91	10.77	25T2-NBOMe 1	121	59	10
362.264	121.1	10.77	25T2-NBOMe 2	121	27	14
348.035	91.1	10.05	25T-NBOMe 1	96	63	14
348.035	121.1	10.05	25T-NBOMe 2	96	27	16
150.209	91	6.08	2-AMINO-1-PHENYLBUTANE 1	61	23	12
150.209	65	6.08	2-AMINO-1-PHENYLBUTANE 2	61	49	10
134.257	117.1	3.87	2-AMINOINDANE 1	51	19	14
134.257	115.1	3.87	2-AMINOINDANE 2	51	33	14
214.186	169	7.04	2-BROMOAMPHETAMINE 1	61	27	8
216.192	170.9	7.04	2-BROMOAMPHETAMINE 2	56	27	20
228.188	169	7.10	2-BROMOMETHAMPHETAMINE 1	71	29	20
230.177	171	7.10	2-BROMOMETHAMPHETAMINE 2	71	27	10
259.957	243	7.70	2C-B 1	51	17	12
259.957	227.9	7.70	2C-B 2	51	29	10
283.976	267	7.99	2C-B_FLY 1	106	21	12
283.976	188.1	7.99	2C-B_FLY 2	106	33	24
216.441	199	7.28	2C-C 1	76	15	24
216.441	184	7.28	2C-C 2	76	27	22
195.583	179	7.50	2C-D 1	71	15	24

195.583	164.1	7.50	2C-D 2	71	25	20
210.052	178	8.54	2C-G 1	76	23	22
210.052	163	8.54	2C-G 2	76	37	20
170.196	125	6.56	2-CHLOROAMPHETAMINE 1	61	25	16
170.196	89	6.56	2-CHLOROAMPHETAMINE 2	61	51	14
307.947	291	8.39	2C-I 1	66	19	12
307.947	276	8.39	2C-I 2	66	31	12
224.065	207.1	10.09	2C-P 1	66	15	10
224.065	192.1	10.09	2C-P 2	66	25	24
256.022	239.1	9.58	2C-T-7 1	71	17	10
256.022	91.1	9.58	2C-T-7 2	71	63	12
250.269	233.1	8.67	2C-TFM 1	91	17	10
250.269	218	8.67	2C-TFM 2	91	29	12
196.255	148.1	4.67	2-FEC 1	76	41	18
196.255	135.1	4.67	2-FEC 2	76	37	10
168.199	123.1	3.17	2-FIC 1	61	21	14
168.199	103.1	3.17	2-FIC 2	61	33	14
154.13	109	5.10	2-FLUOROAMPHETAMINE 1	61	23	14
154.13	137.1	5.10	2-FLUOROAMPHETAMINE 2	61	13	16
168.247	109.1	5.35	2-FLUOROMETHAMPHETAMINE (2-FMA) 1	61	25	12
168.247	83.1	5.35	2-FLUOROMETHAMPHETAMINE (2-FMA) 2	61	53	12
182.187	164.1	4.02	2-FLUOROMETHCATHINONE (2-FMC) 1	81	19	22
182.187	149	4.02	2-FLUOROMETHCATHINONE (2-FMC) 2	81	29	16
262.178	216.9	7.76	2-IODOAMPHETAMINE 1	81	27	12
262.178	90	7.76	2-IODOAMPHETAMINE 2	81	47	12
190.239	58	7.05	2-MAPB 1	51	19	8
190.239	91.1	7.05	2-MAPB 2	51	47	14
194.219	176.1	5.30	2-MeOMC 1	61	17	10
194.219	161.1	5.30	2-MeOMC 2	61	27	16
152.214	120.1	4.95	2-METHOXY-2-PHENYLETHYLAMINE 1	61	15	14
152.214	77	4.95	2-METHOXY-2-PHENYLETHYLAMINE 2	61	45	12
166.068	121.1	6.16	2-METHOXYAMPHETAMINE (2-MA) 1	56	21	16
166.068	149	6.16	2-METHOXYAMPHETAMINE (2-MA) 2	56	13	18
180.322	120.9	6.34	2-METHOXYMETHAMPHETAMINE (2-MeOMA) 1	66	23	14
180.322	91.1	6.34	2-METHOXYMETHAMPHETAMINE (2-MeOMA) 2	66	39	8
164.237	91	6.20	2-METHYLAMINO-1-PHENYLBUTANE 1	71	25	14
164.237	65	6.20	2-METHYLAMINO-1-PHENYLBUTANE 2	71	55	8
178.06	160.1	5.73	2-METHYLMETHCATHINONE (2-MMC) 1	76	17	22
178.06	145.1	5.73	2-METHYLMETHCATHINONE (2-MMC) 2	76	27	18
232.265	105.1	7.34	2-METHYL-PBP 1	116	33	12
232.265	91	7.34	2-METHYL-PBP 2	116	53	12
218.291	98.1	6.47	2-METHYL-PPP 1	116	31	16
218.291	119.1	6.47	2-METHYL-PPP 2	116	31	8
303.454	84.1	9.94	3.4-DICHLOROMETHYLPHENIDATE (3.4-CTMP) 1	121	27	12
303.454	56	9.94	3.4-DICHLOROMETHYLPHENIDATE (3.4-CTMP) 2	121	77	8

292.246	151	7.44	3.4-DIMETHOXY-ALPHA-PVP 1	116	35	22
292.246	126.1	7.44	3.4-DIMETHOXY-ALPHA-PVP 2	116	33	12
192.031	174.1	7.32	3.4-DIMETHYLMETHCATHINONE (3.4-DMMC) 1	81	17	20
192.031	159.2	7.32	3.4-DIMETHYLMETHCATHINONE (3.4-DMMC) 2	81	27	18
206.146	158.1	7.74	3.4-DMEC 1	86	43	14
206.146	115.1	7.74	3.4-DMEC 2	86	67	6
210.063	179.1	5.21	3.4-DMMA 1	61	17	22
210.063	151.1	5.21	3.4-DMMA 2	61	29	20
208.248	177.1	5.61	3.4-EDMA 1	61	19	10
208.248	149.1	5.61	3.4-EDMA 2	61	29	20
222.191	204	5.23	3.4-EDMC 1	61	19	10
222.191	189.1	5.23	3.4-EDMC 2	61	29	10
194.025	163.1	5.27	3.4-MDMA (ECSTAZY) 1	76	17	20
194.025	105.1	5.27	3.4-MDMA (ECSTAZY) 2	76	33	14
222.051	163	6.74	3.4-MDPA 1	81	19	20
222.051	105.1	6.74	3.4-MDPA 2	81	35	14
290.285	135.1	8.66	3.4-MDPHP 1	131	35	16
290.285	140.2	8.66	3.4-MDPHP 2	131	35	18
276.144	126.1	7.50	3.4-METHYLENDIOXYPYROVALERONE 1	76	31	12
276.144	135.1	7.50	3.4-METHYLENDIOXYPYROVALERONE 2	76	41	8
318.23	135.1	10.83	3.4-METHYLENEDIOXY_PV9 1	166	35	8
318.23	168.2	10.83	3.4-METHYLENEDIOXY_PV9 2	166	39	20
396.257	181.1	9.73	30C-NBOMe 1	61	23	10
396.257	148.1	9.73	30C-NBOMe 2	61	59	18
214.192	168.9	7.31	3-BROMOAMPHETAMINE 1	46	25	20
216.189	171.1	7.31	3-BROMOAMPHETAMINE 2	66	25	14
228.18	169	7.38	3-BROMOMETHAMPHETAMINE 1	86	27	22
230.202	170.9	7.38	3-BROMOMETHAMPHETAMINE 2	66	27	20
244.143	145	6.64	3-BROMOMETHCATHINONE (3-BMC) 1	86	23	20
242.128	145.1	6.64	3-BROMOMETHCATHINONE (3-BMC) 2	96	25	22
383.161	239	15.28	3-CAF 1	101	19	12
383.161	210	15.28	3-CAF 2	101	65	24
298.069	280.9	8.54	3C-B-FLY 1	66	21	12
300.079	283	8.54	3C-B-FLY 2	46	17	16
170.206	125.1	6.83	3-CHLOROAMPHETAMINE 1	66	25	14
170.206	89	6.83	3-CHLOROAMPHETAMINE 2	66	53	12
198.231	145.1	5.95	3-CHLOROMETHCATHINONE (3-CMC) 1	76	25	18
198.231	144.1	5.95	3-CHLOROMETHCATHINONE (3-CMC) 2	76	41	18
197.249	154.1	6.78	3-CHLOROPHENYLPIPERAZINE (mCPP) 1	101	27	18
197.249	118.1	6.78	3-CHLOROPHENYLPIPERAZINE (mCPP) 2	101	47	14
254.286	195.1	8.42	3C-P 1	56	19	10
254.286	107.1	8.42	3C-P 2	56	35	14
274.249	126.1	7.99	3-DESOXY-3.4-MDPV 1	126	31	18
274.249	133.1	7.99	3-DESOXY-3.4-MDPV 2	126	37	16
192.22	174.1	7.45	3-ETHYLMETHCATHINONE (3-EMC) 1	66	17	22
192.22	144.1	7.45	3-ETHYLMETHCATHINONE (3-EMC) 2	66	43	18

196.262	135.1	4.96	3-FEC 1	81	39	18
196.262	148.1	4.96	3-FEC 2	81	41	18
222.28	123.1	5.30	3-FLUORO-ALFA-PPP 1	86	31	12
222.28	98.1	5.30	3-FLUORO-ALFA-PPP 2	86	33	14
154.134	109	5.10	3-FLUOROAMPHETAMINE 1	76	25	14
154.134	137.1	5.10	3-FLUOROAMPHETAMINE 2	76	13	16
168.223	109.1	5.35	3-FLUOROMETHAMPHETAMINE (3-FMA) 1	76	27	18
168.223	83.1	5.35	3-FLUOROMETHAMPHETAMINE (3-FMA) 2	76	53	10
182.014	164.1	4.38	3-FLUOROMETHCATHINONE (3-FMC) 1	81	19	20
182.014	149.1	4.38	3-FLUOROMETHCATHINONE (3-FMC) 2	81	27	18
331.895	286.9	9.11	3-HYDROXYBROMAZEPAM 1	106	27	12
331.895	314.9	9.11	3-HYDROXYBROMAZEPAM 2	106	21	14
330.031	238	10.15	3-HYDROXYFLUNITRAZEPAM 1	96	43	12
330.031	284	10.15	3-HYDROXYFLUNITRAZEPAM 2	96	27	12
262.179	217	8.06	3-IODOAMPHETAMINE 1	66	25	10
262.179	117.1	8.06	3-IODOAMPHETAMINE 2	66	43	14
192.185	144.2	6.44	3-MEC 1	86	39	16
192.185	91.1	6.44	3-MEC 2	86	47	14
194.225	161.1	5.30	3-MeOMC 1	81	25	20
194.225	118.1	5.30	3-MeOMC 2	81	47	12
166.07	121.1	5.59	3-METHOXYAMPHETAMINE (3-MA) 1	41	21	16
166.07	91	5.59	3-METHOXYAMPHETAMINE (3-MA) 2	41	37	14
274.19	86.1	8.92	3-METHOXYPHENCYCLIDINE 1	46	17	10
274.19	121.1	8.92	3-METHOXYPHENCYCLIDINE 2	46	37	14
178.046	160.1	5.92	3-METHYLMETHCATHINONE (3-MMC) 1	86	17	20
178.046	145.1	5.92	3-METHYLMETHCATHINONE (3-MMC) 2	86	27	18
232.266	105.1	7.47	3-METHYL-PBP 1	106	31	14
232.266	91	7.47	3-METHYL-PBP 2	106	55	12
218.209	119.3	6.64	3-METHYL-PPP 1	116	31	6
218.209	91	6.64	3-METHYL-PPP 2	116	49	8
191.255	148.1	7.31	4.4'-DMAR 1	61	17	18
191.255	91	7.31	4.4'-DMAR 2	61	39	12
275.216	86	6.36	4-AcO-DET 1	81	23	12
275.216	160	6.36	4-AcO-DET 2	81	35	20
247.314	58.1	5.45	4-AcO-DMT 1	81	21	6
247.314	160.1	5.45	4-AcO-DMT 2	81	33	16
261.3	72	5.92	4-AcO-MET 1	76	21	10
261.3	160	5.92	4-AcO-MET 2	76	35	22
176.148	131.1	6.67	4-APB 1	66	25	16
176.148	91	6.67	4-APB 2	66	39	12
178.238	161.1	5.56	4-APDB 1	71	13	22
178.238	133.1	5.56	4-APDB 2	71	25	16
288.233	257	8.31	4-BROMO-2.5-DMMA 1	61	19	12
290.24	259	8.31	4-BROMO-2.5-DMMA 2	56	19	12
214.182	169	7.44	4-BROMOAMPHETAMINE 1	76	25	20
216.181	170.9	7.44	4-BROMOAMPHETAMINE 2	56	25	22

228.205	168.9	7.52	4-BROMOMETHAMPHETAMINE 1	91	29	20
230.2	170.9	7.52	4-BROMOMETHAMPHETAMINE 2	91	27	20
243.495	145.1	6.64	4-BROMOMETHCATHINONE (BREFEDRONE) 1	101	23	18
243.495	144.1	6.64	4-BROMOMETHCATHINONE (BREFEDRONE) 2	101	45	18
184.174	125.1	7.98	4-CAB 1	46	25	16
184.174	89	7.98	4-CAB 2	46	57	14
212.21	159.3	6.65	4-CEC 1	66	25	8
212.21	144.1	6.65	4-CEC 2	66	39	18
238.267	139.1	6.85	4-CHLORO-ALPHA-PPP 1	111	33	16
238.267	98.1	6.85	4-CHLORO-ALPHA-PPP 2	111	33	12
266.3	125.1	8.93	4-CHLORO-ALPHA-PVP 1	101	33	10
266.3	126.1	8.93	4-CHLORO-ALPHA-PVP 2	101	37	18
170.197	125	6.93	4-CHLOROAMPHETAMINE 1	51	25	12
170.197	89	6.93	4-CHLOROAMPHETAMINE 2	51	53	12
198	145.1	6.15	4-CHLOROMETHCATHINONE (4-CMC) 1	76	25	18
198.008	144.1	6.15	4-CHLOROMETHCATHINONE (4-CMC) 2	71	41	18
184.235	125.1	7.05	4-CMA 1	81	29	14
184.235	89	7.05	4-CMA 2	81	57	12
204.264	131.1	7.34	4-EAPB 1	76	29	10
204.264	91	7.34	4-EAPB 2	76	45	12
206.207	133.2	7.50	4-ETHYL-N.N-DMC 1	61	27	14
206.207	105.2	7.50	4-ETHYL-N.N-DMC 2	61	35	18
196.26	148.1	4.97	4-FEC 1	71	41	18
196.26	135.1	4.97	4-FEC 2	71	37	16
196.234	149.1	5.73	4-FLUORO BUPHEDRONE 1	76	31	18
196.234	148.1	5.73	4-FLUORO BUPHEDRONE 2	76	47	18
210.264	109	7.20	4-FLUORO PENTEDRONE 1	86	33	14
210.264	74	7.20	4-FLUORO PENTEDRONE 2	86	111	10
278.165	109	10.00	4-FLUORO PV8 1	126	33	16
278.165	95.1	10.00	4-FLUORO PV8 2	126	71	12
292.257	109.1	11.02	4-FLUORO PV9 1	116	35	14
292.257	95	11.02	4-FLUORO PV9 2	116	71	14
222.267	123.1	5.30	4-FLUORO-ALFA-PPP 1	86	31	8
222.267	98.1	5.30	4-FLUORO-ALFA-PPP 2	86	33	14
168.214	109.1	5.34	4-FLUOROMETHAMPHETAMINE (4-FMA) 1	81	27	12
168.214	137	5.34	4-FLUOROMETHAMPHETAMINE (4-FMA) 2	81	15	18
182.011	164.1	4.37	4-FLUOROMETHCATHINONE (4-FMC) 1	71	19	22
182.011	149	4.37	4-FLUOROMETHCATHINONE (4-FMC) 2	71	29	20
250.25	109	7.55	4F-PVP 1	91	31	12
250.25	126.1	7.55	4F-PVP 2	91	35	16
262.005	161.1	6.30	4-HYDROXY DiPT 1	171	31	20
262.005	114.1	6.30	4-HYDROXY DiPT 2	171	21	14
341.932	325	8.80	4-HYDROXYMIDAZOLAM 1	121	31	14
341.932	297	8.80	4-HYDROXYMIDAZOLAM 2	121	41	14
262.177	245	8.19	4-IODOAMPHETAMINE 1	56	15	12
262.177	216.9	8.19	4-IODOAMPHETAMINE 2	56	27	12

190.254	131.1	6.84	4-MAPB 1	76	27	18
190.254	91	6.84	4-MAPB 2	76	41	10
220.297	144.1	8.56	4-MEAP 1	66	43	18
220.297	105.1	8.56	4-MEAP 2	66	29	12
262.212	121.1	8.02	4-MEO-ALPHA-PVP 1	91	33	12
262.212	191.2	8.02	4-MEO-ALPHA-PVP 2	91	25	18
248.282	112.1	6.90	4-MeOPBP 1	101	31	14
248.282	121.1	6.90	4-MeOPBP 2	101	37	16
274.176	121.1	8.92	4-METHOXY PHENCYCLIDINE 1	61	39	14
274.176	189.1	8.92	4-METHOXY PHENCYCLIDINE 2	61	17	10
290.295	121.1	10.17	4-METHOXY PV8 1	126	35	16
290.295	154.2	10.17	4-METHOXY PV8 2	126	33	8
304.286	121.1	11.12	4-METHOXY PV9 1	101	35	14
304.286	168.2	11.12	4-METHOXY PV9 2	101	35	8
180.289	149	5.58	4-METHOXYMETHAMPHETAMINE (PMMA) 1	66	15	20
180.289	121.1	5.58	4-METHOXYMETHAMPHETAMINE (PMMA) 2	66	27	14
206.274	144.1	8.28	4-METHYL PENTEDRONE 1	86	47	18
206.274	105.1	8.28	4-METHYL PENTEDRONE 2	86	29	14
206.11	188.3	7.43	4-METHYL-ALPHA-ETHYLAMINOBUTIOPHENONE 1	56	19	22
206.11	144.2	7.43	4-METHYL-ALPHA-ETHYLAMINOBUTIOPHENONE 2	56	43	10
150.227	105.1	6.68	4-METHYLAMPHETAMINE 1	56	23	16
150.227	133.1	6.68	4-METHYLAMPHETAMINE 2	56	11	8
164.232	146.1	5.65	4-METHYLCATHINONE 1	71	15	18
164.232	131	5.65	4-METHYLCATHINONE 2	71	27	16
164.25	105.1	6.82	4-METHYLMETHAMPHETAMINE (4-MMA) 1	66	25	14
164.25	133.1	6.82	4-METHYLMETHAMPHETAMINE (4-MMA) 2	66	15	16
178.066	160.1	5.92	4-METHYLMETHCATHINONE (4-MMC) 1	71	17	20
178.066	145.1	5.92	4-METHYLMETHCATHINONE (4-MMC) 2	71	27	18
192.249	119.1	6.01	4-METHYL-N.N-DMC 1	101	27	16
192.249	72.1	6.01	4-METHYL-N.N-DMC 2	101	33	12
206.209	105	7.07	4-METHYL-N-METHYLBUPHEDRONE 1	51	29	16
206.209	90.9	7.07	4-METHYL-N-METHYLBUPHEDRONE 2	51	47	12
220.287	144.1	9.42	4-METHYL-N-METHYLHEXANOPHENONE 1	86	47	16
220.287	105.1	9.42	4-METHYL-N-METHYLHEXANOPHENONE 2	86	29	14
232.31	105.1	7.47	4-METHYL-PBP 1	81	33	14
232.31	91	7.47	4-METHYL-PBP 2	81	55	12
260.347	105.1	9.62	4-METHYL-PHP 1	131	33	14
260.347	91.1	9.62	4-METHYL-PHP 2	131	63	10
203.04	144.1	8.36	4-METHYL-α-ETHYLTRYPTAMINE 1	56	29	20
203.04	186	8.36	4-METHYL-α-ETHYLTRYPTAMINE 2	56	13	24
176.082	44	6.98	5-APB 1	46	23	8
176.082	91	6.98	5-APB 2	46	47	10
178.29	161	5.56	5-APDB 1	56	13	22
178.29	133.1	5.56	5-APDB 2	56	27	18
176.173	159.2	8.71	5-APDI 1	71	13	22
176.173	131.2	8.71	5-APDI 2	71	27	10

365.216	320.1	12.99	5-CHLORO AB-PINACA 1	91	21	14
367.248	322.2	12.99	5-CHLORO AB-PINACA 2	86	21	14
391.226	247.9	14.09	5-CHLORO-NNEI 1	86	31	12
391.226	144.1	14.09	5-CHLORO-NNEI 2	86	55	8
204.961	132.1	7.09	5-EAPB 1	86	29	16
204.961	131.6	7.09	5-EAPB 2	86	29	16
348.07	232.1	12.10	5F-ABICA 1	71	29	12
348.07	144.1	12.10	5F-ABICA 2	71	53	18
349.193	233.1	12.23	5F-AB-PINACA 1	86	33	10
349.193	304.1	12.23	5F-AB-PINACA 2	86	21	14
378.193	233.1	14.03	5F-ADB (5F-MDMB-PINACA) 1	116	33	10
378.193	318.2	14.03	5F-ADB (5F-MDMB-PINACA) 2	116	23	14
364.092	233.1	13.50	5F-AMB (5F-AMB-PINACA) 1	101	31	10
364.092	304.2	13.50	5F-AMB (5F-AMB-PINACA) 2	101	21	14
383.14	135.1	15.01	5F-APICA (STS-135) 1	156	39	16
383.14	77	15.01	5F-APICA (STS-135) 2	156	119	12
384.207	135.1	15.46	5F-APINACA (AKB-48-5F) 1	106	29	16
384.207	77.1	15.46	5F-APINACA (AKB-48-5F) 2	106	121	12
368.294	135.1	15.30	5-F-JWH-018 ADAMANTYL ANALOG 1	171	39	10
368.294	77	15.30	5-F-JWH-018 ADAMANTYL ANALOG 2	171	113	12
375.043	232.1	13.54	5-FLUORO MN-24 (5-FLUORO NNEI) 1	111	31	10
375.043	144.1	13.54	5-FLUORO MN-24 (5-FLUORO NNEI) 2	111	57	18
377.255	233.1	15.13	5-FLUORO THJ 1	91	29	12
377.255	145.1	15.13	5-FLUORO THJ 2	91	53	14
363.254	145.1	12.29	5-FLUORO-2-ADB-PINACA_ISOMER_2 1	116	47	10
363.254	318.1	12.29	5-FLUORO-2-ADB-PINACA_ISOMER_2 2	116	29	14
367.233	249.1	13.78	5-FLUORO-CUMYL-PICA 1	96	21	12
367.233	91	13.78	5-FLUORO-CUMYL-PICA 2	96	77	14
376.497	233.1	14.60	5-FLUORO-MN-18 1	126	23	10
376.497	145.1	14.60	5-FLUORO-MN-18 2	126	53	18
376.066	145.1	9.85	5-FLUORO-MN-21 (5-FLUORO-PCN) 1	201	55	18
376.066	117	9.85	5-FLUORO-MN-21 (5-FLUORO-PCN) 2	201	89	14
339.222	91	13.04	5-FLUORO-SDB-006 1	141	63	14
339.222	232	13.04	5-FLUORO-SDB-006 2	141	31	10
378.028	233.1	14.03	5F-NPB-22 1	81	23	10
378.028	145.1	14.03	5F-NPB-22 2	81	55	18
377.092	232.1	13.60	5F-PB-22 1	81	27	10
377.092	144.1	13.60	5F-PB-22 2	81	57	20
311.223	144.1	12.11	5-F-PENTYL-3-PYRIDINOYLINDOLE 1	136	51	18
311.223	89	12.11	5-F-PENTYL-3-PYRIDINOYLINDOLE 2	136	99	12
377.212	233.1	14.79	5F-SDB-005 1	121	15	10
377.212	145.1	14.79	5F-SDB-005 2	121	51	10
205.058	58.1	2.86	5-HYDROXY DMT 1	81	17	8
205.058	160.1	2.86	5-HYDROXY DMT 2	81	25	20
175.275	158.1	4.98	5-IT 1	61	13	18
175.275	130.1	4.98	5-IT 2	61	31	18

190.252	159.1	6.61	5-MAPB 1	56	15	16
190.252	131.1	6.61	5-MAPB 2	56	29	20
192.202	161.1	5.67	5-MAPDB 1	56	17	18
192.202	133.1	5.67	5-MAPDB 2	56	31	14
219.295	160.1	7.06	5-MeO-ALPHA-ET 1	71	27	18
219.295	117.1	7.06	5-MeO-ALPHA-ET 2	71	55	14
271.063	110.1	7.20	5-MeO-DALT 1	86	21	14
271.063	174.1	7.20	5-MeO-DALT 2	86	27	22
205.05	188	5.90	5-METHOXY AMT 1	56	15	24
205.05	147.1	5.90	5-METHOXY AMT 2	56	27	20
275.078	114.2	7.16	5-METHOXY DiPT 1	91	21	14
275.078	174.1	7.16	5-METHOXY DiPT 2	91	29	22
219.968	58.1	5.16	5-METHOXY DMT 1	146	21	8
219.968	175	5.16	5-METHOXY DMT 2	146	21	22
238.277	190.1	5.53	5-METHOXY METHYLONE 1	96	21	24
238.277	147.1	5.53	5-METHOXY METHYLONE 2	96	37	16
247.988	86.1	6.16	5-METHOXY MiPT 1	156	19	10
247.988	87.1	6.16	5-METHOXY MiPT 2	156	19	10
176.049	159.1	6.45	6-APB 1	66	13	20
176.049	131.1	6.45	6-APB 2	66	25	18
178.157	161	5.80	6-APDB 1	36	15	22
178.157	132.9	5.80	6-APDB 2	36	29	8
272.17	240.9	7.47	6-BROMO-MDMA 1	86	19	12
274.156	242.8	7.47	6-BROMO-MDMA 2	76	19	12
228.238	169	7.09	6-CHLORO-MDMA 1	61	29	12
228.238	77	7.09	6-CHLORO-MDMA 2	61	53	12
204.15	131.1	7.10	6-EAPB 1	56	29	16
204.15	159.1	7.10	6-EAPB 2	56	17	8
175.258	158.1	5.85	6-IT 1	51	15	8
175.258	130.1	5.85	6-IT 2	51	31	18
328.01	165	5.06	6-MAM 1	141	51	20
328.01	43	5.06	6-MAM 2	141	95	8
190.239	131.1	6.60	6-MAPB 1	71	27	10
190.239	91	6.60	6-MAPB 2	71	43	10
286.241	121.1	6.51	7-AMINOCLONAZEPAM 1	111	39	14
286.241	222.1	6.51	7-AMINOCLONAZEPAM 2	111	33	26
270.396	121.1	5.51	7-AMINODESMETHYLFLUNITRAZEPAM 1	146	37	14
270.396	77	5.51	7-AMINODESMETHYLFLUNITRAZEPAM 2	146	75	10
283.767	135.1	7.55	7-AMINOFLUNITRAZEPAM 1	121	37	18
283.767	77.1	7.55	7-AMINOFLUNITRAZEPAM 2	121	87	12
252.005	121.1	4.57	7-AMINONITRAZEPAM 1	111	35	16
252.005	77.1	4.57	7-AMINONITRAZEPAM 2	111	73	10
176.239	131.1	6.68	7-APB 1	46	25	14
176.239	77	6.68	7-APB 2	46	53	10
178.233	161.1	6.38	7-APDB 1	61	15	10
178.233	133.1	6.38	7-APDB 2	61	25	18

355.053	125.1	11.59	A-796260 1	106	27	16
355.053	114.1	11.59	A-796260 2	106	35	14
340.308	125.1	14.21	A-834735 1	156	29	16
340.308	55	14.21	A-834735 2	156	61	10
311.15	187.1	12.39	A-836339 1	101	23	12
311.15	125.2	12.39	A-836339 2	101	33	10
350.211	135.1	16.10	AB-001 1	146	39	16
350.211	77.1	16.10	AB-001 2	146	117	12
352.92	98.2	11.39	AB005 1	116	53	12
352.92	112.1	11.39	AB005 2	116	29	16
357.16	241.1	14.11	AB-CHMINACA 1	91	37	12
357.16	312.1	14.11	AB-CHMINACA 2	91	23	14
369.13	352	12.67	AB-FUBINACA 1	81	13	14
369.13	109.1	12.67	AB-FUBINACA 2	81	47	14
369.269	253	12.86	AB-FUBINACA 2-FLUOROBENZYL ISOMER 1	86	33	12
369.269	324.2	12.86	AB-FUBINACA 2-FLUOROBENZYL ISOMER 2	86	19	14
369.241	253	12.67	AB-FUBINACA 3-FLUOROBENZYL ISOMER 1	66	35	12
369.241	324.1	12.67	AB-FUBINACA 3-FLUOROBENZYL ISOMER 2	66	21	14
331.065	215.1	13.49	AB-PINACA 1	86	33	10
331.065	286.1	13.49	AB-PINACA 2	86	21	14
382.972	253	13.27	ADB-FUBINACA 1	101	33	12
382.972	109.1	13.27	ADB-FUBINACA 2	101	55	12
345.052	215	14.01	ADB-PINACA 1	91	35	10
345.052	328.2	14.01	ADB-PINACA 2	91	13	14
345.335	215.1	13.69	ADB-PINACA ISOMER_1 1	86	33	10
345.335	300.2	13.69	ADB-PINACA ISOMER_1 2	86	21	14
345.304	215.1	14.06	ADB-PINACA ISOMER_2 1	71	35	10
345.304	300.1	14.06	ADB-PINACA ISOMER_2 2	71	19	14
345.292	215.1	14.05	ADB-PINACA ISOMER_3 1	71	33	10
345.292	300.2	14.05	ADB-PINACA ISOMER_3 2	71	19	14
345.305	215.1	13.98	ADB-PINACA ISOMER_4 1	81	33	10
345.305	300.1	13.98	ADB-PINACA ISOMER_4 2	81	19	14
329.174	284	9.70	AH-7921 1	91	23	12
329.174	173	9.70	AH-7921 2	91	35	18
404.265	135.1	15.64	AKB48_N-(4-FLUOROBENZYL)_ANALOG 1	136	29	16
404.265	77	15.64	AKB48_N-(4-FLUOROBENZYL)_ANALOG 2	136	121	14
206.323	188.1	7.09	ALFA-ETHYLAMINOPENTIOPHENONE 1	86	17	22
206.323	91	7.09	ALFA-ETHYLAMINOPENTIOPHENONE 2	86	39	12
220.315	202.1	7.83	ALFA-PROPYLAMINOPENTIOPHENONE 1	91	19	10
220.315	91.1	7.83	ALFA-PROPYLAMINOPENTIOPHENONE 2	91	33	10
238.321	221.1	6.95	ALLYLESCALINE 1	51	13	10
238.321	77	6.95	ALLYLESCALINE 2	51	67	12
206.291	91.1	6.84	ALPHA-DIMETHYLAMINOPENTIOPHENONE 1	101	27	14
206.291	77.1	6.84	ALPHA-DIMETHYLAMINOPENTIOPHENONE 2	101	57	12
220.312	91	8.41	ALPHA-ETHYLAMINOHEXANOPHENONE 1	106	33	12
220.312	130.1	8.41	ALPHA-ETHYLAMINOHEXANOPHENONE 2	106	47	14

188.767	130.1	7.09	ALPHA-ETHYLTRYPTAMINE 1	76	27	16
188.767	172.1	7.09	ALPHA-ETHYLTRYPTAMINE 2	76	11	20
175.029	158.1	5.68	ALPHA-METHYLTRYPTAMINE 1	56	15	20
175.029	143.1	5.68	ALPHA-METHYLTRYPTAMINE 2	56	35	16
246.318	91	8.41	ALPHA-PHP 1	76	33	10
246.318	77	8.41	ALPHA-PHP 2	76	65	10
280.193	105.1	11.76	ALPHA-PHTALIMIDOPROPIOPHENONE 1	116	31	14
280.193	77	11.76	ALPHA-PHTALIMIDOPROPIOPHENONE 2	116	79	12
232.294	91.1	6.48	ALPHA-PIPBP 1	106	33	8
232.294	77	6.48	ALPHA-PIPBP 2	106	61	10
204.261	105.1	5.00	ALPHA-PPP 1	71	31	14
204.261	98.1	5.00	ALPHA-PPP 2	71	33	8
232.243	91.1	7.17	ALPHA-PVP 1	71	39	8
232.243	126.1	7.17	ALPHA-PVP 2	71	57	6
238.017	126.2	6.24	ALPHA-PVT 1	91	29	16
238.017	97	6.24	ALPHA-PVT 2	91	31	12
224.19	112.2	4.95	ALPHA-PYRROLIDINOBUTHIOPHENONE 1	81	29	12
224.19	97	4.95	ALPHA-PYRROLIDINOBUTHIOPHENONE 2	81	39	12
309.934	282	11.35	ALPRAZOLAM 1	171	37	12
309.934	206	11.35	ALPRAZOLAM 2	171	57	26
383.315	98	10.51	AM1220 1	101	49	14
383.315	112.1	10.51	AM1220 2	101	27	12
391.166	135.2	12.07	AM-1248 1	131	39	16
391.166	112.1	12.07	AM-1248 2	131	39	14
360.031	127.1	14.16	AM-2201 1	171	65	16
360.031	155.1	14.16	AM-2201 2	171	33	18
376.237	232.1	14.94	AM2201 8-QUINOLINYL CARBOXAMIDE 1	86	23	12
376.237	144.1	14.94	AM2201 8-QUINOLINYL CARBOXAMIDE 2	86	55	16
361.184	127.1	14.44	AM2201 BENZIMIDAZOLE ANALOG 1	131	73	16
361.184	155.1	14.44	AM2201 BENZIMIDAZOLE ANALOG 2	131	41	20
353.245	155.1	12.76	AM2232 1	131	31	18
353.245	127	12.76	AM2232 2	131	63	14
278.073	91	10.85	AMITRIPTYLINE 1	101	33	12
278.073	105.1	10.85	AMITRIPTYLINE 2	101	31	14
136.03	91	4.73	AMPHETAMINE 1	51	23	12
136.03	119.1	4.73	AMPHETAMINE 2	51	11	16
267.122	145.1	3.91	ATENOLOL 1	101	35	20
267.122	56.1	3.91	ATENOLOL 2	101	43	8
216.245	174	11.12	ATRAZYNA 1	126	23	24
216.245	104	11.12	ATRAZYNA 2	126	39	14
268.279	250.1	8.69	AZACYCLONOL 1	81	17	20
268.279	91	8.69	AZACYCLONOL 2	81	51	14
385.123	240.1	15.13	BB-22 1	101	19	16
385.123	144	15.13	BB-22 2	101	51	18
194.03	135	6.36	BDB 1	56	25	18
194.03	177	6.36	BDB 2	56	11	24

300.293	215.1	10.62	BENOCYCLIDINE 1	66	17	10
300.293	147	10.62	BENOCYCLIDINE 2	66	39	18
254.273	91.1	9.14	BENZEDRONE 1	111	31	12
254.273	65.1	9.14	BENZEDRONE 2	111	77	10
166.03	120	8.84	BENZOCAINE 1	71	25	16
166.03	94	8.84	BENZOCAINE 2	71	23	12
290.034	168.1	6.54	BENZOYLECGONINE 1	91	27	20
290.034	77	6.54	BENZOYLECGONINE 2	91	77	10
310.213	86.1	10.20	BENZYDAMINE 1	106	23	10
310.213	58.1	10.20	BENZYDAMINE 2	106	71	10
274.896	163	6.96	bk-2C-B 1	81	39	39
274.896	178.1	6.96	bk-2C-B 2	81	21	21
194.195	146	4.23	bk-MDA 1	56	19	14
194.195	118.1	4.23	bk-MDA 2	56	31	14
136.133	91	4.86	BMPEA 1	46	25	10
136.133	119.1	4.86	BMPEA 2	46	11	16
293.977	276.9	10.04	BROMO-DRAGON-FLY 1	71	15	42
296.128	278.9	10.04	BROMO-DRAGON-FLY 2	81	17	12
468.189	55	9.63	BUPRENORPHINE 1	116	95	12
468.189	152	9.63	BUPRENORPHINE 2	116	117	10
239.672	184	8.02	BUPROPION 1	66	17	24
239.672	131.1	8.02	BUPROPION 2	66	37	16
222.185	174.1	5.77	BUTYLONE (bk-MBDB) 1	66	25	20
222.185	204.1	5.77	BUTYLONE (bk-MBDB) 2	66	17	10
202.289	91	8.22	CAMFETAMINE 1	76	43	14
202.289	67	8.22	CAMFETAMINE 2	76	25	14
315.323	193	15.06	CANNABIDIOL 1	121	29	10
315.323	123	15.06	CANNABIDIOL 2	121	43	16
237.209	194.1	10.49	CARBAMAZEPINE 1	111	27	24
237.209	192.1	10.49	CARBAMAZEPINE 2	111	45	24
152.256	134.1	3.67	CATHINE 1	51	13	22
152.256	117.1	3.67	CATHINE 2	51	23	14
150.03	132.1	3.71	CATHINONE 1	56	17	18
150.03	117.1	3.71	CATHINONE 2	56	31	14
369.1	127	16.51	CB-13 1	151	61	20
369.1	170.7	16.51	CB-13 2	151	39	24
358.214	214.1	15.81	CBL-018 1	76	21	10
358.214	144.1	15.81	CBL-018 2	76	49	20
394.203	188.9	14.95	CI2201 1	151	37	24
396.214	191	14.95	CI2201 2	151	35	24
301.995	260	11.09	CLOBAZAM 1	151	29	12
301.995	225	11.09	CLOBAZAM 2	151	45	26
315.043	86.1	11.59	CLOMIPRAMINE 1	106	23	12
315.043	58	11.59	CLOMIPRAMINE 2	106	65	8
316.097	270.1	10.73	CLONAZEPAM 1	151	35	12
316.097	214.3	10.73	CLONAZEPAM 2	151	45	22

318.094	196.1	8.04	COCAETHYLENE 1	101	27	24
318.094	82	8.04	COCAETHYLENE 2	101	39	12
304.198	182.1	7.06	COCAINE 1	106	27	22
304.198	77.1	7.06	COCAINE 2	106	79	12
300.058	152	4.32	CODEINE 1	136	85	18
300.058	115.1	4.32	CODEINE 2	136	95	16
349.217	231.1	14.69	CUMYL-PICA 1	86	21	12
349.217	91	14.69	CUMYL-PICA 2	86	73	12
254.299	236.2	7.95	D2PM 1	81	19	12
254.299	130.1	7.95	D2PM 2	81	39	8
286.956	179.9	10.20	DEMOXEPAM 1	131	31	22
286.956	269	10.20	DEMOXEPAM 2	131	37	12
289.917	140	11.56	DESALKYLFLURAZEPAM 1	116	39	18
289.917	141	11.56	DESALKYLFLURAZEPAM 2	116	39	18
310.255	281	11.39	DESCHLOROETIZOLAM 1	151	33	12
310.255	256	11.39	DESCHLOROETIZOLAM 2	151	31	12
218.287	91	6.21	DESCHLORO-N-ETHYL-KETAMINE 1	96	39	10
218.287	145.1	6.21	DESCHLORO-N-ETHYL-KETAMINE 2	96	23	8
267.085	72.1	10.70	DESIPRAMINE 1	71	21	10
267.085	44.1	10.70	DESIPRAMINE 2	71	63	8
271.978	209.1	11.89	DESMETHYLDIAZEPAM (NORDIAZEPAM) 2	141	39	26
271.978	140	11.89	DESMETHYLDIAZEPAM (NORDIAZEPAM) 1	141	39	18
299.977	254.1	10.31	DESMETHYLFLUNITRAZEPAM 1	116	35	12
299.977	198	10.31	DESMETHYLFLUNITRAZEPAM 2	116	53	24
272.254	167.1	5.08	DESOMORPHINE 1	126	49	20
272.254	152.1	5.08	DESOMORPHINE 2	126	73	18
238.301	91	8.68	DESOXY-D2PM 1	101	33	12
238.301	117.1	8.68	DESOXY-D2PM 2	101	23	8
252.331	91.1	9.03	DESOXYPIPRADROL (2-DPMP) 1	91	49	12
252.331	65	9.03	DESOXYPIPRADROL (2-DPMP) 2	91	85	10
272.289	128.1	9.23	DEXTROMETHORPHAN 1	126	81	16
272.289	171	9.23	DEXTROMETHORPHAN 2	126	51	20
285.397	154	12.30	DIAZEPAM 1	166	37	20
285.397	193	12.30	DIAZEPAM 2	166	43	24
320.306	228	12.33	DICLAZEPAM 1	166	43	28
320.306	89	12.33	DICLAZEPAM 2	166	103	12
322.115	121.1	11.03	DICLOFENSINE 1	151	33	16
322.115	279	11.03	DICLOFENSINE 2	151	29	14
206.061	105.1	5.24	DIETHYLCATHINONE (AMFEPRAMONE) 1	81	31	12
206.061	100.1	5.24	DIETHYLCATHINONE (AMFEPRAMONE) 2	81	29	14
302.062	199	4.26	DIHYDROCODEINE 1	121	43	26
302.062	128.1	4.26	DIHYDROCODEINE 2	121	81	16
279.175	120.1	6.17	DIMETHOCAINE 1	106	31	14
279.175	65	6.17	DIMETHOCAINE 2	106	81	10
222.209	72.2	4.77	DIMETHYLONE (bk-MDDMA) 1	86	25	10
222.209	91	4.77	DIMETHYLONE (bk-MDDMA) 2	86	49	12

256.071	167.1	9.27	DIPHENHYDRAMINE 1	56	17	22
256.071	165.1	9.27	DIPHENHYDRAMINE 2	56	57	22
266.099	181.1	8.71	DIPHENIDINE 1	76	25	22
266.099	103.1	8.71	DIPHENIDINE 2	76	47	12
244.891	114.2	7.30	DiPT 1	81	21	14
244.891	144.1	7.30	DiPT 2	81	31	20
266.292	248.1	7.33	DL-4662 1	86	19	12
266.292	188	7.33	DL-4662 2	86	35	22
322.068	304.9	8.92	DOI 1	61	17	12
322.068	277	8.92	DOI 2	61	27	12
296.089	202	10.16	DOTHIEPIN 1	86	75	26
296.089	220.9	10.16	DOTHIEPIN 2	86	61	28
279.918	107.1	9.52	DOXEPIN 1	101	31	14
279.918	77	9.52	DOXEPIN 2	101	73	10
271.067	167.1	5.77	DOXYLAMINE 1	61	49	22
271.067	182	5.77	DOXYLAMINE 2	61	23	22
388.297	183.1	14.95	EAM-2201 1	81	35	10
388.297	153	14.95	EAM-2201 2	81	65	20
278.507	234.2	9.25	EDDP 1	86	41	10
278.507	249.1	9.25	EDDP 2	86	33	10
410.225	155	15.66	EG-2201 1	181	33	22
410.225	127.1	15.66	EG-2201 2	181	71	16
326.4	223.1	5.32	ERGOMETRINE 1	116	31	10
326.4	208.1	5.32	ERGOMETRINE 2	116	39	10
295.921	268	10.99	ESTAZOLAM 1	101	33	12
295.921	206	10.99	ESTAZOLAM 2	101	55	24
264.918	146.1	11.91	ETAQUALONE 1	116	37	18
264.918	77	11.91	ETAQUALONE 2	116	89	12
180.064	162.1	4.72	ETHCATHINONE METABOLITE 1	76	17	20
180.064	115.1	4.72	ETHCATHINONE METABOLITE 2	76	39	14
222.228	174.1	5.14	ETHYLONE (bk-MDEA) 1	71	25	20
222.228	204.1	5.14	ETHYLONE (bk-MDEA) 2	71	19	10
248.328	84.1	8.17	ETHYLPHENIDATE 1	111	25	12
248.328	56	8.17	ETHYLPHENIDATE 2	111	69	8
343.91	315	11.69	ETIZOLAM 1	121	35	14
343.91	224.1	11.69	ETIZOLAM 2	121	65	10
236.294	188.1	6.18	EUTYLONE (bk-EBDB) 1	96	25	24
236.294	189.1	6.18	EUTYLONE (bk-EBDB) 2	96	29	22
396.194	109.1	15.21	FDU-PB-22 1	96	47	12
396.194	252	15.21	FDU-PB-22 2	96	17	12
232.018	159	8.34	FENFLURAMINE 1	86	31	20
232.018	109	8.34	FENFLURAMINE 2	86	57	14
337.171	188	8.81	FENTANYL 1	131	29	10
337.171	105	8.81	FENTANYL 2	131	57	12
334.716	226.1	11.77	FLUBROMAZEPAM 1	161	39	10
334.716	186	11.77	FLUBROMAZEPAM 2	161	41	22

303.922	212	11.99	FLUDIAZEPAM 1	141	43	26
303.922	89	11.99	FLUDIAZEPAM 2	141	93	12
303.986	258.1	9.20	FLUMAZENIL 1	81	23	12
303.986	217	9.20	FLUMAZENIL 2	81	35	26
313.814	268	10.83	FLUNITRAZEPAM 1	136	35	12
313.814	239	10.83	FLUNITRAZEPAM 2	136	47	12
310.021	44.1	11.20	FLUOXETINE 1	51	43	8
310.021	148.1	11.20	FLUOXETINE 2	51	11	18
388.023	315	9.32	FLURAZEPAM 1	91	31	14
388.023	107	9.32	FLURAZEPAM 2	91	111	14
350.227	109.1	14.95	FUB-144 1	111	61	14
350.227	125.1	14.95	FUB-144 2	111	29	14
380.203	155.1	14.47	FUB-JWH-018 1	176	33	8
380.203	109	14.47	FUB-JWH-018 2	176	63	18
398.186	253	13.65	FUB-NPB-22 1	86	23	12
398.186	109.1	13.65	FUB-NPB-22 2	86	47	8
396.975	109.1	15.21	FUB-PB-22 1	116	45	14
396.975	253.1	15.21	FUB-PB-22 2	116	17	12
375.29	105.1	8.86	FURANYLFENTANYL (Fu-F) 1	136	55	14
375.29	188.1	8.86	FURANYLFENTANYL (Fu-F) 2	136	29	20
102.935	85	1.31	GHB 1	-75	-10	-12
102.935	57	1.31	GHB 2	-75	-10	-18
215.051	174	7.45	HARMALINE 1	61	29	10
215.051	171.9	7.45	HARMALINE 2	61	37	18
212.795	170.1	7.85	HARMINE 1	121	41	20
212.795	198	7.85	HARMINE 2	121	31	26
387.195	243.1	15.91	HU-210 1	146	25	12
387.195	43	15.91	HU-210 2	146	71	8
300.05	199	4.83	HYDROCODONE 1	131	39	24
300.05	128.1	4.83	HYDROCODONE 2	131	77	16
312.288	122.1	7.91	IBOGAINE 1	281	43	14
312.288	77	7.91	IBOGAINE 2	281	119	12
281.078	86.1	10.55	IMIPRAMINE 1	66	21	12
281.078	58.1	10.55	IMIPRAMINE 2	66	59	8
192.055	91	6.81	ISOPENTEDRONE 1	71	33	12
192.055	161	6.81	ISOPENTEDRONE 2	71	17	22
343.221	126.6	15.44	JWH 018 BENZIMIDAZOLE ANALOG 1	121	109	16
343.221	155.1	15.44	JWH 018 BENZIMIDAZOLE ANALOG 2	121	41	20
384.202	155.1	15.80	JWH-011 1	151	37	16
384.202	127.1	15.80	JWH-011 2	151	71	14
342.097	127.1	15.16	JWH-016 1	146	67	16
342.097	155.1	15.16	JWH-016 2	146	33	20
342.063	127.1	14.91	JWH-018 1	146	65	16
342.063	155	14.91	JWH-018 2	146	33	20
365.291	135.1	15.72	JWH-018 ADAMANTYL CARBOXAMIDE 1	156	37	20
365.291	77	15.72	JWH-018 ADAMANTYL CARBOXAMIDE 2	156	109	12

370.197	127.1	15.90	JWH-020 1	156	67	16
370.197	155	15.90	JWH-020 2	156	35	20
340.223	155.1	14.75	JWH-022 1	136	31	8
340.223	127.1	14.75	JWH-022 2	136	61	16
306.155	127.1	14.85	JWH-031 1	131	51	8
306.155	76.9	14.85	JWH-031 2	131	95	6
300.22	127.1	13.63	JWH-071 1	111	57	16
300.22	155.1	13.63	JWH-071 2	111	29	8
328.077	127.1	14.71	JWH-073 1	131	63	16
328.077	155.1	14.71	JWH-073 2	131	31	20
358.107	185	14.96	JWH-080 1	61	33	24
358.107	127.1	14.96	JWH-080 2	61	69	16
372.132	185.1	15.37	JWH-081 1	156	35	24
372.132	114.1	15.37	JWH-081 2	156	93	14
386.111	185	15.50	JWH-098 1	146	35	22
386.111	114.1	15.50	JWH-098 2	146	101	14
370.219	155.2	15.65	JWH-116 1	121	33	16
370.219	127.1	15.65	JWH-116 2	121	69	6
356.234	169.1	15.53	JWH-122 1	126	33	20
356.234	115.1	15.53	JWH-122 2	126	91	14
367.929	154.8	15.59	JWH-145 1	91	35	22
367.929	127.1	15.59	JWH-145 2	91	69	18
396.312	155.1	16.20	JWH-146 1	141	27	18
396.312	127	16.20	JWH-146 2	141	71	22
382.164	155	15.91	JWH-147 1	136	27	20
382.164	127.1	15.91	JWH-147 2	136	69	16
370.172	169.1	15.65	JWH-149 1	156	35	26
370.172	115.2	15.65	JWH-149 2	156	95	14
306.156	91.1	14.55	JWH-167 1	86	31	12
306.156	214.2	14.55	JWH-167 2	86	35	30
328.281	141.1	16.76	JWH-175 1	106	29	18
328.281	115.1	16.76	JWH-175 2	106	83	14
384.268	197	16.06	JWH-182 1	196	33	10
384.268	141	16.06	JWH-182 2	196	61	14
399.123	169.1	11.73	JWH-193 1	116	31	10
399.123	115	11.73	JWH-193 2	116	97	6
415.117	185.1	11.51	JWH-198 1	181	33	22
415.117	114.2	11.51	JWH-198 2	181	35	10
385.076	155.1	10.92	JWH-200 1	121	29	20
385.076	127.1	10.92	JWH-200 2	121	71	16
336.263	121.1	14.46	JWH-201 1	151	35	16
336.263	77	14.46	JWH-201 2	151	77	10
384.326	183.1	15.91	JWH-213 1	181	35	22
384.326	153.1	15.91	JWH-213 2	181	61	18
386.153	155	15.47	JWH-307 1	66	27	24
386.153	127.1	15.47	JWH-307 2	66	81	16

418.325	155	16.09	JWH-309 1	141	29	20
418.325	127.1	16.09	JWH-309 2	141	77	16
386.132	155.1	15.59	JWH-368 1	106	29	20
386.132	127	15.59	JWH-368 2	106	69	16
402.279	155.1	15.69	JWH-369 1	126	29	20
402.279	127	15.69	JWH-369 2	126	65	18
360.213	173	15.41	JWH-412 1	161	33	10
360.213	145.1	15.41	JWH-412 2	161	63	18
422.179	235	14.95	JWH-424 1	131	37	12
420.174	233	14.95	JWH-424 2	111	37	12
238.083	125	6.41	KETAMINE 1	61	37	16
238.083	89	6.41	KETAMINE 2	61	73	12
324.164	223	8.19	LAMPA 1	116	33	28
324.164	208	8.19	LAMPA 2	116	41	26
235.081	86.1	5.70	LIDOCAINE 1	126	23	10
235.081	58.1	5.70	LIDOCAINE 2	126	51	10
464.983	252	9.21	LOPRAZOLAM 1	126	57	12
464.983	111.1	9.21	LOPRAZOLAM 2	126	35	14
321.924	275.9	11.33	LORAZEPAM 1	111	29	12
321.924	303.9	11.33	LORAZEPAM 2	111	21	14
335.939	289.9	11.79	LORMETAZEPAM 1	86	29	14
335.939	177.9	11.79	LORMETAZEPAM 2	86	45	12
324.277	223	8.02	LSD 1	101	33	28
324.277	207	8.02	LSD 2	101	57	26
374.126	169	14.60	MAM-2201 1	126	35	22
374.126	115.1	14.60	MAM-2201 2	126	97	14
278.114	191	10.71	MAPROTILINE 1	116	47	24
278.114	189	10.71	MAPROTILINE 2	116	83	22
208.04	135	6.39	MBDB 1	51	27	18
208.04	77	6.39	MBDB 2	51	55	10
192.204	175.1	5.49	MDAT 1	66	15	10
192.204	117.1	5.49	MDAT 2	66	35	8
221.272	135	2.36	MDBP 1	61	23	10
221.272	77	2.36	MDBP 2	61	53	12
208.054	163	5.80	MDEA 1	66	19	20
208.054	105	5.80	MDEA 2	66	35	14
385.124	240.1	15.12	MDMB-CHMICA (MMB-CHMINACA) 1	81	27	12
385.124	144	15.12	MDMB-CHMICA (MMB-CHMINACA) 2	81	53	18
386.303	241.1	15.49	MDMB-CHMINACA 1	156	33	12
386.303	145	15.49	MDMB-CHMINACA 2	156	57	18
262.024	161	6.30	MDPBP 1	86	31	20
262.024	112.1	6.30	MDPBP 2	86	35	14
329.969	284	11.40	MECLONAZEPAM 1	91	37	14
329.969	238	11.40	MECLONAZEPAM 2	91	57	12
271.019	206.9	9.31	MEDAZEPAM 1	126	37	26
271.019	165.1	9.31	MEDAZEPAM 2	126	61	20

180.261	163.2	9.37	MEMANITINE 1	56	19	8
180.261	107.2	9.37	MEMANITINE 2	56	33	10
248.14	220.1	7.50	MEPERIDINE 1	121	31	20
248.14	91.1	7.50	MEPERIDINE 2	121	59	8
190.139	44	5.33	MEPHTETRAMINE (MTTA) 1	101	31	8
190.139	147.1	5.33	MEPHTETRAMINE (MTTA) 2	101	13	18
314.241	214.1	10.12	MEPIRAPIM 1	66	21	10
314.241	144.1	10.12	MEPIRAPIM 2	66	47	8
219.029	158.1	8.76	MEPROBAMATE 1	66	11	20
219.029	55.1	8.76	MEPROBAMATE 2	66	31	8
212.183	195.1	5.11	MESCALINE 1	76	13	24
212.183	77	5.11	MESCALINE 2	76	63	12
310.094	265.1	10.75	METHADONE 1	66	21	12
310.094	105	10.75	METHADONE 2	66	35	14
150.063	91	4.96	METHAMPHETAMINE 1	51	25	12
150.063	119.1	4.96	METHAMPHETAMINE 2	51	15	16
301.06	121.2	12.42	METHANDIENONE 1	131	35	14
301.06	149.1	12.42	METHANDIENONE 2	131	21	18
251.007	132.1	11.03	METHAQUALONE 1	131	37	18
251.007	91	11.03	METHAQUALONE 2	131	57	12
164.056	131.1	4.07	METHCATHINONE 1	61	27	18
164.056	130.1	4.07	METHCATHINONE 2	61	41	16
193.998	176	5.29	METHEDRONE (bk-PMMA) 1	56	15	10
193.998	161	5.29	METHEDRONE (bk-PMMA) 2	56	31	6
263.072	221	11.80	METHOHEXITAL 1	116	19	10
263.072	77.1	11.80	METHOHEXITAL 2	116	67	10
248.059	121.1	7.08	METHOXETAMINE 1	76	37	16
248.059	203	7.08	METHOXETAMINE 2	76	19	26
297.324	129.1	9.25	METHOXPHENIDINE 1	101	27	16
297.324	117.1	9.25	METHOXPHENIDINE 2	101	31	14
116.066	57	5.74	METHYLHEXANAMINE 1	71	17	8
116.066	41.1	5.74	METHYLHEXANAMINE 2	71	31	6
208.272	160	4.56	METHYLONE (bk-MDMA) 1	86	25	20
208.272	132.1	4.56	METHYLONE (bk-MDMA) 2	86	37	14
234.3	84.1	7.11	METHYLPHENIDATE 1	71	23	10
234.3	56	7.11	METHYLPHENIDATE 2	71	65	8
208.3	91	6.34	MEXEDRONE 1	76	47	16
208.3	119	6.34	MEXEDRONE 2	76	29	6
265.493	208.1	9.27	MIANSERIN 1	146	29	24
265.493	58.1	9.27	MIANSERIN 2	146	45	10
326.065	291.1	9.28	MIDAZOLAM 1	136	37	12
326.065	248.9	9.28	MIDAZOLAM 2	136	51	30
399.094	174	9.16	MITRAGYNINE 1	136	41	22
399.094	159.1	9.16	MITRAGYNINE 2	136	63	20
178.131	161	6.85	MMAI 1	61	15	22
178.131	103	6.85	MMAI 2	61	53	14

345.251	214.1	14.15	MMB018 1	66	19	10
345.251	144	14.15	MMB018 2	66	51	20
363.251	232.1	13.10	MMB2201 1	81	21	10
363.251	144.1	13.10	MMB2201 2	81	53	16
358.061	215.1	15.53	MN-18 1	126	25	10
358.061	145	15.53	MN-18 2	126	49	18
440.336	114.1	12.76	MN-25 1	141	41	12
440.336	261.1	12.76	MN-25 2	141	33	12
454.347	114.1	13.18	MN-25-2-METHYL DERIVATIVE 1	151	41	18
454.347	275.1	13.18	MN-25-2-METHYL DERIVATIVE 2	151	31	14
387.261	241.1	15.46	MO-CHMINACA 1	121	27	22
387.261	145.1	15.46	MO-CHMINACA 2	121	47	8
286.043	152.1	2.36	MORPHINE 1	176	79	20
286.043	128.1	2.36	MORPHINE 2	176	77	16
232.059	105.1	7.46	MPBP 1	116	33	14
232.059	91.1	7.46	MPBP 2	116	57	12
349.38	181	10.78	MT-45 1	176	37	24
349.38	77	10.78	MT-45 2	176	93	12
191.273	105.1	3.89	N-(3-METHYLBENZYL)PIPERAZINE 1	81	27	14
191.273	77	3.89	N-(3-METHYLBENZYL)PIPERAZINE 2	81	55	10
178.273	105.1	5.31	N.N-DIETHYLPHENETHYLAMINE 1	101	25	10
178.273	77	5.31	N.N-DIETHYLPHENETHYLAMINE 2	101	55	12
250.302	100.1	7.20	N.N-DIMETHYLPENTYLONE (bk-DMBDP) 1	101	27	12
250.302	135	7.20	N.N-DIMETHYLPENTYLONE (bk-DMBDP) 2	101	31	14
189.572	58	4.73	N.N-DMT 1	116	19	8
189.572	144.1	4.73	N.N-DMT 2	116	23	18
250.245	208.1	9.24	N-ACETYL-3.4-MDMC 1	76	19	22
250.245	160.1	9.24	N-ACETYL-3.4-MDMC 2	76	35	18
282.065	140.9	10.07	NAPHYRONE 1	51	37	10
282.065	127	10.07	NAPHYRONE 2	51	59	24
282.125	127	9.59	NAPHYRONE-1-NAPHTYL ISOMER 1	51	57	22
282.125	141	9.59	NAPHYRONE-1-NAPHTYL ISOMER 2	51	37	10
298.241	91.1	8.71	N-BENZYLNORBUTYLONE 1	96	41	14
298.241	65	8.71	N-BENZYLNORBUTYLONE 2	96	91	16
194.253	121	6.10	N-ETHYL-4-METHOXYAMPHETAMNE 1	66	29	16
194.253	91	6.10	N-ETHYL-4-METHOXYAMPHETAMNE 2	66	45	14
192.296	130.1	5.78	N-ETHYLBUPHEDRONE 1	66	39	10
192.296	91	5.78	N-ETHYLBUPHEDRONE 2	66	35	14
192.099	105	4.85	N-ETHYL-N-METHYLCATHINONE 1	76	29	6
192.099	77.2	4.85	N-ETHYL-N-METHYLCATHINONE 2	76	57	14
299.364	165.1	12.84	N-ETHYLNORDAZEPAM 1	216	59	20
299.364	77	12.84	N-ETHYLNORDAZEPAM 2	216	89	10
252.18	125	7.10	N-ETHYLNORKETAMINE 1	71	41	16
252.18	89.1	7.10	N-ETHYLNORKETAMINE 2	71	75	14
315.994	270	12.19	N-ETHYLOXAZEPAM 1	116	29	12
315.994	242	12.19	N-ETHYLOXAZEPAM 2	116	47	12

250.269	232.2	7.42	N-ETHYLPENTYLONE 1	71	21	22
250.269	202	7.42	N-ETHYLPENTYLONE 2	71	27	12
296.187	250.1	10.91	NIMETAZEPAM 1	171	35	12
296.187	221	10.91	NIMETAZEPAM 2	171	45	26
309.822	92	7.76	NITRACAINE 1	216	57	12
309.822	76	7.76	NITRACAINE 2	216	91	12
281.974	236	10.55	NITRAZEPAM 1	141	33	30
281.974	180.1	10.55	NITRAZEPAM 2	141	51	24
376.276	232	14.93	NM2201 1	131	21	12
376.276	144.1	14.93	NM2201 2	131	51	18
148.043	117.1	4.24	N-METHYL-2AI 1	81	23	14
148.043	115.1	4.24	N-METHYL-2AI 2	81	37	14
136.182	105.1	3.68	N-METHYL-PEA 1	51	19	18
136.182	77	3.68	N-METHYL-PEA 2	51	43	12
175.508	144.1	4.73	N-METHYLTRYPTAMINE 1	66	17	18
175.508	117.1	4.73	N-METHYLTRYPTAMINE 2	66	37	14
178.233	105	4.29	NN-DMC 1	91	29	14
178.233	72.1	4.29	NN-DMC 2	91	29	10
357.005	214.2	14.48	NNEI 1	81	29	10
357.005	144	14.48	NNEI 2	81	53	20
286.954	245.1	10.65	NORCLOBAZAM 1	141	27	12
286.954	210	10.65	NORCLOBAZAM 2	141	43	26
301.026	72.1	11.72	NORCLOMIPRAMINE 1	101	21	10
301.026	44.1	11.72	NORCLOMIPRAMINE 2	101	65	8
224.176	125.1	6.37	NORKETAMINE 1	51	13	12
224.176	207.2	6.37	NORKETAMINE 2	51	21	12
264.066	91.1	10.99	NORTRIPTYLINE 1	81	29	12
264.066	105.1	10.99	NORTRIPTYLINE 2	81	27	14
178.103	119.1	6.64	N-PROPYLAMPHETAMINE 1	86	17	16
178.103	65	6.64	N-PROPYLAMPHETAMINE 2	86	61	10
242.25	181.1	9.83	NRG-3 1	81	35	8
242.25	180.1	9.83	NRG-3 2	81	53	16
197.229	154.1	6.76	o-CPP 1	121	27	20
197.229	118.1	6.76	o-CPP 2	121	45	8
235.279	100.1	6.08	OCTACAINE 1	81	23	14
235.279	72.1	6.08	OCTACAINE 2	81	51	10
384.309	270.2	11.55	ORG-28611 1	71	25	12
384.309	174	11.55	ORG-28611 2	71	47	22
288.031	242.1	11.31	OXAZEPAM 1	91	31	12
288.031	269.9	11.31	OXAZEPAM 2	91	21	12
302.251	284	2.59	OXYMORPHONE 1	151	25	14
302.251	227.1	2.59	OXYMORPHONE 2	151	37	12
152.016	110	3.78	PARACETAMOL 1	81	21	14
152.016	65	3.78	PARACETAMOL 2	81	39	10
330.014	70	10.51	PAROXETINE 1	111	49	10
330.014	44.1	10.51	PAROXETINE 2	111	71	8

359.081	214.2	14.60	PB-22 1	71	21	10
359.081	144.1	14.60	PB-22 2	71	51	16
248.346	91	9.17	PCEEA 1	56	45	12
248.346	90.1	9.17	PCEEA 2	56	13	12
248.342	91	8.94	PCMPA 1	66	43	14
248.342	90.1	8.94	PCMPA 2	66	15	12
218.345	91	9.07	PCPr 1	46	39	6
218.345	159.1	9.07	PCPr 2	46	15	22
192.062	91	6.81	PENTEDRONE 1	81	31	12
192.062	132.1	6.81	PENTEDRONE 2	81	25	16
194.308	176.1	6.88	PENTEDRONE METABOLITE 1	81	17	22
194.308	91	6.88	PENTEDRONE METABOLITE 2	81	43	12
235.658	188.1	7.12	PENTYLONE (bk-MBDP) 1	136	25	24
235.658	218.1	7.12	PENTYLONE (bk-MBDP) 2	136	19	10
350.845	206	12.06	PHENAZEPAM 1	131	49	26
350.845	179	12.06	PHENAZEPAM 2	131	63	22
244.103	86.1	8.43	PHENCYCLIDINE (PCP) 1	56	17	12
244.103	91	8.43	PHENCYCLIDINE (PCP) 2	56	43	12
231.014	42	8.46	PHENOBARBITAL 1	-100	-10	-44
231.014	188	8.46	PHENOBARBITAL 2	-100	-10	-14
150.067	91	5.93	PHENTERMINE 1	41	27	12
150.067	133.1	5.93	PHENTERMINE 2	41	13	16
253.004	182.1	10.17	PHENYTOIN 1	116	25	24
253.004	104.1	10.17	PHENYTOIN 2	116	45	12
379.06	135.1	10.20	PRAVADOLINE 1	76	23	14
379.06	77.1	10.20	PRAVADOLINE 2	76	89	12
325.365	271	13.48	PRAZEPAM 1	126	31	12
325.365	140	13.48	PRAZEPAM 2	126	49	18
160.078	142.1	4.61	PREGABALIN 1	116	15	18
160.078	55	4.61	PREGABALIN 2	116	29	8
237.063	100.1	4.01	PROCAINE 1	81	21	12
237.063	120.1	4.01	PROCAINE 2	81	37	14
218.162	91.1	7.95	PROLINTANE 1	86	33	12
218.162	72.1	7.95	PROLINTANE 2	86	23	10
285.029	86.1	10.13	PROMETHAZINE 1	76	21	12
285.029	71.1	10.13	PROMETHAZINE 2	76	63	10
342.045	116.1	10.65	PROPAFENONE 1	86	29	14
342.045	72.1	10.65	PROPAFENONE 2	86	47	10
260.069	56	9.06	PROPRANOLOL 1	86	45	8
260.069	58.1	9.06	PROPRANOLOL 2	86	45	10
155.882	69.1	7.99	PROPYLHEXEDRINE 1	81	23	10
155.882	55	7.99	PROPYLHEXEDRINE 2	81	37	8
367.248	259.1	15.96	PSB-SB-1202 1	121	23	12
367.248	121.1	15.96	PSB-SB-1202 2	121	23	8
356.299	283	12.52	PTI-1 1	106	29	14
356.299	213.1	12.52	PTI-1 2	106	47	10

400.341	283	12.77	PTI-2 1	116	31	14
400.341	213.1	12.77	PTI-2 2	116	51	10
260.116	91.1	9.63	PV-8 1	96	33	12
260.116	77.1	9.63	PV-8 2	96	73	10
274.307	91	10.68	PV9 1	126	33	12
274.307	77	10.68	PV9 2	126	73	12
396.09	144	12.62	PX-1 1	76	59	18
396.09	231.9	12.62	PX-1 2	76	31	10
397.253	233	12.76	PX-2 1	86	33	12
397.253	352.2	12.76	PX-2 2	86	21	14
353.943	167.1	9.35	PYRAZOLAM 1	151	47	20
353.943	206	9.35	PYRAZOLAM 2	151	41	26
384.09	253.1	9.53	QUETIAPINE 1	116	31	12
384.09	221	9.53	QUETIAPINE 2	116	51	28
322.05	135.1	14.62	RCS-4 1	136	31	16
322.05	77	14.62	RCS-4 2	136	73	10
326.3	121.1	8.12	RH-34 1	91	25	14
326.3	91.1	8.12	RH-34 2	91	57	10
236.144	188.2	6.86	R-MMC 1	61	25	10
236.144	218.1	6.86	R-MMC 2	61	17	18
303.805	138.1	4.73	SCOPOLAMINE 1	96	29	18
303.805	156.1	4.73	SCOPOLAMINE 2	96	23	20
359.177	215.2	15.57	SDB-005 1	51	21	10
359.177	145	15.57	SDB-005 2	51	45	20
321.153	91	14.09	SDB-006 1	171	61	12
321.153	214.1	14.09	SDB-006 2	171	29	10
306.988	276	11.51	SERTRALINE 1	66	17	12
306.988	159	11.51	SERTRALINE 2	66	37	20
475.047	58.1	10.22	SILDENAFIL 1	91	103	10
475.047	100.1	10.22	SILDENAFIL 2	91	35	12
329.138	81.1	13.96	STANOZOLOL 1	241	79	12
329.138	95.1	13.96	STANOZOLOL 2	241	51	12
222.343	107.1	7.32	TAPENTADOL 1	86	35	14
222.343	77	7.32	TAPENTADOL 2	86	63	12
301.993	256	11.62	TEMAZEPAM 1	116	31	12
301.993	284.1	11.62	TEMAZEPAM 2	116	19	12
265.226	176.1	9.01	TETRACAINE 1	96	21	18
265.226	72	9.01	TETRACAINE 2	96	37	10
315.093	193.1	15.93	THC 1	106	31	24
315.093	123	15.93	THC 2	106	43	16
345.2	299.2	14.97	THCCOOH 1	106	23	10
345.2	193.1	14.97	THCCOOH 2	120	45	10
142.098	125	3.73	THIOPROPAMINE 1	51	13	8
142.098	97	3.73	THIOPROPAMINE 2	51	25	12
359.247	215.2	15.98	THJ 1	121	29	10
359.247	145	15.98	THJ 2	121	49	16

343.076	215.1	15.53	THJ-018 1	136	25	10
343.076	145.1	15.53	THJ-018 2	136	45	18
361.067	233.1	14.62	THJ-2201 (5-FLUORO THJ-018) 1	131	25	10
361.067	145.1	14.62	THJ-2201 (5-FLUORO THJ-018) 2	131	49	18
224.246	179	5.68	TILETAMINE 1	51	13	10
224.246	151.1	5.68	TILETAMINE 2	51	23	18
264.304	58.1	6.88	TRAMADOL 1	96	47	8
264.304	42.1	6.88	TRAMADOL 2	96	113	8
372.082	176	8.24	TRAZODONE 1	126	33	24
372.082	148	8.24	TRAZODONE 2	126	45	20
343.99	309.1	11.35	TRIAZOLAM 1	106	37	14
343.99	239.9	11.35	TRIAZOLAM 2	106	57	30
294.788	100.2	10.95	TRIMIPRAMINE 1	81	23	12
294.788	58.1	10.95	TRIMIPRAMINE 2	81	61	8
329.037	284	9.09	U-47700 1	56	25	14
331.017	286	9.09	U-47700 2	96	25	14
312.107	125.1	15.56	UR-144 1	96	29	16
312.107	214	15.56	UR-144 2	96	33	10
328.092	125.1	13.77	UR-144 metabolite 1	96	27	16
328.092	230.1	13.77	UR-144 metabolite 2	96	33	10
377.154	105.1	13.30	W-15 1	141	33	16
379.165	105.2	13.30	W-15 2	166	33	12
457.176	135.1	12.36	WIN 54.461 1	126	29	12
457.176	77	12.36	WIN 54.461 2	126	95	12
427.117	155.1	13.63	WIN 55.212-2 1	161	33	18
427.117	127.2	13.63	WIN 55.212-2 2	161	75	12
330.293	125.1	14.69	XLR-11 1	116	31	16
330.293	232.1	14.69	XLR-11 2	116	33	10
352.216	125.1	14.79	XLR12 1	141	31	8
352.216	254	14.79	XLR12 2	141	35	12
259.148	161	11.88	YANGONIN 1	121	29	22
259.148	89	11.88	YANGONIN 2	121	93	10
305.911	264	9.91	ZALEPLON 1	141	31	12
305.911	236.1	9.91	ZALEPLON 2	141	37	10
308.323	235.1	7.76	ZOLPIDEM 1	111	47	10
308.323	236	7.76	ZOLPIDEM 2	111	37	30
389.014	244.9	6.70	ZOPICLONE 1	81	23	12
389.014	112	6.70	ZOPICLONE 2	81	79	16
401.024	221	12.12	ZUCLOPENTHIXOL 1	101	73	26
401.024	231	12.12	ZUCLOPENTHIXOL 2	101	49	28
341.989	324	9.92	α-HYDROXYMIDAZOLAM 1	121	29	14
341.989	203	9.92	α-HYDROXYMIDAZOLAM 2	121	37	26

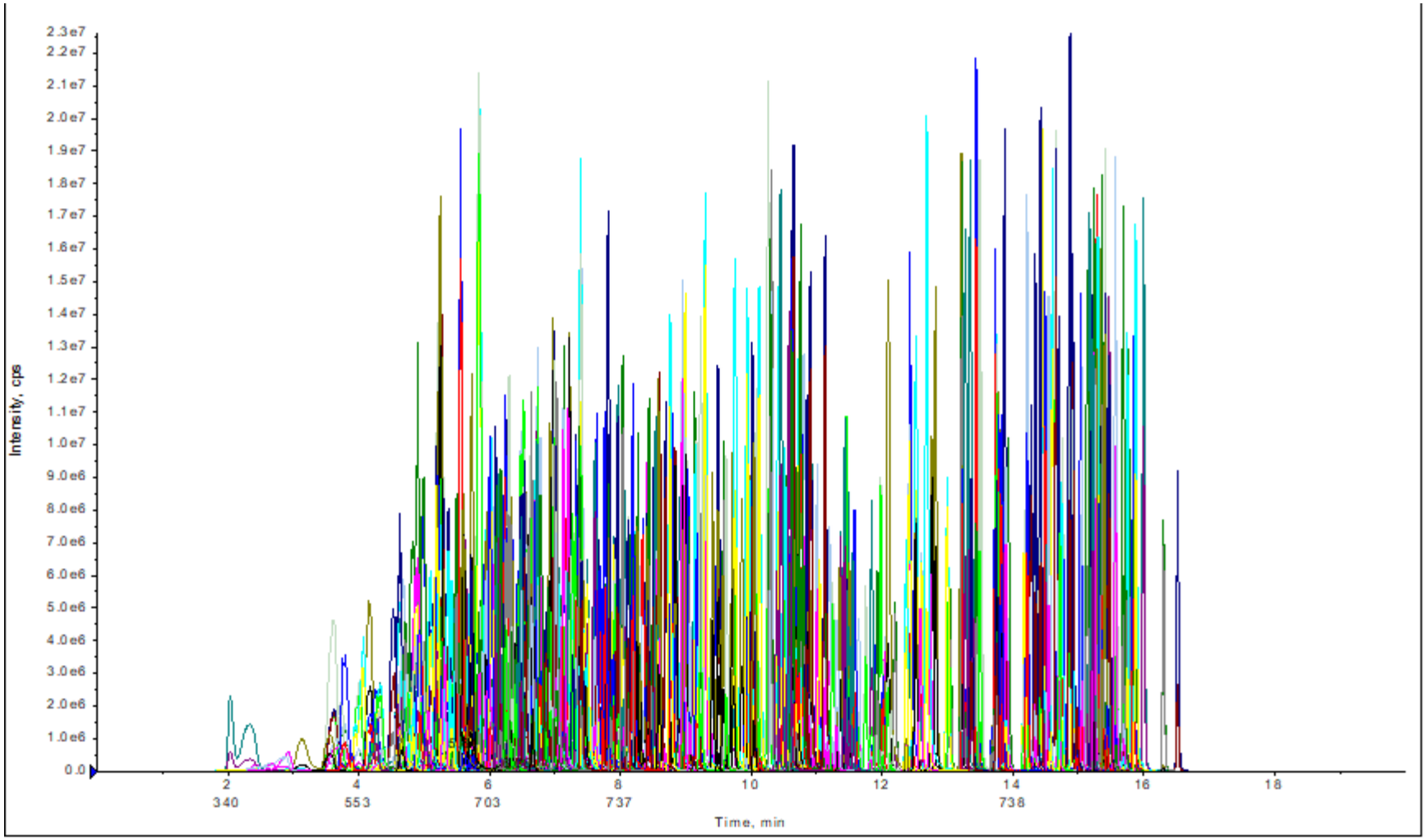

Figure S1. The chromatogram obtained for the Kinetex C18 column (Phenomenex 3.0 x 100 mm; 2.6 μm)

Table 2. The results of precision, BIAS and recovery values for identification of compounds.

ANALYTE	CONCENTRATION (ng/mg)	RECOVERY (%)	SD (%)	CV (%)	BIAS (%)	LOQ (ng/mg)
1-(2-METHOXYPHENYL)PIPERAZINE	0.025	134.2	10.0	7.43	34.2	0.125
	0.125	99.0	9.2	9.29	-1.0	
	1.25	100.3	12.9	12.89	0.3	
	5	112.2	4.7	4.21	12.2	
1-(3-TRIFLUOROMETHYLPHENYL)PIPERAZINE (TFMPP)	0.025	124.5	12.8	10.31	24.5	0.125
	0.125	106.3	6.7	6.34	6.3	
	1.25	99.6	5.4	5.45	-0.4	
	5	112.9	8.2	7.29	12.9	
1-(4-CHLOROPHENYL)PIPERAZINE (pCPP)	0.025	89.1	69.9	78.45	-10.9	0.125
	0.125	92.8	16.0	17.25	-7.2	
	1.25	90.8	15.3	16.87	-9.2	
	5	100.8	20.1	19.97	0.8	
1-(4-FLUOROPHENYL)PIPERAZINE (FPP)	0.025	124.9	19.1	15.30	24.9	0.125
	0.125	95.6	5.9	6.20	-4.4	
	1.25	94.8	8.8	9.28	-5.2	
	5	95.8	6.8	7.11	-4.2	
1.4-DIBENZYLPIPERAZINE (DBZP)	0.025	109.6	28.6	26.09	9.6	0.125
	0.125	103.7	14.9	14.38	3.7	
	1.25	90.9	10.5	11.51	-9.1	
	5	107.3	17.8	16.59	7.3	
1-AMINOINDAN	0.125	98.0	17.4	17.78	-2.0	0.125
	1.25	103.3	11.6	11.26	3.3	
	5	110.2	14.2	12.88	10.2	
1-METHYL-4-BENZYLPIPERAZINE (MBZP)	0.025	135.7	43.4	32.00	35.7	0.125
	0.125	98.5	12.3	12.51	-1.5	
	1.25	80.4	5.4	6.71	-19.6	
	5	92.2	8.5	9.24	-7.8	
1-METHYLAMINO-1-(3.4-METHYLENEDIOXYPHENYL)PROPANE	0.025	106.2	25.7	24.16	6.2	0.125
	0.125	108.5	13.9	12.79	8.5	
	1.25	116.0	11.3	9.74	16.0	
	5	119.2	9.3	7.76	19.2	
2.3-DICHLOROPHENYLPIPERAZINE (DCPP)	0.025	125.2	26.0	20.76	25.2	0.125
	0.125	109.1	10.3	9.40	9.1	
	1.25	95.7	10.0	10.49	-4.3	
	5	87.7	7.6	8.71	-12.3	
2.3-DIMETHYLETHCATHINONE (2.3-DMEC)	0.025	118.1	27.0	22.88	18.1	0.125
	0.125	101.8	6.0	5.91	1.8	
	1.25	97.7	3.7	3.77	-2.3	
	5	102.0	10.8	10.57	2.0	
2.3-DIMETHYLMETHCATHINONE (2.3-DMMC)	0.025	109.5	38.2	34.90	9.5	0.125
	0.125	102.1	18.9	18.47	2.1	
	1.25	88.0	8.3	9.44	-12.0	
	5	94.5	14.6	15.42	-5.5	
2.3-ETHYLONE ISOMER	0.025	125.5	17.8	14.17	25.5	0.125

	0.125	114.6	5.5	4.82	14.6	
	1.25	98.5	11.1	11.30	-1.5	
	5	99.7	13.2	13.20	-0.3	
2.3-MDMA	0.025	187.9	49.7	26.47	87.9	0.125
	0.125	103.2	12.4	12.00	3.2	
	1.25	102.3	3.8	3.75	2.3	
	5	99.5	7.2	7.27	-0.5	
2.3-MDPV	0.025	99.6	8.9	8.91	-0.4	0.125
	0.125	101.7	4.5	4.41	1.7	
	1.25	104.7	8.7	8.28	4.7	
	5	109.6	9.2	8.39	9.6	
2.4.5-TRIMETHOXYAMPHETAMINE	0.125	102.5	19.1	18.67	2.5	0.125
	1.25	97.6	12.8	13.08	-2.4	
	5	93.2	5.6	5.97	-6.8	
2.4-DIMETHYLMETHCATHINONE (2.4-DMMC)	0.025	95.2	29.2	30.64	-4.8	0.125
	0.125	95.6	5.7	5.96	-4.4	
	1.25	94.6	8.4	8.88	-5.4	
	5	112.5	8.5	7.58	12.5	
2.4-DMEC	0.025	99.1	21.9	22.06	-1.0	0.125
	0.125	85.2	12.1	14.18	-14.8	
	1.25	80.5	6.0	7.49	-19.5	
	5	89.4	13.9	15.53	-10.6	
2.5-DMMA	0.025	104.2	22.2	21.32	4.2	0.125
	0.125	106.7	10.8	10.08	6.7	
	1.25	112.8	6.3	5.59	12.8	
	5	110.6	5.6	5.03	10.6	
25B-NBF	0.025	99.4	9.9	9.96	-0.6	0.125
	0.125	93.4	7.9	8.44	-6.6	
	1.25	81.4	14.8	18.17	-18.6	
	5	103.7	8.9	8.55	3.7	
25C-NBF	0.025	110.4	11.6	10.49	10.4	0.125
	0.125	107.3	11.1	10.35	7.3	
	1.25	100.2	12.9	12.87	0.2	
	5	110.3	8.9	8.06	10.3	
25C-NBOH	0.025	108.2	20.8	19.19	8.2	0.125
	0.125	98.7	15.5	15.74	-1.3	
	1.25	87.6	12.0	13.71	-12.4	
	5	101.4	10.7	10.55	1.4	
25C-NBOMe	0.025	101.7	12.7	12.48	1.7	0.125
	0.125	99.8	10.5	10.57	-0.2	
	1.25	88.5	14.0	15.79	-11.5	
	5	111.7	7.2	6.44	11.7	
25D-NBOMe	0.025	109.2	9.5	8.68	9.2	0.125
	0.125	107.2	8.5	7.89	7.2	
	1.25	91.0	9.2	10.15	-9.0	
	5	101.7	13.0	12.77	1.7	

25E-NBOMe	0.025	102.6	12.6	12.26	2.6	0.125
	0.125	108.2	5.0	4.64	8.2	
	1.25	89.9	12.5	13.86	-10.1	
	5	113.7	9.6	8.41	13.7	
25G-NBOMe	0.025	110.6	9.1	8.23	10.6	0.125
	0.125	107.9	4.9	4.57	7.9	
	1.25	97.7	9.8	10.00	-2.3	
	5	113.0	12.1	10.70	13.0	
25H-NBOMe	0.025	110.4	10.9	9.87	10.4	0.125
	0.125	110.8	5.4	4.88	10.8	
	1.25	101.3	4.8	4.78	1.3	
	5	111.1	7.4	6.62	11.1	
25-I-NB2OMe	0.025	102.1	11.6	11.32	2.1	0.125
	0.125	102.2	18.5	18.10	2.2	
	1.25	81.4	11.6	14.22	-18.6	
	5	115.1	14.2	12.35	15.1	
25I-NB3OMe	0.025	71.7	15.6	21.74	-28.3	0.125
	0.125	120.0	5.8	4.81	20.0	
	1.25	83.8	11.1	13.23	-16.2	
	5	100.7	10.5	10.42	0.7	
25I-NB4OMe	0.025	99.2	14.7	14.78	-0.8	0.125
	0.125	119.6	17.1	14.33	19.6	
	1.25	91.5	12.2	13.31	-8.5	
	5	118.9	5.8	4.89	18.9	
25I-NBF	0.025	89.5	14.9	16.64	-10.6	0.125
	0.125	108.1	12.0	11.14	8.1	
	1.25	92.3	7.3	7.95	-7.7	
	5	110.5	11.7	10.60	10.5	
25I-NBMD	0.025	97.1	14.1	14.56	-2.9	0.125
	0.125	96.3	6.4	6.66	-3.7	
	1.25	97.6	6.5	6.64	-2.4	
	5	110.1	14.2	12.86	10.1	
25I-NBOH	0.025	106.0	7.0	6.58	6.0	0.125
	0.125	102.7	9.6	9.34	2.7	
	1.25	83.5	4.8	5.72	-16.5	
	5	98.3	6.9	7.00	-1.7	
25N-NBOMe	0.025	90.2	12.6	13.97	-9.8	0.125
	0.125	105.5	9.9	9.35	5.5	
	1.25	96.8	8.9	9.16	-3.2	
	5	108.6	8.0	7.38	8.6	
25T2-NBOMe	0.025	88.5	14.8	16.73	-11.5	0.125
	0.125	99.8	8.7	8.73	-0.2	
	1.25	91.3	10.7	11.75	-8.7	
	5	107.8	11.7	10.88	7.8	
25T-NBOMe	0.025	107.3	10.0	9.30	7.3	0.125
	0.125	100.7	3.7	3.63	0.7	

	1.25	95.0	3.0	3.20	-5.0	
	5	114.9	10.7	9.33	14.9	
2-AMINO-1-PHENYLBUTANE	0.025	113.1	19.7	17.42	13.1	0.125
	0.125	99.7	15.6	15.66	-0.3	
	1.25	99.0	12.2	12.30	-1.0	
	5	106.5	15.6	14.61	6.5	
2-AMINOINDANE	0.025	125.3	32.1	25.61	25.3	0.125
	0.125	104.1	9.0	8.61	4.1	
	1.25	97.1	6.6	6.74	-2.9	
	5	102.7	8.9	8.67	2.7	
2-BROMOAMPHETAMINE	0.025	123.5	26.7	21.63	23.5	0.125
	0.125	115.4	8.3	7.18	15.4	
	1.25	109.5	10.1	9.19	9.5	
	5	107.5	11.9	11.08	7.5	
2-BROMOMETHAMPHETAMINE	0.025	107.0	22.7	21.26	7.0	0.125
	0.125	109.6	9.1	8.31	9.6	
	1.25	107.1	16.0	14.93	7.1	
	5	113.2	10.5	9.25	13.2	
2C-B	0.025	47.7	30.3	63.44	-52.3	0.125
	0.125	83.0	9.3	11.22	-17.0	
	1.25	90.3	11.1	12.32	-9.7	
	5	113.2	4.6	4.09	13.2	
2C-B_FLY	0.025	99.7	25.9	25.97	-0.3	0.125
	0.125	119.2	19.6	16.46	19.2	
	1.25	102.4	8.9	8.64	2.4	
	5	112.5	18.0	16.04	12.5	
2C-C	0.025	176.0	125.3	71.22	76.0	0.125
	0.125	98.1	16.6	16.96	-1.9	
	1.25	93.5	13.1	13.96	-6.5	
	5	94.3	6.7	7.11	-5.7	
2C-D	0.025	1513.1	929.0	61.40	1413.1	-
	0.125	307.3	181.5	59.07	207.3	
	1.25	129.3	59.1	45.69	29.3	
	5	168.5	66.0	39.18	68.5	
2C-G	0.025	95.1	22.9	24.12	-4.9	0.125
	0.125	103.4	19.5	18.86	3.4	
	1.25	86.3	8.8	10.17	-13.7	
	5	101.0	12.1	11.97	1.0	
2-CHLOROAMPHETAMINE	0.025	101.9	16.5	16.23	1.9	0.125
	0.125	111.1	9.3	8.38	11.1	
	1.25	100.6	15.3	15.17	0.6	
	5	108.1	11.0	10.20	8.1	
2C-I	0.025	114.7	35.3	30.77	14.7	0.125
	0.125	87.6	14.1	16.14	-12.4	
	1.25	88.3	11.2	12.64	-11.7	
	5	114.8	12.3	10.73	14.8	

2C-P	0.025	179.1	121.1	67.61	79.1	0.125
	0.125	109.0	14.4	13.26	9.0	
	1.25	92.0	12.6	13.70	-8.0	
	5	113.0	16.7	14.75	13.0	
2C-T-7	0.025	125.1	30.6	24.48	25.1	0.125
	0.125	94.6	11.2	11.81	-5.4	
	1.25	105.4	13.0	12.30	5.4	
	5	118.1	18.8	15.94	18.1	
2C-TFM	0.025	125.6	31.0	24.69	25.6	0.125
	0.125	115.7	12.0	10.41	15.7	
	1.25	92.5	18.5	19.99	-7.5	
	5	100.0	14.9	14.88	0.0	
2-FEC	0.025	81.3	24.2	29.82	-18.7	0.125
	0.125	94.5	13.7	14.54	-5.5	
	1.25	80.3	5.7	7.08	-19.7	
	5	83.2	4.9	5.91	-16.8	
2-FIC	0.025	104.4	21.3	20.36	4.4	0.125
	0.125	99.5	13.2	13.31	-0.5	
	1.25	110.4	9.2	8.30	10.4	
	5	110.2	7.3	6.62	10.2	
2-FLUOROAMPHETAMINE	0.025	110.4	9.2	8.36	10.4	0.125
	0.125	103.2	10.9	10.57	3.2	
	1.25	107.8	15.5	14.38	7.8	
	5	111.0	7.2	6.45	11.0	
2-FLUOROMETHAMPHETAMINE (2-FMA)	0.025	120.8	17.3	14.35	20.8	0.125
	0.125	113.0	8.1	7.21	13.0	
	1.25	102.7	5.3	5.14	2.7	
	5	105.2	7.8	7.36	5.2	
2-FLUOROMETHCATHINONE (2-FMC)	0.025	97.7	20.8	21.28	-2.3	0.125
	0.125	96.8	4.8	4.93	-3.2	
	1.25	89.0	4.0	4.48	-11.0	
	5	86.2	9.2	10.66	-13.8	
2-IODOAMPHETAMINE	0.025	109.0	25.8	23.66	9.0	0.125
	0.125	111.1	12.6	11.35	11.1	
	1.25	88.7	6.2	6.95	-11.3	
	5	96.7	8.7	9.02	-3.3	
2-MAPB	0.025	85.2	22.2	26.08	-14.8	0.125
	0.125	98.8	15.9	16.09	-1.2	
	1.25	93.3	12.8	13.70	-6.7	
	5	92.4	10.4	11.22	-7.6	
2-MeOMC	0.025	100.1	22.4	22.40	0.1	0.125
	0.125	111.9	7.0	6.27	11.9	
	1.25	94.2	10.5	11.10	-5.8	
	5	103.3	9.2	8.86	3.3	
2-METHOXY-2-PHENYLETHYLAMINE	0.025	79.4	15.2	19.09	-20.6	0.125
	0.125	90.9	11.6	12.81	-9.1	

	1.25	99.6	8.0	8.02	-0.4	
	5	100.6	9.5	9.44	0.6	
2-METHOXYAMPHETAMINE (2-MA)	0.025	111.2	12.3	11.07	11.2	0.125
	0.125	96.7	11.0	11.41	-3.3	
	1.25	98.9	12.8	12.95	-1.1	
	5	109.3	7.3	6.69	9.3	
2-METHOXYMETHAMPHETAMINE (2-MeOMA)	0.025	45.6	15.5	33.87	-54.4	0.125
	0.125	101.7	18.9	18.60	1.7	
	1.25	81.6	7.0	8.61	-18.4	
	5	93.9	9.3	9.85	-6.1	
2-METHYLAMINO-1-PHENYLBUTANE	0.025	56.4	30.7	54.54	-43.6	0.125
	0.125	100.2	13.0	12.98	0.2	
	1.25	99.3	11.9	11.94	-0.7	
	5	98.6	10.6	10.79	-1.4	
2-METHYLMETHCATHINONE (2-MMC)	0.025	104.6	18.2	17.35	4.6	0.125
	0.125	93.3	5.4	5.76	-6.7	
	1.25	97.5	10.4	10.67	-2.5	
	5	102.0	14.2	13.89	2.0	
2-METHYL-PBP	0.025	124.7	41.6	33.37	24.7	0.125
	0.125	96.8	9.2	9.53	-3.2	
	1.25	91.4	11.9	12.98	-8.6	
	5	107.0	6.7	6.23	7.0	
2-METHYL-PPP	0.025	106.0	23.0	21.71	6.0	0.125
	0.125	92.9	9.5	10.21	-7.1	
	1.25	91.2	13.9	15.26	-8.8	
	5	105.4	9.1	8.65	5.4	
3.4-DICHLOROMETHYLPHENIDATE (3.4-CTMP)	0.025	115.9	29.4	25.41	15.9	0.125
	0.125	102.3	15.1	14.80	2.3	
	1.25	94.6	13.3	14.02	-5.4	
	5	115.5	14.3	12.41	15.5	
3.4-DIMETHOXY-ALPHA-PVP	0.025	80.6	14.8	18.35	-19.4	0.125
	0.125	106.6	8.9	8.38	6.6	
	1.25	107.3	8.2	7.67	7.3	
	5	119.5	9.9	8.29	19.5	
3.4-DIMETHYLMETHCATHINONE (3.4-DMMC)	0.025	89.8	26.1	29.06	-10.2	0.125
	0.125	108.3	19.0	17.55	8.3	
	1.25	100.4	13.5	13.42	0.4	
	5	109.7	11.6	10.54	9.7	
3.4-DMEC	0.025	89.4	29.7	33.15	-10.6	0.125
	0.125	97.5	8.6	8.80	-2.5	
	1.25	106.2	13.6	12.84	6.2	
	5	111.5	16.0	14.35	11.5	
3.4-DMMA	0.025	112.1	21.3	19.04	12.1	0.125
	0.125	105.7	12.1	11.40	5.7	
	1.25	116.4	11.1	9.56	16.4	
	5	117.4	7.5	6.42	17.4	

3.4-EDMA	0.025	101.9	14.7	14.42	1.9	0.125
	0.125	95.8	7.4	7.74	-4.2	
	1.25	97.6	12.6	12.91	-2.4	
	5	110.2	12.8	11.62	10.2	
3.4-EDMC	0.025	94.8	21.3	22.43	-5.2	0.125
	0.125	100.6	12.3	12.24	0.6	
	1.25	89.7	9.1	10.12	-10.3	
	5	101.7	7.4	7.26	1.7	
3.4-MDMA (ECSTAZY)	0.025	86.9	12.6	14.50	-13.1	0.125
	0.125	95.6	13.3	13.87	-4.4	
	1.25	114.2	7.7	6.72	14.2	
	5	116.8	11.9	10.19	16.8	
3.4-MDPA	0.025	134.5	29.3	21.82	34.5	0.125
	0.125	111.6	9.5	8.48	11.6	
	1.25	102.0	8.3	8.14	2.0	
	5	119.7	14.1	11.76	19.7	
3.4-MDPHP	0.025	84.5	26.7	31.57	-15.5	0.125
	0.125	88.7	9.4	10.56	-11.3	
	1.25	91.4	11.0	12.05	-8.6	
	5	108.6	14.9	13.71	8.6	
3.4-METHYLENDIOXYPYROVALERONE	0.025	83.6	16.0	19.13	-16.4	0.125
	0.125	101.4	15.7	15.49	1.4	
	1.25	107.1	8.4	7.83	7.1	
	5	117.2	8.9	7.60	17.2	
3.4-METHYLENEDIOXY_PV9	0.025	107.9	5.5	5.14	7.9	0.125
	0.125	113.5	6.6	5.83	13.5	
	1.25	96.5	7.5	7.80	-3.5	
	5	109.4	11.2	10.25	9.4	
30C-NBOMe	0.025	96.0	10.4	10.80	-4.0	0.125
	0.125	95.4	9.0	9.41	-4.6	
	1.25	101.0	18.3	18.12	1.0	
	5	116.9	9.8	8.39	16.9	
3-BROMOAMPHETAMINE	0.025	149.7	55.0	36.72	49.7	0.125
	0.125	114.9	11.5	9.99	14.9	
	1.25	117.9	11.8	10.02	17.9	
	5	112.3	21.2	18.87	12.3	
3-BROMOMETHAMPHETAMINE	0.025	106.8	10.1	9.44	6.8	0.125
	0.125	106.2	14.8	13.89	6.2	
	1.25	105.5	16.7	15.81	5.5	
	5	109.7	13.8	12.60	9.7	
3-BROMOMETHCATHINONE (3-BMC)	0.025	90.6	15.8	17.47	-9.4	0.125
	0.125	98.4	6.8	6.90	-1.6	
	1.25	94.3	6.0	6.36	-5.7	
	5	97.4	8.0	8.23	-2.6	
3-CAF	0.025	118.8	13.6	11.48	18.8	0.125
	0.125	118.0	5.9	4.97	18.0	

	1.25	181.2	21.3	11.73	81.2	
3C-B-FLY	0.025	84.3	26.1	30.91	-15.7	0.125
	0.125	93.5	14.1	15.04	-6.5	
	1.25	93.0	12.8	13.76	-7.0	
	5	108.2	5.8	5.36	8.2	
3-CHLOROAMPHETAMINE	0.025	99.6	56.3	56.47	-0.4	0.125
	0.125	86.6	16.9	19.51	-13.4	
	1.25	96.8	12.4	12.79	-3.2	
	5	105.9	11.2	10.54	5.9	
3-CHLOROMETHCATHINONE (3-CMC)	0.025	96.1	14.9	15.48	-3.9	0.125
	0.125	105.5	9.9	9.40	5.5	
	1.25	98.8	12.7	12.85	-1.2	
	5	93.0	11.2	12.06	-7.0	
3-CHLOROPHENYLPIPERAZINE (mCPP)	0.025	105.6	21.9	20.76	5.6	0.125
	0.125	89.4	4.8	5.38	-10.6	
	1.25	94.7	9.3	9.82	-5.3	
	5	90.6	9.3	10.23	-9.4	
3C-P	0.025	108.8	12.7	11.68	8.8	0.125
	0.125	85.6	9.3	10.90	-14.4	
	1.25	99.8	17.4	17.45	-0.2	
	5	99.1	6.3	6.37	-0.9	
3-DESOXY-3.4-MDPV	0.025	97.0	13.9	14.35	-3.0	0.125
	0.125	92.8	9.2	9.88	-7.2	
	1.25	92.3	10.6	11.45	-7.7	
	5	92.4	11.1	12.07	-7.6	
3-ETHYLMETHCATHINONE (3-EMC)	0.025	97.2	7.0	7.23	-2.8	0.125
	0.125	97.4	11.7	12.02	-2.6	
	1.25	109.4	15.3	13.98	9.4	
	5	100.4	6.1	6.06	0.4	
3-FEC	0.025	149.7	16.1	10.78	49.7	0.125
	0.125	117.1	10.2	8.70	17.1	
	1.25	103.7	6.1	5.89	3.7	
	5	104.3	8.9	8.57	4.3	
3-FLUORO-ALFA-PPP	0.025	116.1	9.5	8.18	16.1	0.125
	0.125	99.5	7.6	7.67	-0.5	
	1.25	104.4	9.3	8.91	4.4	
	5	111.3	11.9	10.65	11.3	
3-FLUOROAMPHETAMINE	0.025	72.6	9.0	12.37	-27.4	0.125
	0.125	92.0	13.8	15.05	-8.0	
	1.25	99.2	5.5	5.59	-0.8	
	5	107.9	17.1	15.84	7.9	
3-FLUOROMETHAMPHETAMINE (3-FMA)	0.025	127.1	17.0	13.42	27.1	0.125
	0.125	106.1	7.7	7.27	6.1	
	1.25	96.7	7.0	7.26	-3.3	
	5	103.7	4.1	3.93	3.7	
3-FLUOROMETHCATHINONE (3-FMC)	0.025	96.4	17.1	17.76	-3.6	0.125

	0.125	95.2	3.8	3.96	-4.8	
	1.25	95.3	7.6	7.94	-4.7	
	5	94.7	5.7	6.02	-5.3	
3-HYDROXYBROMAZEPAM	0.025	87.5	33.2	37.98	-12.5	0.125
	0.125	83.4	12.8	15.30	-16.6	
	1.25	90.5	10.0	11.06	-9.5	
	5	98.2	8.2	8.32	-1.8	
3-HYDROXYFLUNITRAZEPAM	0.125	93.6	17.6	18.81	-6.4	0.125
	1.25	97.9	12.4	12.66	-2.1	
	5	110.3	6.7	6.04	10.3	
3-IODOAMPHETAMINE	0.025	92.2	25.1	27.27	-7.8	0.125
	0.125	119.6	7.1	5.96	19.6	
	1.25	109.5	11.9	10.89	9.5	
	5	101.5	15.6	15.36	1.5	
3-MEC	0.025	125.1	29.0	23.15	25.1	0.125
	0.125	105.1	11.9	11.33	5.1	
	1.25	92.2	12.3	13.35	-7.8	
	5	104.1	13.3	12.74	4.1	
3-MeOMC	0.025	93.9	10.7	11.42	-6.1	0.125
	0.125	91.1	8.8	9.65	-8.9	
	1.25	89.7	4.7	5.20	-10.3	
	5	88.7	8.7	9.85	-11.3	
3-METHOXYAMPHETAMINE (3-MA)	0.025	134.1	20.4	15.23	34.1	0.125
	0.125	94.0	18.1	19.31	-6.0	
	1.25	109.6	6.1	5.58	9.6	
	5	109.3	10.8	9.87	9.3	
3-METHOXYPHENCYCLIDINE	0.025	99.9	21.5	21.54	-0.1	0.125
	0.125	110.8	11.2	10.11	10.8	
	1.25	85.3	6.2	7.31	-14.7	
	5	107.2	6.3	5.88	7.2	
3-METHYLMETHCATHINONE (3-MMC)	0.025	100.4	7.9	7.91	0.4	0.125
	0.125	95.4	8.4	8.77	-4.6	
	1.25	108.8	5.9	5.40	8.8	
	5	105.3	9.1	8.64	5.3	
3-METHYL-PBP	0.025	103.9	14.3	13.76	3.9	0.125
	0.125	105.0	5.8	5.55	5.0	
	1.25	99.1	12.2	12.35	-0.9	
	5	105.4	7.6	7.23	5.4	
3-METHYL-PPP	0.025	109.0	27.1	24.87	9.0	0.125
	0.125	106.0	9.0	8.52	6.0	
	1.25	103.2	8.9	8.62	3.2	
	5	108.6	12.3	11.36	8.6	
4.4'-DMAR	0.025	82.0	11.6	14.09	-18.0	0.125
	0.125	95.0	11.6	12.25	-5.0	
	1.25	107.9	6.7	6.20	7.9	
	5	115.0	13.8	11.97	15.0	

4-AcO-DET	0.025	86.4	17.9	20.66	-13.6	0.125
	0.125	109.6	9.4	8.56	9.6	
	1.25	94.5	18.0	19.03	-5.5	
	5	100.3	11.7	11.71	0.3	
4-AcO-DMT	0.025	108.5	23.9	21.98	8.5	0.125
	0.125	108.3	11.2	10.32	8.3	
	1.25	91.0	14.9	16.37	-9.0	
	5	85.5	10.4	12.22	-14.5	
4-AcO-MET	0.025	72.2	31.6	43.79	-27.8	0.125
	0.125	105.1	10.9	10.34	5.1	
	1.25	96.8	13.8	14.30	-3.2	
	5	108.4	12.5	11.54	8.4	
4-APB	0.025	110.7	12.9	11.61	10.7	0.125
	0.125	94.5	10.1	10.71	-5.5	
	1.25	109.7	20.1	18.33	9.7	
	5	115.0	14.6	12.67	15.0	
4-APDB	0.025	163.7	110.3	67.38	63.7	0.125
	0.125	117.4	12.6	10.75	17.4	
	1.25	98.0	12.2	12.42	-2.0	
	5	105.8	12.7	11.97	5.8	
4-BROMO-2.5-DMMA	0.025	105.3	21.6	20.52	5.3	0.125
	0.125	102.8	16.3	15.84	2.8	
	1.25	105.3	17.0	16.16	5.3	
	5	115.5	14.6	12.66	15.5	
4-BROMOAMPHETAMINE	0.025	109.8	45.6	41.55	9.8	0.125
	0.125	98.1	11.1	11.31	-1.9	
	1.25	103.9	7.4	7.14	3.9	
	5	111.0	16.1	14.53	11.0	
4-BROMOMETHAMPHETAMINE	0.025	130.7	18.2	13.93	30.7	0.125
	0.125	102.5	14.3	13.98	2.5	
	1.25	86.5	7.3	8.45	-13.5	
	5	101.4	14.6	14.39	1.4	
4-BROMOMETHCATHINONE (BREFEDRONE)	0.025	138.7	55.3	39.84	38.7	0.125
	0.125	85.6	15.9	18.63	-14.4	
	1.25	103.9	11.1	10.69	3.9	
	5	119.8	11.8	9.83	19.8	
4-CAB	0.025	89.4	23.5	26.25	-10.7	0.125
	0.125	103.1	10.9	10.55	3.1	
	1.25	100.7	11.4	11.33	0.7	
	5	114.2	5.5	4.79	14.2	
4-CEC	0.025	66.3	34.2	51.48	-33.7	0.125
	0.125	97.2	19.4	19.92	-2.8	
	1.25	93.9	3.4	3.64	-6.1	
	5	97.9	8.2	8.37	-2.1	
4-CHLORO-ALPHA-PPP	0.025	105.6	15.5	14.71	5.6	0.125
	0.125	92.3	7.5	8.17	-7.7	

	1.25	102.5	10.8	10.49	2.5	
	5	110.0	8.4	7.68	10.0	
4-CHLORO-ALPHA-PVP	0.025	100.0	16.1	16.08	0.0	0.125
	0.125	97.8	9.4	9.59	-2.2	
	1.25	81.8	7.8	9.50	-18.2	
	5	96.3	4.3	4.45	-3.7	
4-CHLOROAMPHETAMINE	0.025	103.5	39.1	37.75	3.5	0.125
	0.125	104.0	7.4	7.08	4.0	
	1.25	80.7	2.7	3.33	-19.3	
	5	110.1	18.7	17.00	10.1	
4-CHLOROMETHCATHINONE (4-CMC)	0.025	89.7	17.4	19.38	-10.4	0.125
	0.125	96.5	15.4	15.92	-3.5	
	1.25	92.9	11.7	12.59	-7.1	
	5	95.7	12.3	12.89	-4.3	
4-CMA	0.025	123.6	10.8	8.77	23.6	0.125
	0.125	102.9	11.6	11.31	2.9	
	1.25	102.8	12.8	12.49	2.8	
	5	107.5	13.2	12.27	7.5	
4-EAPB	0.025	85.1	5.9	6.95	-14.9	0.125
	0.125	91.3	6.7	7.30	-8.7	
	1.25	97.4	11.9	12.18	-2.6	
	5	100.1	8.2	8.19	0.1	
4-ETHYL-N.N-DMC	0.025	80.0	17.1	21.43	-20.0	0.125
	0.125	92.2	8.4	9.06	-7.8	
	1.25	103.5	7.3	7.06	3.5	
	5	106.4	6.7	6.34	6.4	
4-FEC	0.025	100.3	15.4	15.32	0.3	0.125
	0.125	104.8	10.3	9.84	4.8	
	1.25	90.3	4.1	4.57	-9.7	
	5	89.8	4.8	5.30	-10.2	
4-FLUORO BUPHEDRONE	0.025	81.6	14.6	17.90	-18.4	0.125
	0.125	106.4	10.4	9.82	6.4	
	1.25	102.8	10.2	9.90	2.8	
	5	107.4	10.2	9.52	7.4	
4-FLUORO PENTEDRONE	0.025	108.1	21.5	19.85	8.1	0.125
	0.125	116.3	12.8	11.00	16.3	
	1.25	94.1	13.4	14.21	-5.9	
	5	109.1	7.3	6.74	9.1	
4-FLUORO PV8	0.025	108.5	6.5	5.97	8.5	0.125
	0.125	97.7	7.1	7.26	-2.3	
	1.25	98.2	8.5	8.69	-1.8	
	5	110.3	7.0	6.36	10.3	
4-FLUORO PV9	0.025	104.9	8.8	8.40	4.9	0.125
	0.125	104.1	5.1	4.95	4.1	
	1.25	92.3	7.8	8.39	-7.7	
	5	98.7	8.7	8.80	-1.3	

4-FLUORO-ALFA-PPP	0.025	111.1	31.6	28.48	11.1	0.125
	0.125	108.3	10.0	9.20	8.3	
	1.25	97.7	8.1	8.25	-2.3	
	5	108.6	11.8	10.89	8.6	
4-FLUOROMETHAMPHETAMINE (4-FMA)	0.025	103.1	7.8	7.59	3.1	0.125
	0.125	101.9	6.8	6.66	1.9	
	1.25	91.7	10.8	11.78	-8.3	
	5	99.3	13.7	13.84	-0.7	
4-FLUOROMETHCATHINONE (4-FMC)	0.025	107.3	10.3	9.65	7.3	0.125
	0.125	97.5	13.5	13.86	-2.5	
	1.25	99.9	4.3	4.28	-0.1	
	5	102.5	5.9	5.76	2.5	
4F-PVP	0.025	112.5	12.3	10.97	12.5	0.125
	0.125	105.7	7.2	6.79	5.7	
	1.25	101.8	10.4	10.18	1.8	
	5	115.8	7.7	6.64	15.8	
4-HYDROXY DiPT	0.025	97.9	28.9	29.56	-2.1	0.125
	0.125	99.1	15.5	15.66	-0.9	
	1.25	102.6	15.3	14.94	2.6	
	5	113.4	8.7	7.68	13.4	
4-HYDROXYMIDAZOLAM	0.025	34.7	26.5	76.51	-65.3	1.25
	0.125	42.5	16.8	39.57	-57.5	
	1.25	90.7	11.7	12.90	-9.3	
	5	86.2	12.5	14.46	-13.8	
4-IODOAMPHETAMINE	0.025	182.6	61.4	33.60	82.6	0.125
	0.125	95.9	16.8	17.55	-4.1	
	1.25	101.4	19.5	19.24	1.4	
	5	111.4	7.7	6.92	11.4	
4-MAPB	0.025	92.6	20.8	22.42	-7.4	0.125
	0.125	113.2	18.7	16.52	13.2	
	1.25	93.3	8.5	9.14	-6.7	
	5	105.7	17.5	16.51	5.7	
4-MEAP	0.025	99.4	17.3	17.36	-0.6	0.125
	0.125	105.8	14.3	13.50	5.8	
	1.25	96.8	12.7	13.14	-3.2	
	5	112.4	12.0	10.70	12.4	
4-MEO-ALPHA-PVP	0.025	74.8	23.2	30.97	-25.2	0.125
	0.125	99.7	7.8	7.82	-0.3	
	1.25	118.5	17.3	14.61	18.5	
	5	111.0	9.3	8.36	11.0	
4-MeOPBP	0.025	120.9	11.0	9.10	20.9	0.125
	0.125	93.5	9.7	10.32	-6.5	
	1.25	105.0	6.4	6.10	5.0	
	5	111.9	6.9	6.14	11.9	
4-METHOXY PHENCYCLIDINE	0.025	98.5	11.7	11.88	-1.5	0.125
	0.125	103.0	12.3	11.92	3.0	

	1.25	112.4	6.6	5.90	12.4	
	5	107.5	6.7	6.26	7.5	
4-METHOXY PV8	0.025	104.1	9.9	9.56	4.1	0.125
	0.125	101.5	6.7	6.62	1.5	
	1.25	91.4	3.5	3.83	-8.6	
	5	109.2	15.3	14.05	9.2	
4-METHOXY PV9	0.025	99.2	11.5	11.57	-0.8	0.125
	0.125	101.2	7.9	7.80	1.2	
	1.25	87.4	8.8	10.08	-12.6	
	5	110.7	17.4	15.73	10.7	
4-METHOXYMETHAMPHETAMINE (PMMA)	0.025	101.0	33.6	33.23	1.0	0.125
	0.125	96.6	8.4	8.74	-3.4	
	1.25	93.2	8.1	8.72	-6.8	
	5	106.1	9.7	9.18	6.1	
4-METHYL PENTEDRONE	0.025	100.9	5.5	5.49	0.9	0.125
	0.125	97.8	10.8	11.07	-2.2	
	1.25	87.5	4.6	5.30	-12.5	
	5	95.5	15.0	15.70	-4.5	
4-METHYL-ALPHA-ETHYLAMINOBUTIOPHENONE	0.025	60.3	11.4	18.88	-39.8	0.125
	0.125	88.3	13.3	15.04	-11.7	
	1.25	98.7	10.2	10.36	-1.3	
	5	108.0	14.5	13.43	8.0	
4-METHYLAMPHETAMINE	0.025	103.0	49.3	47.92	3.0	0.125
	0.125	91.2	5.4	5.91	-8.8	
	1.25	105.1	14.2	13.54	5.1	
	5	118.4	16.7	14.10	18.4	
4-METHYLCATHINONE	0.025	88.5	29.8	33.72	-11.5	0.125
	0.125	93.0	6.6	7.07	-7.0	
	1.25	115.2	17.2	14.93	15.2	
	5	105.0	8.7	8.32	5.0	
4-METHYLMETHAMPHETAMINE (4-MMA)	0.025	99.0	19.7	19.92	-1.1	0.125
	0.125	99.2	8.3	8.35	-0.8	
	1.25	115.5	11.0	9.52	15.5	
	5	114.7	5.8	5.06	14.7	
4-METHYLMETHCATHINONE (4-MMC)	0.025	109.6	5.6	5.09	9.6	0.125
	0.125	102.6	7.2	6.99	2.6	
	1.25	109.7	14.4	13.16	9.7	
	5	113.4	9.1	8.03	13.4	
4-METHYL-N.N-DMC	0.025	125.2	35.5	28.37	25.2	0.125
	0.125	93.1	10.3	11.07	-6.9	
	1.25	105.4	7.4	7.01	5.4	
	5	118.2	9.0	7.62	18.2	
4-METHYL-N-METHYLBUPHEDRONE	0.025	132.2	35.4	26.75	32.2	0.125
	0.125	99.0	12.0	12.14	-1.0	
	1.25	97.6	6.9	7.04	-2.4	
	5	106.1	7.4	6.95	6.1	

4-METHYL-N-METHYLHEXANOPHENONE	0.025	82.4	13.4	16.27	-17.6	0.125
	0.125	90.6	10.7	11.82	-9.4	
	1.25	90.7	16.8	18.47	-9.3	
	5	98.0	11.0	11.20	-2.0	
4-METHYL-PBP	0.025	106.4	18.2	17.14	6.4	0.125
	0.125	107.5	7.4	6.91	7.5	
	1.25	117.3	13.6	11.63	17.3	
	5	113.8	6.9	6.07	13.8	
4-METHYL-PHP	0.025	106.1	14.0	13.16	6.1	0.125
	0.125	101.1	2.5	2.49	1.1	
	1.25	97.6	9.6	9.80	-2.4	
	5	109.5	7.1	6.49	9.5	
4-METHYL-α-ETHYLTRYPTAMINE	0.025	109.8	56.0	51.00	9.8	0.125
	0.125	104.3	10.7	10.22	4.3	
	1.25	109.8	11.8	10.74	9.8	
	5	100.9	11.7	11.58	0.9	
5-APB	0.125	93.2	16.7	17.89	-6.8	0.125
	1.25	82.6	11.6	14.02	-17.4	
	5	105.7	13.7	12.94	5.7	
5-APDB	0.125	112.4	21.9	19.46	12.4	0.125
	1.25	93.1	10.0	10.78	-6.9	
	5	93.6	13.4	14.37	-6.4	
5-APDI	0.125	106.6	9.0	8.49	6.6	0.125
	1.25	101.3	17.5	17.25	1.3	
	5	99.0	17.2	17.40	-1.0	
5-CHLORO AB-PINACA	0.025	96.7	10.0	10.34	-3.3	0.025
	0.125	103.6	5.7	5.45	3.6	
	1.25	111.1	20.2	18.14	11.1	
5-CHLORO-NNEI	0.025	97.5	17.1	17.53	-2.5	0.025
	0.125	106.1	4.2	3.97	6.1	
	1.25	117.2	8.2	7.00	17.2	
5-EAPB	0.025	46.6	53.3	114.26	-53.4	0.125
	0.125	86.7	6.1	7.01	-13.4	
	1.25	94.2	17.2	18.23	-5.8	
	5	101.1	9.1	9.02	1.1	
5F-ABICA	0.025	106.2	6.6	6.21	6.2	0.025
	0.125	107.3	9.2	8.58	7.3	
	1.25	95.7	10.6	11.03	-4.3	
5F-AB-PINACA	0.025	118.3	8.1	6.86	18.3	0.025
	0.125	104.3	9.1	8.75	4.3	
	1.25	110.8	3.4	3.04	10.8	
5F-ADB (5F-MDMB-PINACA)	0.025	87.3	15.3	17.50	-12.7	0.025
	0.125	106.4	6.8	6.38	6.4	
	1.25	104.3	7.6	7.29	4.3	
5F-AMB (5F-AMB-PINACA)	0.025	103.5	1.1	1.05	3.5	0.025
	0.125	99.3	3.4	3.43	-0.7	

	1.25	101.2	9.0	8.92	1.2	
5F-APICA (STS-135)	0.025	118.1	9.4	7.98	18.1	0.025
	0.125	110.7	8.4	7.63	10.7	
	1.25	115.1	9.8	8.48	15.1	
5F-APINACA (AKB-48-5F)	0.025	115.2	9.2	8.02	15.2	0.025
	0.125	116.2	14.2	12.23	16.2	
	1.25	114.3	20.3	17.75	14.3	
5-F-JWH-018 ADAMANTYL ANALOG	0.025	109.7	9.9	9.02	9.7	0.025
	0.125	111.8	10.3	9.20	11.8	
	1.25	113.4	8.2	7.23	13.4	
5-FLUORO MN-24 (5-FLUORO NNEI)	0.025	111.3	7.0	6.33	11.3	0.025
	0.125	106.7	4.2	3.93	6.7	
	1.25	98.8	8.5	8.60	-1.2	
5-FLUORO THJ	0.025	99.4	8.3	8.34	-0.6	0.025
	0.125	102.6	15.2	14.81	2.6	
	1.25	116.3	17.1	14.67	16.3	
5-FLUORO-2-ADB-PINACA_ISOMER_2	0.025	108.9	15.9	14.62	8.9	0.025
	0.125	110.7	9.4	8.48	10.7	
	1.25	106.9	8.3	7.77	6.9	
5-FLUORO-CUMYL-PICA	0.025	112.0	10.1	8.99	12.0	0.025
	0.125	114.1	5.1	4.43	14.1	
	1.25	102.4	11.5	11.27	2.4	
5-FLUORO-MN-18	0.025	93.9	8.1	8.66	-6.1	0.025
	0.125	99.3	3.9	3.97	-0.7	
	1.25	113.7	15.4	13.51	13.7	
5-FLUORO-MN-21 (5-FLUORO-PCN)	0.025	87.8	9.9	11.33	-12.3	0.025
	0.125	92.0	3.1	3.42	-8.0	
	1.25	85.2	14.9	17.47	-14.8	
5-FLUORO-SDB-006	0.025	113.1	6.4	5.70	13.1	0.025
	0.125	101.5	6.0	5.96	1.5	
	1.25	110.9	8.3	7.49	10.9	
5F-NPB-22	0.025	90.1	14.5	16.09	-9.9	0.025
	0.125	116.8	13.9	11.88	16.8	
	1.25	113.7	12.0	10.56	13.7	
5F-PB-22	0.025	106.9	5.1	4.79	6.9	0.025
	0.125	113.7	9.9	8.74	13.7	
	1.25	91.8	11.2	12.17	-8.2	
5-F-PENTYL-3-PYRIDINOYLINDOLE	0.025	97.1	11.6	11.95	-2.9	0.025
	0.125	107.4	6.7	6.26	7.4	
	1.25	93.1	10.9	11.72	-6.9	
5F-SDB-005	0.025	87.5	11.2	12.80	-12.5	0.025
	0.125	112.9	4.6	4.09	12.9	
	1.25	113.6	10.7	9.42	13.6	
5-HYDROXY DMT	0.025	174.4	24.9	14.28	74.4	0.125
	0.125	113.2	7.0	6.21	13.2	
	1.25	109.2	4.3	3.93	9.2	

	5	115.2	4.7	4.09	15.2	
5-IT	0.025	106.6	66.3	62.18	6.6	0.125
	0.125	82.9	13.3	16.09	-17.1	
	1.25	98.2	11.3	11.52	-1.8	
	5	102.7	10.3	10.06	2.7	
5-MAPB	0.025	114.3	9.9	8.65	14.3	0.125
	0.125	96.2	10.0	10.37	-3.8	
	1.25	108.0	10.7	9.90	8.0	
	5	119.6	14.0	11.72	19.6	
5-MAPDB	0.025	106.8	9.7	9.07	6.8	0.125
	0.125	93.3	9.4	10.05	-6.7	
	1.25	88.6	6.5	7.31	-11.4	
	5	95.7	10.8	11.26	-4.3	
5-MeO-ALPHA-ET	0.025	65.1	27.7	42.57	-34.9	0.125
	0.125	97.6	18.6	19.06	-2.4	
	1.25	119.6	9.3	7.80	19.6	
	5	114.3	8.8	7.73	14.3	
5-MeO-DALT	0.025	98.1	10.2	10.41	-1.9	0.125
	0.125	98.9	7.3	7.42	-1.1	
	1.25	100.3	8.1	8.04	0.3	
	5	114.6	11.2	9.80	14.6	
5-METHOXY AMT	0.025	110.3	35.3	31.99	10.3	0.125
	0.125	98.8	12.8	12.97	-1.2	
	1.25	108.4	12.6	11.67	8.4	
	5	109.9	16.8	15.28	9.9	
5-METHOXY DiPT	0.025	120.2	16.5	13.70	20.2	0.125
	0.125	97.3	6.7	6.86	-2.7	
	1.25	98.2	9.6	9.80	-1.8	
	5	97.7	9.0	9.22	-2.3	
5-METHOXY DMT	0.125	118.7	9.3	7.80	18.7	0.125
	1.25	91.9	10.0	10.88	-8.1	
	5	115.9	21.5	18.52	15.9	
5-METHOXY METHYLONE	0.025	69.1	12.2	17.68	-30.9	0.125
	0.125	105.5	6.4	6.08	5.5	
	1.25	94.7	14.2	14.95	-5.3	
	5	99.7	9.3	9.29	-0.3	
5-METHOXY MiPT	0.125	96.5	16.6	17.20	-3.5	0.125
	1.25	104.9	19.9	18.97	4.9	
	5	118.4	14.8	12.53	18.4	
6-APB	0.125	97.2	17.1	17.57	-2.8	0.125
	1.25	98.0	9.7	9.86	-2.0	
	5	112.5	6.8	6.04	12.5	
6-APDB	0.025	185.7	139.0	74.85	85.7	0.125
	0.125	107.9	17.5	16.20	7.9	
	1.25	94.0	16.1	17.17	-6.0	
	5	117.4	3.9	3.28	17.4	

6-BROMO-MDMA	0.025	109.4	9.9	9.10	9.4	0.125
	0.125	110.0	5.9	5.38	10.0	
	1.25	92.3	16.4	17.73	-7.7	
	5	102.2	17.7	17.32	2.2	
6-CHLORO-MDMA	0.025	94.8	15.1	15.91	-5.2	0.125
	0.125	105.8	11.4	10.77	5.8	
	1.25	97.3	8.7	8.96	-2.7	
	5	101.5	10.8	10.69	1.5	
6-EAPB	0.025	89.2	19.0	21.29	-10.8	0.125
	0.125	104.9	9.6	9.13	4.9	
	1.25	102.2	8.6	8.37	2.2	
	5	109.6	9.6	8.79	9.6	
6-IT	0.025	157.1	62.6	39.85	57.1	0.125
	0.125	110.1	6.6	6.04	10.1	
	1.25	102.8	4.8	4.66	2.8	
	5	105.4	8.0	7.61	5.4	
6-MAM	0.025	136.6	23.3	17.04	36.6	0.125
	0.125	89.0	11.4	12.81	-11.0	
	1.25	96.6	7.1	7.39	-3.4	
	5	104.0	10.9	10.50	4.0	
6-MAPB	0.025	109.6	11.9	10.84	9.6	0.125
	0.125	93.1	11.4	12.27	-7.0	
	1.25	99.7	8.5	8.52	-0.3	
	5	107.0	10.1	9.47	7.0	
7-AMINOCLONAZEPAM	0.025	83.3	44.3	53.18	-16.7	0.125
	0.125	92.5	11.8	12.81	-7.6	
	1.25	101.5	9.1	8.95	1.5	
	5	96.9	7.2	7.42	-3.1	
7-AMINODESMETHYLFLUNITRAZEPAM	0.025	100.3	13.7	13.70	0.3	0.125
	0.125	88.1	7.1	8.06	-11.9	
	1.25	88.0	13.7	15.60	-12.0	
	5	89.9	5.4	5.96	-10.1	
7-AMINOFLUNITRAZEPAM	0.025	89.6	25.8	28.75	-10.4	0.125
	0.125	92.1	13.8	15.00	-7.9	
	1.25	92.0	11.4	12.40	-8.0	
	5	119.8	13.5	11.25	19.8	
7-AMINONITRAZEPAM	0.025	117.3	31.3	26.70	17.3	0.125
	0.125	88.6	11.5	12.99	-11.4	
	1.25	91.4	7.7	8.47	-8.6	
	5	104.2	3.4	3.30	4.2	
7-APB	0.025	117.7	26.6	22.62	17.7	0.125
	0.125	104.1	16.0	15.34	4.1	
	1.25	88.1	9.4	10.68	-11.9	
	5	107.7	13.4	12.42	7.7	
7-APDB	0.025	258.0	163.1	63.20	158.0	0.125
	0.125	104.9	17.6	16.80	4.9	

	1.25	110.0	17.5	15.95	10.0	
	5	112.0	15.1	13.48	12.0	
A-796260	0.025	106.8	12.7	11.86	6.8	0.025
	0.125	101.1	5.3	5.27	1.1	
	1.25	86.8	9.5	10.97	-13.2	
A-834735	0.025	97.5	10.9	11.15	-2.5	0.025
	0.125	106.2	8.3	7.78	6.2	
	1.25	113.5	5.4	4.73	13.5	
A-836339	0.025	102.9	11.8	11.46	2.9	0.025
	0.125	114.4	7.9	6.89	14.4	
	1.25	97.0	9.3	9.61	-3.0	
AB-001	0.025	111.0	12.8	11.58	11.0	0.025
	0.125	114.2	4.2	3.68	14.2	
	1.25	118.4	6.0	5.11	18.4	
AB005	0.025	101.6	13.7	13.50	1.6	0.025
	0.125	103.4	12.0	11.60	3.4	
	1.25	87.2	10.4	11.92	-12.8	
AB-CHMINACA	0.025	110.7	9.3	8.44	10.7	0.025
	0.125	111.4	4.3	3.86	11.4	
	1.25	113.8	9.1	7.97	13.8	
AB-FUBINACA	0.025	141.1	51.2	36.28	41.1	0.125
	0.125	104.9	15.5	14.75	4.9	
	1.25	105.5	7.5	7.08	5.5	
AB-FUBINACA 2-FLUOROBENZYL ISOMER	0.025	104.9	7.0	6.69	4.9	0.025
	0.125	110.3	7.9	7.15	10.3	
	1.25	104.4	11.9	11.38	4.4	
AB-FUBINACA 3-FLUOROBENZYL ISOMER	0.025	99.8	11.0	11.00	-0.2	0.025
	0.125	107.7	9.5	8.84	7.7	
	1.25	99.5	12.8	12.88	-0.5	
AB-PINACA	0.025	100.5	8.1	8.06	0.5	0.025
	0.125	114.4	11.1	9.70	14.4	
	1.25	110.2	7.5	6.78	10.2	
ADB-FUBINACA	0.025	111.1	12.2	10.94	11.1	0.025
	0.125	112.4	11.6	10.35	12.4	
	1.25	107.3	4.8	4.45	7.3	
ADB-PINACA	0.025	107.8	5.1	4.75	7.8	0.025
	0.125	107.2	6.4	5.93	7.2	
	1.25	100.5	15.2	15.17	0.5	
ADB-PINACA ISOMER_1	0.025	107.4	13.2	12.25	7.4	0.025
	0.125	101.5	19.8	19.48	1.5	
	1.25	102.4	10.8	10.59	2.4	
ADB-PINACA ISOMER_2	0.025	109.4	13.9	12.67	9.4	0.025
	0.125	99.4	16.4	16.49	-0.6	
	1.25	103.4	12.8	12.40	3.4	
ADB-PINACA ISOMER_3	0.025	88.3	7.1	8.00	-11.8	0.025
	0.125	99.6	13.5	13.56	-0.4	

	1.25	100.0	5.3	5.29	0.0	
ADB-PINACA ISOMER_4	0.025	101.3	6.5	6.46	1.3	0.025
	0.125	105.3	5.8	5.52	5.3	
	1.25	94.8	9.0	9.44	-5.2	
AH-7921	0.025	91.1	10.7	11.77	-8.9	0.125
	0.125	94.3	8.4	8.96	-5.7	
	1.25	90.4	4.5	4.94	-9.6	
	5	103.4	14.4	13.97	3.4	
AKB48_N-(4-FLUOROBENZYL)_ANALOG	0.025	96.9	16.9	17.41	-3.1	0.025
	0.125	111.7	9.0	8.07	11.7	
	1.25	181.7	22.9	12.58	81.7	
ALFA-ETHYLAMINOPENTIOPHENONE	0.025	86.5	36.8	42.52	-13.5	0.125
	0.125	104.5	9.1	8.69	4.5	
	1.25	101.0	6.3	6.29	1.0	
	5	102.7	6.7	6.54	2.7	
ALFA-PROPYLAMINOPENTIOPHENONE	0.025	109.8	11.3	10.29	9.8	0.125
	0.125	102.5	11.6	11.27	2.5	
	1.25	116.0	6.6	5.68	16.0	
	5	117.7	13.2	11.25	17.7	
ALLYLESCALINE	0.125	101.0	20.0	19.80	1.0	0.125
	1.25	99.1	9.9	10.00	-0.9	
	5	116.4	8.9	7.68	16.4	
ALPHA-DIMETHYLAMINOPENTIOPHENONE	0.025	86.6	18.8	21.71	-13.4	0.125
	0.125	98.0	11.6	11.86	-2.0	
	1.25	95.7	6.7	7.02	-4.3	
	5	110.1	16.3	14.78	10.1	
ALPHA-ETHYLAMINOHEXANOPHENONE	0.025	91.5	36.0	39.31	-8.5	0.125
	0.125	116.6	14.9	12.75	16.6	
	1.25	104.6	15.6	14.90	4.6	
	5	95.9	14.3	14.91	-4.1	
ALPHA-ETHYLTRYPTAMINE	0.025	105.7	44.2	41.84	5.7	0.125
	0.125	95.6	19.1	19.95	-4.4	
	1.25	116.8	15.6	13.37	16.8	
	5	117.3	17.2	14.65	17.3	
ALPHA-METHYLTRYPTAMINE	1.25	114.5	9.1	7.99	14.5	1.25
	5	119.0	16.2	13.59	19.0	
ALPHA-PHP	0.025	101.8	15.9	15.63	1.7	0.125
	0.125	119.5	9.3	7.78	19.5	
	1.25	105.4	9.2	8.74	5.4	
	5	107.0	11.1	10.39	7.0	
ALPHA-PHTALIMIDOPROPIOPHENONE	0.025	102.3	20.9	20.46	2.3	0.125
	0.125	118.5	4.9	4.14	18.5	
	1.25	105.0	9.8	9.30	5.0	
	5	112.9	14.9	13.20	12.9	
ALPHA-PIPBP	0.025	118.1	22.4	18.97	18.1	0.125
	0.125	104.1	11.1	10.70	4.1	

	1.25	101.1	4.0	4.01	1.1	
	5	108.5	11.6	10.67	8.5	
ALPHA-PPP	0.025	109.9	14.9	13.51	9.9	0.125
	0.125	95.3	12.1	12.66	-4.8	
	1.25	93.9	7.5	7.98	-6.1	
	5	98.4	5.1	5.17	-1.6	
ALPHA-PVP	0.025	122.7	17.8	14.53	22.7	0.125
	0.125	97.5	11.1	11.34	-2.5	
	1.25	90.8	9.4	10.32	-9.2	
	5	90.0	10.7	11.91	-10.0	
ALPHA-PVT	0.025	112.6	20.3	18.04	12.6	0.125
	0.125	110.9	6.3	5.71	10.9	
	1.25	93.5	14.0	14.95	-6.5	
	5	116.1	15.5	13.36	16.1	
ALPHA-PYRROLIDINOBUTHIOPHENONE	0.025	102.9	11.5	11.17	2.9	0.125
	0.125	94.7	10.6	11.22	-5.3	
	1.25	98.0	4.8	4.92	-2.0	
	5	105.9	11.9	11.23	5.9	
ALPRAZOLAM	0.025	105.3	14.9	14.14	5.3	0.125
	0.125	87.7	7.0	8.03	-12.3	
	1.25	94.2	11.7	12.37	-5.8	
	5	119.8	12.1	10.07	19.8	
AM1220	0.025	98.7	15.1	15.34	-1.3	0.025
	0.125	94.9	8.7	9.16	-5.1	
	1.25	92.5	6.1	6.61	-7.5	
AM-1248	0.025	99.1	12.5	12.65	-1.0	0.025
	0.125	112.4	4.0	3.59	12.4	
	1.25	112.2	9.8	8.70	12.2	
AM-2201	0.025	116.4	7.9	6.75	16.4	0.025
	0.125	110.1	3.8	3.43	10.1	
	1.25	108.4	10.2	9.42	8.4	
AM2201 8-QUINOLINYL CARBOXAMIDE	0.025	96.9	15.8	16.31	-3.1	0.025
	0.125	94.8	10.9	11.49	-5.2	
	1.25	116.4	19.3	16.54	16.4	
AM2201 BENZIMIDAZOLE ANALOG	0.025	105.6	12.2	11.56	5.6	0.025
	0.125	108.6	6.0	5.57	8.6	
	1.25	109.3	9.7	8.88	9.3	
AM2232	0.025	111.1	9.1	8.20	11.1	0.025
	0.125	100.4	7.9	7.88	0.4	
	1.25	103.4	10.1	9.79	3.4	
AMITRIPTYLINE	0.025	103.1	18.6	18.04	3.1	0.125
	0.125	102.8	7.6	7.43	2.8	
	1.25	92.3	8.4	9.06	-7.7	
	5	105.3	10.6	10.05	5.3	
AMPHETAMINE	0.025	101.1	14.9	14.75	1.1	0.125
	0.125	113.1	16.5	14.62	13.1	

	1.25	89.7	11.6	12.93	-10.3	
	5	104.3	9.2	8.82	4.3	
ATENOLOL	0.025	152.5	32.5	21.32	52.5	0.125
	0.125	119.9	13.0	10.86	19.9	
	1.25	114.4	12.0	10.48	14.4	
	5	120.0	13.4	11.20	20.0	
AZACYCLONOL	0.025	138.0	12.6	9.15	38.0	0.125
	0.125	103.6	16.8	16.20	3.6	
	1.25	111.8	12.2	10.92	11.8	
	5	93.0	10.4	11.13	-7.0	
BB-22	0.025	101.0	11.7	11.60	1.0	0.025
	0.125	112.1	8.0	7.15	12.1	
	1.25	107.6	6.4	5.91	7.6	
BDB	0.125	100.1	14.1	14.12	0.1	0.125
	1.25	104.0	11.1	10.64	4.0	
	5	102.9	17.4	16.94	2.9	
BENOCYCLIDINE	0.025	109.7	10.7	9.78	9.7	0.125
	0.125	99.7	9.4	9.46	-0.3	
	1.25	94.7	10.7	11.34	-5.3	
	5	110.5	8.5	7.73	10.5	
BENZEDRONE	0.025	106.2	9.5	8.96	6.2	0.125
	0.125	96.0	5.8	6.09	-4.0	
	1.25	94.0	7.0	7.45	-6.0	
	5	108.8	14.3	13.14	8.8	
BENZOCAINE	0.025	129.4	72.2	55.78	29.4	0.125
	0.125	102.1	10.0	9.76	2.1	
	1.25	109.5	18.5	16.93	9.5	
	5	117.3	9.2	7.85	17.3	
BENZOYLECGONINE	0.025	107.8	17.6	16.32	7.8	0.025
	0.125	101.3	13.8	13.65	1.3	
	1.25	89.4	9.3	10.45	-10.6	
	5	109.4	19.3	17.61	9.4	
BENZYDAMINE	0.025	101.2	9.3	9.20	1.2	0.125
	0.125	93.5	5.4	5.79	-6.5	
	1.25	93.8	8.3	8.80	-6.2	
	5	99.0	10.6	10.70	-1.0	
bk-MDA	0.025	117.5	6.4	5.42	17.5	0.125
	0.125	101.2	5.3	5.20	1.2	
	1.25	97.4	12.2	12.51	-2.6	
	5	112.1	9.9	8.80	12.1	
BMPEA	0.025	171.2	60.0	35.05	71.2	0.125
	0.125	114.1	20.4	17.88	14.1	
	1.25	113.9	11.1	9.72	13.9	
	5	105.2	10.5	10.01	5.2	
BROMO-DRAGON-FLY	0.025	83.5	15.7	18.81	-16.5	0.125
	0.125	95.6	17.4	18.24	-4.4	

	1.25	84.9	10.0	11.77	-15.1	
	5	106.4	10.8	10.12	6.4	
BUPRENORPHINE	0.025	94.8	23.6	24.88	-5.2	0.125
	0.125	106.3	9.5	8.97	6.3	
	1.25	80.3	7.2	8.92	-19.7	
	5	98.3	13.4	13.62	-1.7	
BUPROPION	0.025	117.4	37.7	32.09	17.4	0.125
	0.125	113.2	16.8	14.85	13.2	
	1.25	107.8	4.2	3.94	7.8	
	5	112.0	2.4	2.15	12.0	
BUTYLONE (bk-MBDB)	0.025	105.7	23.5	22.21	5.7	0.125
	0.125	101.1	13.8	13.62	1.1	
	1.25	98.5	9.2	9.39	-1.5	
	5	115.2	19.8	17.20	15.2	
CAMFETAMINE	0.025	106.1	17.9	16.86	6.1	0.125
	0.125	102.1	19.9	19.54	2.1	
	1.25	116.8	22.0	18.80	16.8	
	5	108.6	9.3	8.53	8.6	
CANNABIDIOL	0.025	40.9	13.8	33.78	-59.1	0.125
	0.125	95.8	14.1	14.76	-4.2	
	1.25	115.3	10.9	9.42	15.3	
CARBAMAZEPINE	0.025	97.1	6.8	6.98	-2.9	0.125
	0.125	110.2	5.3	4.77	10.2	
	1.25	103.2	15.7	15.22	3.2	
	5	103.1	8.6	8.31	3.1	
CATHINE	0.125	98.4	11.5	11.64	-1.6	0.125
	1.25	105.6	6.2	5.88	5.6	
	5	110.9	6.7	6.01	10.9	
CATHINONE	0.025	142.9	30.4	21.26	42.9	0.125
	0.125	108.6	4.9	4.51	8.6	
	1.25	102.3	11.6	11.31	2.3	
	5	108.8	6.0	5.53	8.8	
CB-13	0.025	106.0	5.4	5.13	6.0	0.025
	0.125	109.6	4.5	4.08	9.6	
	1.25	118.2	7.3	6.20	18.2	
CBL-018	0.025	104.2	14.3	13.72	4.1	0.025
	0.125	97.3	4.8	4.91	-2.7	
	1.25	110.1	9.5	8.61	10.1	
CI2201	0.025	122.6	10.1	8.28	22.6	0.125
	0.125	114.0	5.6	4.88	14.0	
	1.25	117.8	13.0	11.02	17.8	
	5	155.2	25.9	16.69	55.2	
CLOBAZAM	0.025	131.3	14.3	10.93	31.3	0.125
	0.125	105.6	15.2	14.42	5.6	
	1.25	108.7	6.3	5.80	8.7	
	5	113.7	15.0	13.23	13.7	

CLOMIPRAMINE	0.025	111.5	8.1	7.24	11.5	0.125
	0.125	110.1	7.3	6.60	10.1	
	1.25	81.8	10.3	12.60	-18.2	
	5	114.8	11.7	10.17	14.8	
CLONAZEPAM	0.025	95.2	8.4	8.83	-4.8	0.125
	0.125	101.9	14.3	13.99	1.9	
	1.25	107.3	7.8	7.25	7.3	
	5	117.5	7.9	6.73	17.5	
COCAETHYLENE	0.025	102.3	15.0	14.69	2.3	0.025
	0.125	91.6	3.7	4.03	-8.4	
	1.25	109.1	7.7	7.10	9.1	
	5	115.2	13.9	12.08	15.2	
COCAINE	0.025	96.9	19.3	19.91	-3.1	0.125
	0.125	109.0	17.6	16.12	9.0	
	1.25	104.5	10.1	9.68	4.5	
	5	110.4	12.8	11.57	10.4	
CODEINE	0.025	125.2	24.2	19.37	25.2	0.125
	0.125	103.3	10.6	10.29	3.3	
	1.25	103.8	7.7	7.42	3.8	
	5	111.5	6.8	6.13	11.5	
CUMYL-PICA	0.025	98.8	6.8	6.88	-1.2	0.025
	0.125	108.7	5.1	4.68	8.7	
	1.25	117.3	10.7	9.09	17.3	
D2PM	0.025	112.3	17.0	15.16	12.3	0.125
	0.125	110.7	7.9	7.15	10.7	
	1.25	108.4	9.5	8.79	8.4	
	5	113.3	14.7	13.00	13.3	
DEMOXEPAM	0.125	101.1	8.4	8.33	1.1	0.125
	1.25	99.0	11.8	11.89	-1.0	
	5	118.3	12.3	10.39	18.3	
DESALKYLFLURAZEPAM	0.125	89.5	17.3	19.38	-10.5	0.125
	1.25	99.3	8.7	8.80	-0.7	
	5	98.4	7.2	7.30	-1.6	
DESCHLOROETIZOLAM	0.025	104.6	14.4	13.80	4.6	0.125
	0.125	91.7	14.5	15.78	-8.3	
	1.25	102.2	7.5	7.35	2.2	
	5	105.9	15.0	14.12	5.9	
DESCHLORO-N-ETHYL-KETAMINE	0.025	116.1	14.4	12.41	16.1	0.125
	0.125	109.1	13.5	12.38	9.1	
	1.25	101.8	9.8	9.65	1.8	
	5	112.6	12.8	11.42	12.6	
DESIPRAMINE	0.025	93.8	9.2	9.83	-6.3	0.125
	0.125	117.5	8.7	7.44	17.5	
	1.25	94.4	10.1	10.67	-5.6	
	5	115.0	11.3	9.85	15.0	
DESMETHYLDIAZEPAM (NORDIAZEPAM)	0.025	46.9	23.9	50.94	-53.1	0.125

	0.125	98.3	13.2	13.39	-1.7	
	1.25	109.8	12.7	11.57	9.8	
	5	113.7	6.7	5.85	13.7	
DESMETHYLFLUNITRAZEPAM	0.025	91.4	17.3	18.94	-8.6	0.125
	0.125	82.9	4.6	5.49	-17.1	
	1.25	80.8	8.0	9.90	-19.2	
	5	80.7	3.9	4.87	-19.3	
DESOMORPHINE	0.025	131.1	23.4	17.89	31.1	0.125
	0.125	95.0	8.9	9.39	-5.0	
	1.25	101.4	13.5	13.31	1.4	
	5	106.4	12.8	12.04	6.4	
DESOXY-D2PM	0.025	125.5	15.6	12.41	25.5	0.125
	0.125	94.0	8.6	9.18	-6.0	
	1.25	94.4	11.5	12.15	-5.6	
	5	100.6	13.9	13.85	0.6	
DESOXYPIPRADROL (2-DPMP)	0.025	99.8	12.1	12.14	-0.2	0.125
	0.125	91.2	6.6	7.23	-8.8	
	1.25	115.1	7.7	6.72	15.1	
	5	119.9	10.5	8.73	19.9	
DEXTROMETHORPHAN	0.025	101.0	22.8	22.53	1.0	0.125
	0.125	95.0	9.8	10.32	-5.0	
	1.25	105.0	9.9	9.44	5.0	
	5	115.6	4.0	3.49	15.6	
DIAZEPAM	0.025	94.0	8.2	8.69	-6.0	0.125
	0.125	88.3	7.0	7.96	-11.8	
	1.25	101.6	9.1	8.91	1.6	
	5	110.4	10.6	9.58	10.4	
DICLAZEPAM	0.025	79.9	30.2	37.77	-20.1	0.125
	0.125	89.9	10.3	11.48	-10.1	
	1.25	109.9	11.7	10.65	9.9	
	5	118.5	6.6	5.53	18.5	
DICLOFENSINE	0.025	120.3	13.0	10.84	20.3	0.125
	0.125	97.5	8.7	8.91	-2.5	
	1.25	94.5	8.6	9.06	-5.5	
	5	118.6	10.3	8.65	18.6	
DIETHYLCATHINONE (AMFEPRAMONE)	0.025	131.1	57.2	43.61	31.1	0.125
	0.125	103.5	6.3	6.09	3.5	
	1.25	109.9	6.5	5.89	9.9	
	5	114.1	12.5	10.98	14.1	
DIHYDROCODEINE	0.025	116.9	23.2	19.87	16.9	0.125
	0.125	107.0	5.0	4.71	7.0	
	1.25	119.0	10.4	8.75	19.0	
	5	117.1	7.9	6.74	17.1	
DIMETHOCAINE	0.025	110.7	8.5	7.68	10.7	0.125
	0.125	101.5	8.8	8.71	1.5	
	1.25	109.5	6.4	5.81	9.5	

	5	119.4	14.6	12.20	19.4	
DIMETHYLONE (bk-MDDMA)	0.025	111.0	22.8	20.58	11.0	0.125
	0.125	93.8	8.3	8.79	-6.2	
	1.25	98.9	14.1	14.26	-1.1	
	5	99.7	7.9	7.90	-0.3	
DIPHENHYDRAMINE	0.025	100.0	17.6	17.56	0.0	0.125
	0.125	102.9	8.7	8.48	2.9	
	1.25	100.2	8.8	8.80	0.2	
	5	106.1	6.5	6.14	6.1	
DIPHENIDINE	0.025	107.2	13.4	12.47	7.1	0.125
	0.125	105.7	7.1	6.71	5.7	
	1.25	94.2	8.6	9.14	-5.8	
	5	111.6	11.2	10.07	11.6	
DiPT	0.125	131.7	101.5	77.07	31.7	1.25
	1.25	112.2	6.9	6.15	12.2	
	5	119.1	9.5	7.97	19.1	
DL-4662	0.025	95.6	22.8	23.80	-4.4	0.125
	0.125	100.7	9.8	9.71	0.7	
	1.25	107.5	13.4	12.48	7.5	
	5	104.5	10.4	9.99	4.5	
DOI	0.025	103.2	31.1	30.17	3.2	0.125
	0.125	95.4	11.7	12.26	-4.6	
	1.25	118.7	17.2	14.45	18.7	
	5	117.0	4.1	3.53	17.0	
DOTHIEPIN	0.025	107.9	18.1	16.81	7.9	0.125
	0.125	103.9	7.2	6.92	3.9	
	1.25	88.5	8.4	9.52	-11.5	
	5	101.8	13.7	13.45	1.8	
DOXEPIN	0.025	114.6	19.2	16.72	14.6	0.125
	0.125	111.3	11.3	10.15	11.3	
	1.25	100.2	12.6	12.56	0.2	
	5	112.0	8.2	7.33	12.0	
DOXYLAMINE	0.025	40.6	46.2	113.81	-59.4	1.25
	0.125	53.2	25.3	47.46	-46.8	
	1.25	100.3	8.8	8.82	0.3	
	5	119.8	4.0	3.37	19.8	
EAM-2201	0.025	113.2	9.6	8.52	13.2	0.025
	0.125	116.3	7.6	6.57	16.3	
	1.25	118.8	21.2	17.84	18.8	
EDDP	0.025	98.0	11.9	12.14	-2.0	0.025
	0.125	106.8	7.9	7.39	6.8	
	1.25	91.7	6.6	7.18	-8.3	
	5	100.9	7.4	7.36	0.9	
EG-2201	0.025	98.3	18.3	18.63	-1.7	0.025
	0.125	97.8	14.5	14.78	-2.2	
	1.25	105.9	8.6	8.10	5.9	

ERGOMETRINE	0.025	115.6	5.7	4.94	15.6	0.125
	0.125	99.1	6.6	6.67	-0.9	
	1.25	89.1	15.4	17.24	-10.9	
	5	94.6	5.9	6.23	-5.4	
ESTAZOLAM	0.025	103.9	32.8	31.57	3.9	0.125
	0.125	112.7	11.3	10.04	12.7	
	1.25	102.0	19.3	18.89	2.0	
	5	119.7	3.1	2.56	19.7	
ETAQUALONE	0.025	96.3	10.0	10.41	-3.8	0.125
	0.125	109.8	10.6	9.63	9.8	
	1.25	119.8	5.6	4.63	19.8	
	5	118.7	8.8	7.38	18.7	
ETHCATHINONE METABOLITE	0.125	95.0	17.7	18.58	-5.0	0.125
	1.25	106.8	16.7	15.60	6.8	
	5	114.3	8.8	7.74	14.3	
ETHYLONE (bk-MDEA)	0.025	80.1	22.1	27.58	-19.9	0.125
	0.125	94.6	5.6	5.91	-5.4	
	1.25	97.1	9.1	9.34	-2.9	
	5	106.6	12.6	11.83	6.6	
ETHYLPHENIDATE	0.025	112.3	14.2	12.68	12.3	0.125
	0.125	93.9	5.4	5.73	-6.1	
	1.25	100.1	12.6	12.54	0.1	
	5	96.4	9.1	9.40	-3.6	
ETIZOLAM	0.025	92.2	16.6	18.00	-7.8	0.125
	0.125	100.3	11.3	11.22	0.3	
	1.25	108.1	19.2	17.77	8.1	
	5	118.9	6.3	5.32	18.9	
EUTYLONE (bk-EBDB)	0.025	101.3	13.6	13.39	1.3	0.125
	0.125	110.9	11.6	10.50	10.9	
	1.25	109.1	15.3	14.02	9.1	
	5	112.2	11.0	9.82	12.2	
FDU-PB-22	0.025	80.9	29.1	35.99	-19.1	0.125
	0.125	99.1	7.4	7.51	-0.9	
	1.25	115.6	7.8	6.79	15.6	
FENFLURAMINE	0.025	111.4	23.0	20.66	11.4	0.125
	0.125	115.8	9.8	8.51	15.8	
	1.25	100.7	13.0	12.89	0.7	
	5	118.0	22.9	19.39	18.0	
FENTANYL	0.025	102.4	22.6	22.05	2.4	0.125
	0.125	111.8	12.0	10.70	11.8	
	1.25	94.8	7.0	7.35	-5.2	
	5	103.7	19.7	19.00	3.7	
FLUBROMAZEPAM	0.025	104.9	28.3	26.99	4.8	0.125
	0.125	93.6	11.5	12.28	-6.4	
	1.25	95.9	8.0	8.31	-4.1	
	5	107.2	11.9	11.11	7.2	

FLUDIAZEPAM	0.025	106.0	26.9	25.35	6.0	0.125
	0.125	87.5	11.9	13.63	-12.5	
	1.25	102.8	2.3	2.19	2.8	
	5	115.7	9.8	8.51	15.7	
FLUMAZENIL	0.025	101.1	10.8	10.65	1.1	0.125
	0.125	100.8	2.7	2.67	0.8	
	1.25	101.8	10.3	10.16	1.8	
	5	115.2	16.0	13.90	15.2	
FLUNITRAZEPAM	0.025	95.5	14.9	15.58	-4.5	0.125
	0.125	103.3	9.8	9.51	3.3	
	1.25	103.8	7.0	6.77	3.8	
	5	118.8	12.0	10.14	18.8	
FLUOXETINE	0.025	111.9	14.3	12.75	11.9	0.125
	0.125	94.8	6.7	7.05	-5.2	
	1.25	102.5	8.4	8.21	2.5	
	5	118.0	12.3	10.44	18.0	
FLURAZEPAM	0.025	108.0	12.7	11.81	7.9	0.125
	0.125	100.4	6.3	6.24	0.4	
	1.25	91.3	8.2	8.97	-8.7	
	5	103.8	10.7	10.34	3.8	
FUB-144	0.025	100.3	6.3	6.28	0.3	0.025
	0.125	101.8	13.8	13.58	1.8	
	1.25	116.2	16.0	13.78	16.2	
FUB-JWH-018	0.025	105.8	3.3	3.16	5.8	0.025
	0.125	103.8	8.5	8.22	3.8	
	1.25	109.8	21.7	19.76	9.8	
FUB-NPB-22	0.025	109.4	14.8	13.54	9.4	0.025
	0.125	108.2	8.6	7.94	8.2	
	1.25	102.0	17.5	17.20	2.0	
FUB-PB-22	0.025	239.2	151.8	63.45	139.2	-
	0.125	146.1	118.4	81.04	46.1	
	1.25	116.6	19.0	16.28	16.6	
FURANYLFENTANYL (Fu-F)	0.025	83.4	14.6	17.49	-16.6	0.125
	0.125	104.9	14.1	13.44	4.9	
	1.25	107.3	15.8	14.72	7.3	
	5	114.7	10.3	8.94	14.7	
HARMALINE	0.025	82.1	19.7	24.01	-17.9	0.125
	0.125	100.8	8.3	8.28	0.8	
	1.25	89.8	9.7	10.77	-10.2	
	5	97.0	12.5	12.90	-3.0	
HARMINE	0.025	141.5	30.8	21.75	41.5	0.125
	0.125	92.1	18.4	20.03	-7.9	
	1.25	94.4	9.4	9.92	-5.6	
	5	107.8	7.5	6.99	7.8	
HU-210	0.025	84.6	9.1	10.80	-15.5	0.025
	0.125	115.6	18.6	16.09	15.6	

	1.25	118.8	5.3	4.42	18.8	
HYDROCODONE	0.025	136.8	25.6	18.68	36.8	0.125
	0.125	103.3	13.5	13.11	3.3	
	1.25	100.5	10.2	10.15	0.5	
	5	103.4	11.3	10.90	3.4	
IBOGAINE	0.125	65.0	26.4	40.69	-35.0	1.25
	1.25	97.4	12.9	13.23	-2.6	
	5	118.0	6.6	5.62	18.0	
IMIPRAMINE	0.025	102.9	13.9	13.54	2.9	0.125
	0.125	114.9	10.9	9.45	14.9	
	1.25	90.6	6.3	6.92	-9.4	
	5	115.6	10.0	8.62	15.6	
ISOPENTEDRONE	0.025	103.1	52.7	51.12	3.1	0.125
	0.125	94.0	14.4	15.28	-6.0	
	1.25	95.7	9.5	9.88	-4.3	
	5	106.6	5.0	4.70	6.6	
JWH 018 BENZIMIDAZOLE ANALOG	0.025	97.7	17.4	17.83	-2.3	0.025
	0.125	98.5	14.4	14.64	-1.5	
	1.25	106.3	14.2	13.39	6.3	
JWH-011	0.025	111.1	9.9	8.92	11.1	0.025
	0.125	110.3	9.5	8.58	10.3	
	1.25	116.7	2.9	2.49	16.7	
JWH-016	0.025	116.8	6.0	5.16	16.8	0.025
	0.125	103.9	5.8	5.55	3.9	
	1.25	118.5	7.5	6.30	18.5	
JWH-018	0.025	98.7	10.4	10.54	-1.3	0.025
	0.125	98.4	4.8	4.86	-1.6	
	1.25	113.1	16.8	14.85	13.1	
JWH-018 ADAMANTYL CARBOXAMIDE	0.025	101.0	10.6	10.54	1.0	0.025
	0.125	115.9	9.8	8.44	15.9	
	1.25	117.8	9.9	8.40	17.8	
JWH-020	0.025	100.5	10.9	10.90	0.5	0.025
	0.125	105.4	5.6	5.27	5.4	
	1.25	115.6	7.8	6.79	15.6	
JWH-022	0.025	104.7	7.6	7.22	4.7	0.025
	0.125	109.5	6.9	6.29	9.5	
	1.25	114.0	9.4	8.23	14.0	
JWH-031	0.025	91.5	9.4	10.26	-8.5	0.025
	0.125	102.3	3.0	2.92	2.3	
	1.25	117.0	12.4	10.61	17.0	
JWH-071	0.025	111.5	6.9	6.14	11.5	0.025
	0.125	106.4	5.5	5.21	6.4	
	1.25	109.8	12.7	11.57	9.8	
JWH-073	0.025	96.6	10.6	10.93	-3.4	0.025
	0.125	107.6	9.5	8.79	7.6	
	1.25	112.9	10.9	9.67	12.9	

JWH-080	0.025	110.6	17.2	15.52	10.6	0.025
	0.125	106.8	5.5	5.11	6.8	
	1.25	118.4	5.9	4.99	18.4	
JWH-081	0.025	114.7	13.1	11.40	14.7	0.025
	0.125	111.9	7.9	7.05	11.9	
	1.25	113.1	14.8	13.08	13.1	
JWH-098	0.025	107.8	12.3	11.37	7.8	0.025
	0.125	105.8	8.0	7.57	5.8	
	1.25	114.6	7.5	6.53	14.6	
JWH-116	0.025	97.5	7.1	7.24	-2.5	0.025
	0.125	108.5	3.8	3.53	8.5	
	1.25	112.8	13.3	11.79	12.8	
JWH-122	0.025	97.3	8.6	8.83	-2.7	0.025
	0.125	104.7	6.5	6.19	4.7	
	1.25	115.3	10.9	9.42	15.3	
JWH-145	0.025	113.4	6.3	5.58	13.4	0.025
	0.125	108.9	6.1	5.56	8.9	
	1.25	110.1	17.2	15.64	10.1	
JWH-146	0.025	105.1	8.5	8.07	5.1	0.025
	0.125	108.8	4.5	4.14	8.8	
	1.25	116.2	16.2	13.98	16.2	
JWH-147	0.025	110.3	12.1	11.00	10.3	0.025
	0.125	105.9	9.4	8.85	5.9	
	1.25	116.4	15.6	13.38	16.4	
JWH-149	0.025	110.2	12.0	10.88	10.2	0.025
	0.125	115.9	11.5	9.95	15.9	
	1.25	116.7	12.7	10.91	16.7	
JWH-167	0.025	100.0	9.3	9.30	0.0	0.025
	0.125	104.9	7.4	7.02	4.8	
	1.25	112.3	9.5	8.49	12.3	
JWH-175	0.025	97.4	4.0	4.12	-2.6	0.025
	0.125	100.8	2.5	2.47	0.8	
	1.25	118.4	5.6	4.72	18.4	
JWH-182	0.025	95.4	7.0	7.36	-4.6	0.025
	0.125	104.3	10.3	9.88	4.3	
	1.25	119.9	7.3	6.07	19.9	
JWH-193	0.025	106.2	17.6	16.62	6.2	0.025
	0.125	106.5	8.6	8.05	6.5	
	1.25	109.0	11.0	10.06	9.0	
JWH-198	0.025	88.2	8.0	9.07	-11.8	0.025
	0.125	109.7	8.5	7.78	9.7	
	1.25	114.8	6.2	5.43	14.8	
JWH-200	0.025	102.8	8.3	8.07	2.8	0.025
	0.125	98.4	10.3	10.50	-1.6	
	1.25	91.7	15.7	17.09	-8.3	
JWH-201	0.025	106.8	16.1	15.04	6.8	0.025

	0.125	109.9	11.6	10.53	9.9	
	1.25	119.4	18.4	15.40	19.4	
JWH-213	0.025	105.2	10.6	10.04	5.1	0.025
	0.125	114.7	6.9	6.04	14.7	
	1.25	114.0	8.1	7.12	14.0	
JWH-307	0.025	104.9	8.3	7.91	4.9	0.025
	0.125	119.4	7.0	5.87	19.4	
	1.25	116.1	11.6	10.00	16.1	
JWH-309	0.025	105.6	3.4	3.18	5.6	0.025
	0.125	111.4	4.8	4.33	11.4	
	1.25	107.3	12.2	11.34	7.3	
JWH-368	0.025	110.1	11.3	10.25	10.1	0.025
	0.125	106.4	9.2	8.66	6.4	
	1.25	110.0	17.5	15.93	10.0	
JWH-369	0.025	101.6	5.8	5.69	1.6	0.025
	0.125	114.2	6.3	5.50	14.2	
	1.25	118.4	11.9	10.04	18.4	
JWH-412	0.025	109.0	10.4	9.54	9.0	0.025
	0.125	114.9	6.1	5.35	14.9	
	1.25	119.7	20.6	17.25	19.7	
JWH-424	0.025	107.3	17.5	16.29	7.3	0.025
	0.125	107.4	6.1	5.72	7.4	
	1.25	115.5	15.8	13.66	15.5	
KETAMINE	0.025	86.2	10.9	12.67	-13.8	0.125
	0.125	114.2	12.5	10.91	14.2	
	1.25	106.9	16.2	15.18	6.9	
	5	111.9	14.6	13.02	11.9	
LAMPA	0.025	99.4	23.3	23.43	-0.6	0.125
	0.125	80.1	6.2	7.72	-19.9	
	1.25	84.6	8.7	10.27	-15.4	
	5	99.9	5.9	5.86	-0.1	
LIDOCAINE	0.025	93.7	13.5	14.38	-6.3	0.125
	0.125	114.3	7.9	6.89	14.3	
	1.25	108.8	9.9	9.07	8.8	
	5	114.1	18.1	15.87	14.1	
LOPRAZOLAM	0.125	82.0	12.8	15.66	-18.0	0.125
	1.25	102.1	12.3	12.02	2.1	
	5	104.7	9.3	8.91	4.7	
LORAZEPAM	0.025	145.2	67.8	46.73	45.2	0.125
	0.125	95.7	17.1	17.90	-4.3	
	1.25	93.0	8.3	8.91	-7.0	
	5	107.4	12.4	11.53	7.4	
LORMETAZEPAM	0.025	82.1	25.8	31.37	-17.9	0.125
	0.125	108.7	18.7	17.18	8.7	
	1.25	104.0	7.6	7.26	4.0	
	5	113.5	7.8	6.85	13.5	

LSD	0.025	101.4	31.7	31.23	1.4	0.125
	0.125	104.9	11.2	10.71	4.9	
	1.25	81.3	9.6	11.75	-18.7	
	5	99.1	8.2	8.31	-0.9	
MAM-2201	0.025	107.8	18.1	16.83	7.8	0.025
	0.125	113.0	9.5	8.39	13.0	
	1.25	116.7	12.6	10.77	16.7	
MAPROTILINE	0.025	123.1	19.4	15.79	23.1	0.125
	0.125	104.6	11.8	11.24	4.6	
	1.25	90.1	8.8	9.81	-9.9	
	5	116.5	11.7	10.01	16.5	
MBDB	0.025	138.3	9.3	6.73	38.3	0.125
	0.125	108.0	3.8	3.47	8.0	
	1.25	113.6	8.4	7.39	13.6	
	5	114.8	13.8	12.00	14.8	
MDAT	0.125	98.1	17.8	18.19	-1.9	0.125
	1.25	99.9	15.4	15.40	-0.1	
	5	103.0	15.1	14.66	3.0	
MDBP	0.025	185.9	25.7	13.80	85.9	0.125
	0.125	119.2	6.9	5.81	19.2	
	1.25	91.2	13.1	14.38	-8.8	
	5	90.1	7.8	8.63	-9.9	
MDEA	0.025	113.1	12.6	11.15	13.1	0.125
	0.125	104.6	6.2	5.89	4.6	
	1.25	101.4	8.5	8.36	1.4	
	5	103.6	10.7	10.36	3.6	
MDMB-CHMICA (MMB-CHMINACA)	0.025	111.3	5.3	4.76	11.3	0.025
	0.125	114.6	5.5	4.82	14.6	
	1.25	119.4	13.0	10.88	19.4	
MDMB-CHMINACA	0.025	98.7	7.0	7.09	-1.3	0.025
	0.125	112.8	10.0	8.87	12.8	
	1.25	117.5	16.9	14.34	17.5	
MDPBP	0.025	113.8	18.5	16.27	13.8	0.125
	0.125	104.3	12.7	12.17	4.3	
	1.25	99.5	10.3	10.32	-0.5	
	5	113.4	6.6	5.82	13.4	
MECLONAZEPAM	0.025	117.1	9.5	8.11	17.1	0.125
	0.125	94.0	10.3	10.95	-6.0	
	1.25	104.4	8.8	8.43	4.4	
	5	119.1	5.8	4.87	19.1	
MEDAZEPAM	0.025	83.2	20.6	24.82	-16.8	0.125
	0.125	82.8	4.8	5.74	-17.2	
	1.25	88.7	3.6	4.02	-11.3	
	5	116.2	15.7	13.50	16.2	
MEMANITINE	1.25	105.0	12.0	11.46	5.0	1.25
	5	108.4	17.6	16.20	8.4	

MEPERIDINE	0.025	107.9	24.6	22.77	7.9	0.125
	0.125	92.7	17.6	19.03	-7.3	
	1.25	101.8	11.6	11.35	1.8	
	5	117.2	15.0	12.82	17.2	
MEPHTETRAMINE (MTTA)	0.025	73.7	24.0	32.58	-26.3	0.125
	0.125	96.6	9.9	10.22	-3.4	
	1.25	86.4	3.8	4.40	-13.6	
	5	99.4	9.8	9.82	-0.6	
MEPIRAPIM	0.025	88.0	11.8	13.46	-12.1	0.025
	0.125	102.9	7.8	7.54	2.9	
	1.25	93.7	6.4	6.83	-6.3	
MEPROBAMATE	0.025	82.9	69.4	83.76	-17.1	0.125
	0.125	114.4	11.6	10.12	14.4	
	1.25	82.2	11.7	14.29	-17.8	
	5	94.0	9.5	10.12	-6.0	
MESCALINE	0.025	1212.9	631.2	52.04	1112.9	1.25
	0.125	294.9	103.1	34.95	194.9	
	1.25	99.8	13.2	13.25	-0.2	
	5	96.3	8.4	8.71	-3.7	
METHADONE	0.025	109.9	12.1	11.02	9.9	0.125
	0.125	107.8	9.6	8.90	7.8	
	1.25	101.5	7.2	7.10	1.5	
	5	116.9	6.0	5.17	16.9	
METHAMPHETAMINE	0.025	149.1	69.8	46.80	49.1	0.125
	0.125	98.9	15.8	16.00	-1.1	
	1.25	87.4	14.1	16.11	-12.6	
	5	103.9	12.9	12.45	3.9	
METHANDIENONE	0.025	101.5	15.9	15.64	1.5	0.125
	0.125	109.1	7.8	7.12	9.1	
	1.25	104.0	12.3	11.81	4.0	
	5	110.0	10.9	9.94	10.0	
METHAQUALONE	0.025	100.7	24.8	24.58	0.7	0.125
	0.125	119.5	4.3	3.60	19.5	
	1.25	103.8	11.6	11.18	3.8	
	5	96.3	4.3	4.42	-3.7	
METHCATHINONE	0.025	109.5	19.8	18.06	9.5	0.125
	0.125	97.6	6.5	6.68	-2.4	
	1.25	95.0	5.7	6.03	-5.0	
	5	106.0	10.9	10.32	6.0	
METHEDRONE (bk-PMMA)	0.025	88.2	6.7	7.64	-11.8	0.125
	0.125	101.8	9.3	9.09	1.8	
	1.25	113.8	10.6	9.33	13.8	
	5	108.7	10.7	9.80	8.7	
METHOHEXITAL	0.125	92.5	17.0	18.37	-7.5	0.125
	1.25	96.6	11.8	12.25	-3.4	
	5	114.5	9.3	8.16	14.5	

METHOXETAMINE	0.025	90.7	30.5	33.66	-9.4	0.125
	0.125	109.8	16.4	14.91	9.8	
	1.25	113.4	8.6	7.57	13.4	
	5	118.7	7.7	6.53	18.7	
METHOXPHENIDINE	0.025	77.4	38.6	49.93	-22.7	0.125
	0.125	91.2	8.4	9.19	-8.8	
	1.25	99.5	11.7	11.73	-0.5	
	5	114.3	10.1	8.79	14.3	
METHYLHEXANAMINE	0.025	286.6	231.6	80.83	186.6	0.125
	0.125	114.5	13.8	12.01	14.5	
	1.25	99.2	10.1	10.22	-0.8	
	5	111.8	17.9	16.01	11.8	
METHYLONE (bk-MDMA)	0.025	105.7	6.5	6.15	5.7	0.125
	0.125	98.7	8.1	8.20	-1.3	
	1.25	97.9	8.6	8.81	-2.1	
	5	99.7	11.0	11.06	-0.3	
METHYLPHENIDATE	0.025	110.4	10.7	9.66	10.4	0.125
	0.125	114.1	19.8	17.38	14.1	
	1.25	94.9	12.2	12.84	-5.1	
	5	99.3	3.6	3.63	-0.7	
MEXEDRONE	0.025	89.8	11.9	13.29	-10.2	0.125
	0.125	102.6	13.4	13.04	2.6	
	1.25	102.1	5.5	5.35	2.1	
	5	114.2	10.1	8.82	14.2	
MIANSERIN	0.025	85.3	10.4	12.18	-14.8	0.125
	0.125	90.9	9.1	10.05	-9.1	
	1.25	84.2	6.0	7.10	-15.8	
	5	103.7	10.8	10.38	3.7	
MIDAZOLAM	0.025	108.3	12.0	11.10	8.3	0.125
	0.125	96.2	8.3	8.62	-3.8	
	1.25	81.2	2.2	2.66	-18.8	
	5	102.3	6.6	6.48	2.3	
MITRAGYNINE	0.025	82.3	20.5	24.96	-17.7	0.125
	0.125	93.4	13.0	13.90	-6.6	
	1.25	100.6	6.6	6.54	0.6	
	5	114.9	9.2	8.05	14.9	
MMAI	0.125	105.2	8.3	7.90	5.2	0.125
	1.25	93.0	11.9	12.82	-7.0	
	5	100.6	12.0	11.93	0.6	
MMB018	0.025	104.9	6.1	5.85	4.9	0.025
	0.125	105.9	8.9	8.42	5.9	
	1.25	117.2	9.9	8.45	17.2	
MMB2201	0.025	107.0	4.9	4.60	7.0	0.025
	0.125	108.2	5.3	4.87	8.2	
	1.25	110.4	11.8	10.68	10.4	
MN-18	0.025	100.1	12.3	12.26	0.1	0.025

	0.125	102.7	11.2	10.87	2.7	
	1.25	113.5	7.0	6.14	13.5	
MN-25	0.025	100.2	17.5	17.44	0.1	0.025
	0.125	98.1	9.5	9.68	-1.9	
	1.25	105.5	7.3	6.90	5.5	
MN-25-2-METHYL DERIVATIVE	0.025	99.3	7.9	7.99	-0.7	0.025
	0.125	105.7	6.5	6.10	5.7	
	1.25	104.2	8.8	8.46	4.2	
MO-CHMINACA	0.025	113.2	11.9	10.54	13.2	0.025
	0.125	115.5	8.9	7.68	15.5	
	1.25	116.9	11.4	9.71	16.9	
MORPHINE	0.025	142.7	12.2	8.55	42.7	0.125
	0.125	111.0	6.1	5.50	11.0	
	1.25	114.9	4.9	4.30	14.9	
	5	119.7	3.8	3.15	19.7	
MT-45	0.025	93.7	18.5	19.77	-6.3	0.125
	0.125	91.6	5.2	5.62	-8.4	
	1.25	114.6	9.8	8.54	14.6	
	5	119.0	16.2	13.62	19.0	
N-(3-METHYLBENZYL)PIPERAZINE	0.025	155.6	15.8	10.18	55.6	0.125
	0.125	109.1	5.1	4.65	9.1	
	1.25	82.6	1.9	2.30	-17.4	
	5	96.7	15.1	15.58	-3.3	
N.N-DIETHYLPHENETHYLAMINE	0.025	105.3	14.8	14.04	5.3	0.125
	0.125	104.0	10.1	9.73	4.0	
	1.25	93.6	6.2	6.63	-6.4	
	5	105.4	6.1	5.75	5.4	
N.N-DIMETHYLPENTYLONE (bk-DMBDP)	0.025	102.5	11.9	11.64	2.5	0.125
	0.125	107.9	14.2	13.18	7.9	
	1.25	95.5	12.2	12.76	-4.5	
	5	112.4	10.5	9.37	12.4	
N.N-DMT	0.125	101.6	19.2	18.85	1.6	0.125
	1.25	96.6	13.1	13.54	-3.4	
	5	104.7	9.0	8.63	4.7	
N-ACETYL-3.4-MDMC	0.025	123.2	19.7	16.00	23.2	0.125
	0.125	91.5	6.3	6.87	-8.5	
	1.25	101.0	9.9	9.84	1.0	
	5	110.3	15.8	14.29	10.3	
NAPHYRONE	0.025	110.0	13.9	12.67	10.0	0.125
	0.125	112.5	6.4	5.66	12.5	
	1.25	101.6	4.8	4.77	1.6	
	5	107.3	3.9	3.64	7.3	
NAPHYRONE-1-NAPHTYL ISOMER	0.025	99.1	14.4	14.56	-0.9	0.125
	0.125	106.4	8.0	7.51	6.4	
	1.25	99.8	9.4	9.45	-0.2	
	5	118.2	13.2	11.18	18.2	

N-BENZYLNORBUTYLONE	0.025	75.0	6.8	9.11	-25.0	0.125
	0.125	96.4	12.2	12.71	-3.6	
	1.25	90.9	10.8	11.91	-9.1	
	5	97.6	12.5	12.85	-2.4	
N-ETHYL-4-METHOXYAMPHETAMNE	0.025	98.6	18.0	18.30	-1.5	0.125
	0.125	107.0	13.6	12.75	6.9	
	1.25	105.3	8.8	8.31	5.3	
	5	112.1	10.3	9.19	12.1	
N-ETHYLBUPHEDRONE	0.025	96.9	19.6	20.25	-3.1	0.125
	0.125	103.8	8.5	8.21	3.8	
	1.25	104.6	8.8	8.38	4.6	
	5	113.9	11.9	10.46	13.9	
N-ETHYL-N-METHYLCATHINONE	0.025	96.6	27.8	28.76	-3.4	0.125
	0.125	97.6	9.1	9.37	-2.4	
	1.25	98.6	9.8	9.95	-1.4	
	5	106.7	15.2	14.22	6.7	
N-ETHYLNORDAZEPAM	0.025	82.7	12.2	14.75	-17.3	0.125
	0.125	89.9	7.1	7.93	-10.1	
	1.25	89.2	6.9	7.75	-10.8	
	5	96.5	9.1	9.45	-3.5	
N-ETHYLNORKETAMINE	0.025	107.8	25.2	23.42	7.8	0.125
	0.125	110.4	19.8	17.94	10.4	
	1.25	114.9	10.5	9.15	14.9	
	5	114.7	6.0	5.27	14.7	
N-ETHYLOXAZEPAM	0.025	91.5	12.9	14.13	-8.5	0.125
	0.125	95.6	13.6	14.19	-4.4	
	1.25	103.3	8.1	7.82	3.3	
	5	117.5	7.5	6.40	17.5	
N-ETHYLPENTYLONE	0.025	113.2	12.2	10.82	13.2	0.125
	0.125	109.1	10.9	9.95	9.1	
	1.25	91.8	10.6	11.55	-8.2	
	5	105.3	11.1	10.53	5.3	
NIMETAZEPAM	0.025	107.9	10.6	9.84	7.9	0.125
	0.125	98.8	8.1	8.20	-1.2	
	1.25	102.1	9.2	9.02	2.1	
	5	108.3	13.6	12.59	8.3	
NITRAZEPAM	0.025	101.5	14.2	14.01	1.5	0.125
	0.125	89.2	8.6	9.67	-10.8	
	1.25	94.4	4.1	4.38	-5.6	
	5	100.1	7.0	7.04	0.1	
NM2201	0.025	104.0	17.6	16.97	4.0	0.025
	0.125	104.7	8.4	8.07	4.7	
	1.25	113.0	13.0	11.54	13.0	
N-METHYL-2AI	0.025	111.5	7.9	7.06	11.5	0.125
	0.125	98.5	5.7	5.75	-1.5	
	1.25	96.5	7.8	8.08	-3.5	

	5	93.0	10.4	11.22	-7.0	
N-METHYL-PEA	0.025	120.5	9.6	7.98	20.5	0.125
	0.125	105.1	4.1	3.87	5.1	
	1.25	99.4	6.5	6.54	-0.6	
	5	103.0	2.7	2.62	3.0	
N-METHYLTRYPTAMINE	0.025	98.3	17.6	17.87	-1.7	0.125
	0.125	98.7	6.7	6.75	-1.3	
	1.25	95.7	8.2	8.57	-4.3	
	5	89.7	14.1	15.76	-10.3	
NN-DMC	0.025	101.2	14.6	14.43	1.1	0.125
	0.125	101.4	4.1	4.03	1.4	
	1.25	99.6	4.4	4.44	-0.4	
	5	104.4	8.8	8.40	4.4	
NNEI	0.025	104.0	16.3	15.70	4.0	0.025
	0.125	105.8	5.7	5.41	5.8	
	1.25	114.3	8.8	7.73	14.3	
NORCLOBAZAM	0.125	87.5	12.0	13.68	-12.5	0.125
	1.25	110.2	9.5	8.66	10.2	
	5	117.2	6.8	5.83	17.2	
NORCLOMIPRAMINE	0.025	105.3	15.4	14.60	5.3	0.125
	0.125	106.1	9.1	8.58	6.1	
	1.25	83.7	11.8	14.15	-16.3	
	5	104.1	15.7	15.10	4.1	
NORKETAMINE	0.125	82.3	15.4	18.68	-17.8	0.125
	1.25	91.9	7.9	8.60	-8.1	
	5	108.1	10.7	9.86	8.1	
NORTRIPTYLINE	0.025	104.2	19.4	18.62	4.2	0.125
	0.125	108.1	6.7	6.20	8.1	
	1.25	94.4	9.7	10.27	-5.6	
	5	106.7	12.2	11.46	6.7	
N-PROPYLAMPHETAMINE	0.025	89.2	30.0	33.65	-10.8	0.125
	0.125	90.5	17.0	18.77	-9.5	
	1.25	108.7	17.5	16.08	8.7	
	5	110.1	12.2	11.09	10.1	
NRG-3	0.025	101.7	13.9	13.66	1.7	0.125
	0.125	86.5	4.1	4.69	-13.5	
	1.25	87.4	6.5	7.39	-12.6	
	5	105.3	7.1	6.71	5.3	
o-CPP	0.025	143.6	22.9	15.96	43.6	0.125
	0.125	100.8	17.1	16.95	0.8	
	1.25	107.5	10.7	9.92	7.5	
	5	110.3	9.3	8.39	10.3	
OCTACAINE	0.025	87.8	10.3	11.78	-12.3	0.125
	0.125	113.5	11.8	10.36	13.5	
	1.25	99.1	6.8	6.90	-0.9	
	5	103.7	8.2	7.87	3.7	

ORG-28611	0.025	98.8	8.4	8.46	-1.2	0.025
	0.125	113.5	7.5	6.61	13.5	
	1.25	85.0	5.7	6.67	-15.0	
OXAZEPAM	0.025	78.0	56.5	72.50	-22.0	0.125
	0.125	93.3	14.8	15.83	-6.7	
	1.25	94.9	10.6	11.21	-5.1	
	5	111.3	6.7	6.06	11.3	
OXYMORPHONE	0.025	572.2	362.7	63.39	472.2	-
	0.125	342.5	14.6	4.27	242.5	
	1.25	250.4	237.3	94.77	150.4	
	5	521.3	285.2	54.71	421.3	
PARACETAMOL	0.025	70.4	19.3	27.35	-29.6	0.125
	0.125	85.4	5.8	6.74	-14.6	
	1.25	102.9	6.7	6.53	2.9	
	5	105.8	5.5	5.24	5.8	
PAROXETINE	0.025	115.3	16.6	14.41	15.3	0.125
	0.125	103.5	17.3	16.70	3.5	
	1.25	82.0	6.6	8.03	-18.0	
	5	104.4	19.0	18.20	4.4	
PB-22	0.025	106.5	11.4	10.73	6.5	0.025
	0.125	109.3	10.8	9.86	9.3	
	1.25	116.0	13.3	11.43	16.0	
PCEEA	0.025	102.3	5.8	5.64	2.3	0.125
	0.125	91.8	9.8	10.73	-8.2	
	1.25	99.9	4.8	4.79	-0.1	
	5	109.6	5.3	4.83	9.6	
PCMPA	0.025	101.9	13.7	13.41	1.9	0.125
	0.125	117.3	15.9	13.58	17.3	
	1.25	118.3	8.9	7.53	18.3	
	5	113.5	13.4	11.83	13.5	
PCPr	0.125	95.7	11.7	12.18	-4.3	0.125
	1.25	116.4	8.6	7.41	16.4	
	5	114.4	2.2	1.91	14.4	
PENTEDRONE	0.025	87.2	22.2	25.51	-12.8	0.125
	0.125	99.2	10.1	10.19	-0.8	
	1.25	89.5	13.0	14.56	-10.5	
	5	101.9	8.6	8.45	1.9	
PENTEDRONE METABOLITE	0.025	114.0	4.8	4.17	14.0	0.125
	0.125	107.1	6.6	6.15	7.1	
	1.25	109.4	10.3	9.45	9.4	
	5	107.4	15.8	14.68	7.4	
PENTYLONE (bk-MBDP)	0.025	47.1	39.4	83.84	-53.0	0.125
	0.125	112.8	17.3	15.37	12.8	
	1.25	111.3	18.6	16.69	11.3	
	5	114.5	14.5	12.62	14.5	
PHENAZEPAM	0.025	81.6	32.7	40.01	-18.4	0.125

	0.125	92.7	15.9	17.15	-7.3	
	1.25	107.6	10.9	10.08	7.6	
	5	113.3	5.2	4.63	13.3	
PHENCYCLIDINE (PCP)	0.025	99.7	33.1	33.23	-0.4	0.125
	0.125	113.2	4.9	4.37	13.2	
	1.25	116.0	8.6	7.42	16.0	
	5	96.7	11.7	12.13	-3.3	
PHENTERMINE	0.025	99.7	58.0	58.17	-0.3	0.125
	0.125	90.9	15.4	16.91	-9.1	
	1.25	112.1	20.3	18.15	12.1	
	5	102.8	13.8	13.40	2.8	
PHENYTOIN	0.025	111.8	18.3	16.39	11.8	0.125
	0.125	98.6	10.0	10.13	-1.4	
	1.25	106.1	9.3	8.72	6.1	
	5	116.6	7.7	6.61	16.6	
PRAVADOLINE	0.025	95.2	13.4	14.03	-4.8	0.125
	0.125	100.0	11.2	11.20	0.0	
	1.25	90.5	15.5	17.12	-9.5	
	5	102.3	14.9	14.55	2.3	
PRAZEPAM	0.025	99.5	6.0	6.02	-0.5	0.125
	0.125	107.9	4.5	4.16	7.9	
	1.25	99.1	4.6	4.64	-0.9	
	5	94.4	4.5	4.76	-5.6	
PREGABALIN	0.125	64.2	12.3	19.23	-35.8	1.25
	1.25	94.6	8.6	9.14	-5.4	
	5	93.8	5.1	5.42	-6.2	
PROCAINE	0.025	118.6	18.8	15.86	18.6	0.125
	0.125	117.1	5.2	4.47	17.1	
	1.25	116.2	6.5	5.63	16.2	
	5	119.2	7.5	6.27	19.2	
PROLINTANE	0.025	123.8	33.8	27.32	23.8	0.125
	0.125	111.1	18.0	16.22	11.1	
	1.25	107.8	9.2	8.51	7.8	
	5	109.9	11.2	10.23	9.9	
PROMETHAZINE	0.025	88.9	4.9	5.46	-11.1	0.125
	0.125	93.1	9.7	10.45	-6.9	
	1.25	80.1	3.6	4.55	-19.9	
	5	96.9	12.6	13.01	-3.1	
PROPAFENONE	0.025	127.6	11.3	8.84	27.6	0.125
	0.125	97.9	8.6	8.74	-2.1	
	1.25	90.0	7.4	8.18	-10.0	
	5	105.7	13.6	12.83	5.7	
PROPRANOLOL	0.025	71.8	24.6	34.18	-28.2	0.125
	0.125	96.1	11.5	11.91	-3.9	
	1.25	86.6	5.4	6.28	-13.4	
	5	110.3	19.6	17.80	10.3	

PROPYLHEXEDRINE	0.025	85.0	57.4	67.53	-15.0	0.125
	0.125	95.0	17.2	18.11	-5.0	
	1.25	113.4	18.0	15.92	13.4	
	5	118.7	9.1	7.65	18.7	
PSB-SB-1202	0.025	106.6	18.5	17.32	6.6	0.025
	0.125	108.6	13.3	12.28	8.6	
	1.25	114.4	7.7	6.74	14.4	
PTI-1	0.025	107.7	7.5	6.98	7.7	0.025
	0.125	103.1	6.3	6.13	3.1	
	1.25	114.9	9.1	7.92	14.9	
PTI-2	0.025	100.8	9.4	9.29	0.8	0.025
	0.125	101.3	3.0	2.94	1.3	
	1.25	118.4	15.6	13.17	18.4	
PV-8	0.025	97.6	18.8	19.23	-2.5	0.125
	0.125	108.9	13.7	12.59	8.9	
	1.25	91.4	8.1	8.90	-8.6	
	5	114.3	5.3	4.67	14.3	
PV9	0.025	115.1	7.9	6.90	15.1	0.125
	0.125	101.8	7.7	7.55	1.8	
	1.25	94.1	6.0	6.36	-5.9	
	5	108.1	5.9	5.45	8.1	
PX-1	0.025	114.6	17.9	15.58	14.6	0.025
	0.125	99.6	5.6	5.59	-0.4	
	1.25	93.4	11.4	12.16	-6.6	
PX-2	0.025	109.2	12.1	11.09	9.2	0.025
	0.125	98.9	5.2	5.21	-1.1	
	1.25	112.6	12.8	11.37	12.6	
PYRAZOLAM	0.025	96.7	17.3	17.89	-3.3	0.125
	0.125	87.0	11.5	13.23	-13.0	
	1.25	95.6	4.5	4.69	-4.4	
	5	117.3	14.3	12.19	17.3	
QUETIAPINE	0.025	84.7	18.0	21.29	-15.4	0.125
	0.125	88.6	10.3	11.58	-11.4	
	1.25	88.0	11.7	13.29	-12.0	
	5	107.7	20.5	19.05	7.7	
RCS-4	0.025	103.4	19.6	18.96	3.4	0.025
	0.125	117.3	9.3	7.91	17.3	
	1.25	112.1	17.1	15.26	12.1	
RH-34	0.025	90.6	19.1	21.06	-9.5	0.125
	0.125	102.6	16.9	16.50	2.6	
	1.25	91.5	13.0	14.20	-8.5	
	5	110.9	16.6	14.96	10.9	
R-MMC	0.025	133.6	24.2	18.12	33.6	0.125
	0.125	112.0	8.8	7.89	12.0	
	1.25	119.9	9.7	8.07	19.9	
	5	114.1	8.9	7.76	14.1	

SCOPOLAMINE	0.025	112.3	13.7	12.23	12.3	0.125
	0.125	110.1	15.8	14.38	10.1	
	1.25	101.2	8.5	8.44	1.2	
	5	99.1	11.1	11.23	-0.9	
SDB-005	0.025	100.5	11.7	11.60	0.5	0.025
	0.125	112.0	5.8	5.18	12.0	
	1.25	107.9	10.0	9.23	7.9	
SDB-006	0.025	97.2	6.2	6.39	-2.8	0.025
	0.125	115.7	7.8	6.71	15.7	
	1.25	112.2	11.6	10.31	12.2	
SERTRALINE	0.025	88.4	23.9	26.99	-11.6	0.125
	0.125	99.1	10.9	11.00	-0.9	
	1.25	101.8	18.2	17.92	1.8	
	5	118.4	4.7	4.00	18.4	
SILDENAFIL	0.025	100.9	21.4	21.17	0.9	0.125
	0.125	117.0	10.5	8.98	17.0	
	1.25	98.2	16.3	16.62	-1.8	
	5	107.4	10.6	9.88	7.4	
STANOZOLOL	0.025	3064.3	2512.9	82.01	2964.3	-
	1.25	120.8	53.7	44.44	20.8	
	5	38.1	4.1	10.81	-61.9	
TAPENTADOL	0.025	116.3	22.1	18.98	16.3	0.125
	0.125	101.0	15.6	15.45	1.0	
	1.25	98.6	10.8	10.93	-1.4	
	5	94.1	7.9	8.42	-5.9	
TEMAZEPAM	0.025	106.7	17.1	16.05	6.7	0.125
	0.125	97.9	15.3	15.65	-2.1	
	1.25	104.3	6.5	6.27	4.3	
	5	112.1	10.4	9.29	12.1	
TETRACAINE	0.025	110.8	14.7	13.28	10.8	0.125
	0.125	100.2	9.6	9.59	0.2	
	1.25	102.2	8.0	7.81	2.2	
	5	118.0	7.6	6.45	18.0	
THC	0.025	94.6	10.2	10.84	-5.5	0.025
	0.125	98.2	13.0	13.26	-1.8	
	1.25	115.1	12.1	10.49	15.1	
THCCOOH	0.021.25	83.6	14.1	16.93	-16.4	0.250
	1.25	90.3	13.6	15.06	-9.7	
	1.25	101.4	16.0	15.81	1.4	
THIOPROPAMINE	0.025	122.9	42.5	34.58	22.9	0.125
	0.125	103.3	11.0	10.66	3.3	
	1.25	101.6	7.0	6.86	1.6	
	5	105.9	9.9	9.37	5.9	
THJ	0.025	95.3	4.5	4.75	-4.7	0.025
	0.125	94.9	5.3	5.59	-5.1	
	1.25	116.0	9.3	8.02	16.0	

THJ-018	0.025	104.9	18.1	17.28	4.9	0.025
	0.125	109.1	5.2	4.78	9.1	
	1.25	118.1	12.0	10.20	18.1	
THJ-2201 (5-FLUORO THJ-018)	0.025	96.8	12.5	12.94	-3.2	0.025
	0.125	107.6	8.9	8.23	7.6	
	1.25	116.8	17.7	15.14	16.8	
TILETAMINE	0.025	91.3	18.6	20.38	-8.7	0.125
	0.125	98.8	10.9	11.01	-1.2	
	1.25	109.4	6.2	5.64	9.4	
	5	111.6	12.1	10.88	11.6	
TRAMADOL	0.025	107.8	11.0	10.22	7.8	0.125
	0.125	101.2	9.1	9.00	1.2	
	1.25	100.1	9.5	9.53	0.1	
	5	104.1	8.4	8.05	4.1	
TRAZODONE	0.025	93.2	22.2	23.85	-6.8	0.125
	0.125	86.2	11.3	13.07	-13.8	
	1.25	88.5	6.0	6.81	-11.5	
	5	99.0	9.5	9.55	-1.0	
TRIAZOLAM	0.025	75.3	20.5	27.26	-24.8	0.125
	0.125	95.2	13.8	14.55	-4.8	
	1.25	94.9	5.6	5.90	-5.1	
	5	112.7	11.9	10.51	12.7	
TRIMIPRAMINE	0.025	93.5	12.5	13.34	-6.6	0.125
	0.125	104.4	8.3	7.91	4.4	
	1.25	95.2	17.4	18.27	-4.8	
	5	111.2	9.6	8.63	11.2	
U-47700	0.025	99.4	13.4	13.53	-0.6	0.125
	0.125	104.2	4.1	3.93	4.2	
	1.25	101.6	6.0	5.94	1.6	
	5	104.5	11.2	10.74	4.5	
UR-144	0.025	103.0	17.9	17.37	3.0	0.025
	0.125	108.6	7.6	7.02	8.6	
	1.25	115.2	14.1	12.21	15.2	
UR-144 metabolite	0.025	96.7	17.5	18.07	-3.3	0.025
	0.125	102.4	9.0	8.81	2.4	
	1.25	108.7	9.7	8.96	8.7	
W-15	0.025	105.5	4.4	4.15	5.5	0.125
	0.125	99.7	6.2	6.22	-0.3	
	1.25	100.7	6.0	5.95	0.7	
	5	114.2	9.3	8.15	14.2	
WIN 54.461	0.025	104.4	8.1	7.79	4.4	0.025
	0.125	105.5	11.5	10.93	5.5	
	1.25	101.5	8.1	8.00	1.5	
WIN 55.212-2	0.025	94.3	10.2	10.86	-5.8	0.025
	0.125	89.0	6.9	7.73	-11.0	
	1.25	93.8	13.0	13.86	-6.2	

XLR-11	0.025	98.6	12.7	12.92	-1.4	0.025
	0.125	101.1	9.6	9.54	1.1	
	1.25	108.8	10.3	9.47	8.8	
XLR12	0.025	101.3	5.5	5.39	1.3	0.025
	0.125	103.5	4.9	4.74	3.5	
	1.25	109.0	10.9	9.97	9.0	
YANGONIN	0.125	90.3	17.2	19.08	-9.7	0.125
	1.25	119.6	14.3	11.93	19.6	
	5	114.5	2.9	2.53	14.5	
ZALEPLON	0.025	100.1	10.5	10.52	0.1	0.125
	0.125	99.3	9.7	9.80	-0.7	
	1.25	102.9	11.9	11.53	2.9	
	5	119.4	6.1	5.07	19.4	
ZOLPIDEM	0.025	89.9	6.9	7.66	-10.1	0.125
	0.125	100.5	7.9	7.90	0.5	
	1.25	97.1	6.8	7.04	-2.9	
	5	95.5	3.0	3.15	-4.5	
ZOPICLONE	0.025	34.8	14.6	42.00	-65.3	0.125
	0.125	99.3	9.1	9.13	-0.7	
	1.25	112.0	17.1	15.28	12.0	
	5	112.3	15.3	13.66	12.3	
ZUCLOPENTHIXOL	0.025	139.8	36.4	26.01	39.8	0.125
	0.125	108.6	17.9	16.46	8.6	
	1.25	117.1	12.6	10.75	17.1	
	5	153.4	27.5	17.91	53.4	
α-HYDROXYMIDAZOLAM	0.025	131.4	26.6	20.22	31.4	0.125
	0.125	86.3	12.6	14.63	-13.7	
	1.25	89.5	4.9	5.43	-10.5	
	5	108.3	6.5	5.98	8.3	

[D3] Jakub Czarny, **Jadwiga Musiał**, Jolanta Powierska-Czarny, Natalia Galant, Michał Raczkowski, Bogusław Buszewski, Renata Gadzała-Kopciuch, *Validation of a simple and quick method for determination of psychoactive substances, drugs and their metabolites from human blood by LC-MS/MS*, Microchemical Journal, 2022, 182: 107922, ISSN 0026-265X, https://doi.org/10.1016/j.microc.2022.107922, IF=5,304

W związku z ciągle wzrastającą liczbą zdarzeń drogowych oraz przestępstw kryminalnych popełnianych pod wpływem substancji psychoaktywnych dostępnych w sprzedaży ulicznej, a także wciąż wzrastającą ilość nowych substancji psychoaktywnych, rosnące zainteresowanie tego typu używkami wśród społeczeństwa, wzrasta także zapotrzebowanie na badania próbek biologicznych pod kątem tego typu substancji. Ze względu na fakt, że najczęściej analizowanymi próbkami biologicznymi w Instytucie Genetyki Sądowej są próbki krwi w opisanej pracy skupiono się na opracowaniu metody analitycznej umożliwiającej oznaczenie jak największej liczby analitów należących do grupy substancji psychoaktywnych/leków/ich metabolitów właśnie dla tej matrycy.

Celem prac było opracowanie metody analitycznej, która jest prosta, ale jednocześnie dająca możliwość łatwego dodania kolejnych analitów, a także stosunkowo łatwego dostosowania jej do innej matrycy biologicznej. Chcąc wykorzystać opracowaną metodykę dla analitów izolowanych z włosów przystąpiono do przygotowania próbek stosując ekstrakcję substancji psychoaktywnych, ich metabolitów i leków z próbek krwi. W procedurze przygotowania próbki podobnie, jak w przypadku próbek włosów skupiono się na uwzględnieniu wpływu matrycy oraz ograniczeniu zanieczyszczeń pochodzących z próbki, dlatego też zdecydowano się również w przypadku tej matrycy na sporządzenie krzywej wzorcowej na bazie matrycy.

Ze względu, że jedną z najczęściej stosowanych technik ekstrakcyjnych jest ekstrakcja do fazy stałej (SPE) podjęto próbę zastosowania właśnie tego sposobu do wyizolowania wybranych do badań analitów. Ze względu na ilość analitów oraz fakt, że należą one do wielu grup spośród substancji psychoaktywnych, konieczne byłoby zastosowanie kilku kolumienek SPE do różnych grup analitów. Wprowadzenie tego sposobu do procedury analitycznej wiązałoby się z wydłużeniem czasu analizy, konieczności posiadania większej objętości prób, a także znacznie zwiększyłoby koszty analiz i ilość odpadów z niej pochodzących. Biorąc pod uwagę powyższe podjęto próbę opracowania innej metody przygotowania próbki. Kolejnym etapem było zastosowanie techiki QuEChERS. Uzyskane wyniki dla tej metody również nie

były dla nas zadowalające. Brak pozytywnych rezultatów skłonił do wykorzystania ekstrakcji ciecz-ciecz (LLE). W celu zminimalizowania wpływu matrycy poza zastosowaniem krzywej wzorcowej w matrycy zastosowano także metodę rozcieńczenia próbki w ostatnim etapie przygotowania próbki zamiast jej wzbogacania poprzez odparowanie do sucha pod strumieniem azotu. Pozwoliło to na uzyskanie czystszych ekstraktów, co w konsekwencji przełożyło się na niższe wartości LOQ dla poszczególnych analitów.

Opracowaną metodę analityczną poddano procesowi walidacji tak jak w przypadku próbek włosów zgodnie z wytycznymi SWGTOX [78]. Linowość sprawdzono poprzez analizę 6 powtórzeń krzywej wzorcowej przygotowanej w matrycy w stężeniach w zakresie od 2 do 200 ng/ml dla kannabinoidów (1 do 200 ng/ml dla THC), od 0,05 do 50 ng/ml dla pozostałych grup analitów. Ponadto, w każdej serii analizowano próbkę ślepą (bez substancji badanych) i matrycę z wzorcem wewnętrznym. Współczynniki korelacji obliczone dla każdego analitu wynosiły ≥0,99. Aby wyznaczyć precyzję i BIAS analizowano sześciokrotnie pięć poziomów stężeń analitów po uwzględnieniu rozcieńczenia próbki (1 ng/ml dla THC, 2, 10, 200,400, 500 i 1000 ng/ml. Dla powyższych parametrów przyjęto zgodnie z wytycznymi granicę ±20%. Pomiary te wykorzystano także do wyznaczenia średniego odzysku analitów. LOQ wyznaczono na podstawie stosunku S/N ≥10, który odpowiadał najniższemu punktowi na krzywej wzorcowej. W celu weryfikacji powtarzalności metody przystąpiono do analizy próbek w badaniach biegłości.

Opracowana procedura analityczna izolowania NPS oraz ich oznaczania została wprowadzona do rutynowych analiz w Instytucie Genetyki Sądowej w Bydgoszczy.

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Validation of a simple and quick method for determination of psychoactive substances, drugs and their metabolites from human blood by LC-MS/MS

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ABSTRACT

The development of the black market, and thus the increase in the number of available psychoactive substances, forces laboratories to take measures to prevent poisoning and deaths caused by the use of, inter alia, new psychoactive substances (NPS). It is important to selectively determine psychoactive substances and their metabolites in blood samples in the shortest possible time, which will allow medical services to act timely. Bearing in mind the above, the aim of our study was to develop an analytical method that would enable the unequivocal identification of over 500 psychoactive substances in blood samples with one analysis. The techniques selected for this purpose were liquid–liquid extraction (LLE) and liquid chromatography coupled with mass spectrometry (LC-MS/MS). Acetonitrile with ammonium formate and formic acid was used for the extraction. The best column was found to be the Kinetex C18 column (Phenomenex, 3.0 × 100 mm; 2.6 μm). MRM pair monitoring mode was used (two pairs for each analyte). 522 psychoactive substances and their metabolites have been validated, and only 2 out of 522 failed to meet the validation criteria recommended by SWGTOX (CV: ± 20 % and BIAS ± 20 %). The developed method enables the quantitative analysis of 520 psychoactive substances during a 30-minute run. Limits of quantification (LOQ) range from 1 to 200 ng/mL. The developed method was introduced into the routine toxicological analysis of blood samples. It also offers opportunities for further development in line with the needs of toxicology.

1. Introduction

In recent years, a dynamic development of civilization has been observed, resulting in an increase in the number of lifestyle-related diseases. There is a greater number of cases of diseases of the cardiovascular and digestive systems, mental diseases, and addictions, including drug addiction. A society chasing professional development and money is increasingly fleeing to psychoactive substances, which often are legal highs, sold as legal drugs that are a cheaper alternative to classic drugs or alcohol. In addition to classic narcotics, new psychoactive substances (NPS) have lately been noted to appear on the market with growing frequency. Due to their diversity, no penalization of their use, the ease with which NPS distributors circumvent legal restrictions, as well as the lack of widespread awareness of the effects they cause in the body, NPS have become a global health problem [1,2]. In recent years, this group includes not only amphetamine, THC, tryptamine and piperazine derivatives, but also compounds from the cathinone group and 2C substances, the consumption of which causes enormous effects in the body that are difficult to predict [3–5]. The number of identified new psychoactive substances is constantly increasing. In 2009, 13 NPS were submitted to the European Monitoring Center for Drugs and Drug Addiction (EMCDDA), in 2010 another 41, in 2011 – 49, while in 2012 – 73. The next year brought notifications about 81 new substances, and in 2014 – as many as 101. Reports of the abovementioned organization indicate that 400 legal highs were detected in 2008–2014 [1,6–7]. Monitoring of NPS emerging on the market made it possible to detect and deaths caused by the use of this type of substance and publish the relevant data [8–16]. Due to the speed at which the black drug market develops new products, toxicology laboratories face a real challenge. They must meet the local community's demand regarding the list of analyzed substances, including new psychoactive substances. The aim of the laboratories is to expand the range of tested analytes to include NPS

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in order to be able to diagnose cases of poisoning with these substances as well as NPS-related causes of deaths, and to monitor symptoms. Identification of the constantly growing number of narcotic drugs is associated with certain difficulties, such as a large variety in chemical structures of such compounds and the need for quick analysis, if only because it is difficult to predict the body's reaction to a given toxin [5,17–19]. What is also noteworthy is that a positive cross-reaction result obtained from the immunochemical test must be confirmed by means of chromatographic techniques due to the lack of unambiguous identification by means of an immunochemical test [20]. The above facts show how important it is to develop constantly new methods of NPS determination so that a maximum number of compounds can be analyzed in the shortest possible time.

2. Material and methods

2.1. Chemicals, reagents and equipment

For the development of this analytical method, certified analytical standards were purchased from the following suppliers: LGC Standards (Łomianki, Poland), Cayman Chemical Company (Ann Arbor, MI, USA), Tusnovics Instruments Sp. z o. o. (Kraków, Poland), Lipomed Services to Health (Arlesheim, Switzerland). All the analytical standards used are certified. Several certificates are attached to the manuscript (Fig. S1), while others will be provided upon request. LC-MS purity solvents used came from S. WITKO CHS (methanol and formic acid) and ammonium formate from Sigma Aldrich (Darmstadt, Germany). Other equipment used to develop the method included Eppendorf tubes (2 mL), vials (2 mL), MS2 Minishaker IKA 200–2500 rpm, laboratory centrifuge Sigma 4-16S, and syringe filters: VWR 0.2 μm.

2.2. Instrumentation and detection method

The analysis of blood samples for new psychoactive substances and their metabolites involved the use of ExionLC AC Pump 2x, ExionLC Degaser, Exion AC Autosampler, ExionLC Column Oven from AB SCIEX coupled to a 5500 QTRAP spectrometer (AB SCIEX). Both positive and negative ionization modes operating in electrospray (ESI) were used. A Kinetex C18 column (Phenomenex, 3.0 × 100 mm; 2.6 μm) was used to separate the analytes. Mobile phase: **A** – water with 2 mM ammonium formate and 0.1 % (v/v) formic acid and **B** – methanol with 2 mM ammonium formate and 0.1 % (v/v) formic acid, were used.

Gradient elution was used, with the following conditions: 5 % of **B** at 0 min, held for 1 min, then increased to 95 % of **B** over 14 min, held until 21 min; then returned to 5 % B at 27 min and held until 30 min. The mobile phase was delivered at a flow rate of 0.5 mL/min. Precursor ion and two fragment ions were monitored for each analyte. The mass detector parameters were as follows: CUR: 30, CAD: medium, TEM: 400, GS1: 40, GS2: 70, dwell time ≥ 5 ms. The transitions, declustering potential (DP), entrance potential (EP), collision energy (CE), and collision cell exit potential (CXP) for individual analytes are presented in Table 1. Data acquisition, data handling and instrument control were performed with Analyst 1.6.3 and MultiQuant 3.0.3 software.

2.3. Blood samples

For the development and validation of the method, blank whole blood samples were used. The blood used in the method validation process came from the person who gave consent to collect, and we have a signed declaration of informed consent to collect blood and use it for research. On the other hand, blood samples that have been analyzed for the presence of psychoactive substances, drugs, and their metabolites are blood samples tested at the request of judicial authorities in forensic cases. This is a particular type of test that, according to the provisions of law, does not require the consent of the tested person or the permission of the Bioethics Committee. These samples were collected in health clinics by qualified medical personnel. Two vials of blood were collected from each test person, which, together with the blood collection protocol, were secured and transported to the laboratory by the requirements for this type of sample. Blood samples from the examined people were collected in Poland, and they were obtained from women and men aged 18–65 years. Most samples were from living people, but some came from dead bodies.

2.4. Standards, calibrators, and control samples

Stock solutions of analytical standards at concentration 1 mg/mL were prepared with methanol and stored below −20 °C. Drug-free blood samples were fortified with a mix of all the investigated psychoactive substances to create a calibration curve in the matrix at the following concentrations: 0.05, 0.1, 0.5, 1.0, 5.0, 10, 20 and 50 ng/mL. Two fortified samples were prepared in each series of analyses (2 ng/mL and 10 ng/mL). Atrazine solution at the concentration of 2500 ng/mL was used as an procedural internal standard (P-IS). This substance was chosen as the internal standard because of its stability and the certainty that it will not be present in the test and control samples. In addition, deuterated standards would be dedicated to a specific analyte, which would not be reliable for other analytes, while increasing the number of internal standards would make the analysis difficult and significantly increase its costs. Extraction solution containing 20 μL ammonium formate, 20 μL formic acid and 60 μL acetonitrile was prepared. Detailed instructions for the preparation of all mixes, dilutions, and other solutions are the subject of a patent application to the Patent Office of the Republic of Poland, application no: P.441164, with the possibility of extending the patent in the EU. As proof of having and using analytical standards, the laboratory can present scans of certificates of purchased standards. The description of the preparation of the standards and the ranges of the concentrations used can be found in the publication sent for review. If needed, the authors of the work will provide all the necessary explanations in this regard.

2.5. Sample preparation procedure

2.5.1. Blood samples

In the first stage of sample preparation, atrazine solution (20 μL; 2500 ng/mL) was added to the test tube. Then a blood sample (0.5 mL) and cold acetonitrile (2 mM ammonium formate, 0.1 % (v/v) formic acid) (0.5 mL) was added. After vortexing, the sample was placed in a shaker (1400 RCF, 10 min, 21 °C) and then transferred to a freezer (10 min). In the next step the sample was centrifuged (2000 RCF, 5 min) and the obtained supernatant was placed in a syringe filter (0.2 μm PTFE). In the last step, the sample applied to the syringe filter was centrifuged (10.000 RCF, 1 min) and 50 μL of the resulting extract was transferred to a autosampler vials with 450 μL mobile phase (A:B; 90:10 v/v). The blood sample preparation procedure described above allowed the isolation of all tested analytes from the blood samples during one process, giving satisfactory recovery results. The injection volume was 20 μL. Each samples was analyzed twice. The analysis of real samples has shown that the difference between the samples analyzed twice does not exceed 20 %.

2.5.2. Fortified samples

Two fortified samples were tested in each series of analyses (2 ng/mL and 10 ng/mL). 20 μL of 2500 ng/mL methanolic solutions of atrazine (IS) and 50 μL of mix of analytical standards 10 or 100 ng/mL, depending on the level of fortifications, was introduced into an Eppendorf tube containing 0.5 mL of blood without analytes. For precipitation, 0.5 mL of cold acetonitrile (2 mM ammonium formate, 0.1 % (v/v) formic acid) was used. The samples were vortexed and placed in a minishaker (1400 rpm, 21 °C) for 10 min. After 10 min in the freezer, and the obtained supernatant was placed in a syringe filter (0.2 PTFE). In the last step, the sample applied to the syringe filter was centrifuged

Table 1
Summary of operating parameters LC-MS/MS.

Precursor Ion (Q1)	Product Ion (Q3)	Retention time [min]	Analyte	Declustering potential (DP)	Collision energy (CE)	Cell exit potential (CXP)
266.3	125.1	8.93	4-CHLORO-ALPHA-PVP 1	101	33	10
266.3	126.1	8.93	4-CHLORO-ALPHA-PVP 2	101	37	18
193.263	120.1	5.30	1-(2-METHOXYPHENYL)PIPERAZINE 1	106	43	8
193.263	150.1	5.30	1-(2-METHOXYPHENYL)PIPERAZINE 2	106	25	18
231.278	188	7.95	1-(3-TRIFLUOROMETHYLPHENYL)PIPERAZINE (TFMPP) 1	141	31	22
231.278	118	7.95	1-(3-TRIFLUOROMETHYLPHENYL)PIPERAZINE (TFMPP) 2	141	51	16
197.469	119.1	6.67	1-(4-CHLOROPHENYL)PIPERAZINE (pCPP) 1	121	33	14
197.469	118.1	6.67	1-(4-CHLOROPHENYL)PIPERAZINE (pCPP) 2	121	45	16
181.26	138.1	4.69	1-(4-FLUOROPHENYL)PIPERAZINE (FPP) 1	106	27	16
181.26	74	4.69	1-(4-FLUOROPHENYL)PIPERAZINE (FPP) 2	106	103	12
267.107	91	7.73	1,4-DIBENZYLPIPERAZINE (DBZP) 1	111	47	12
267.107	65.1	7.73	1,4-DIBENZYLPIPERAZINE (DBZP) 2	111	91	10
134.019	117.1	4.09	1-AMINOINDAN 1	56	15	14
134.019	115.1	4.09	1-AMINOINDAN 2	56	33	14
191.061	91	3.20	1-METHYL-4-BENZYLPIPERAZINE (MBZP) 1	86	31	12
191.061	65	3.20	1-METHYL-4-BENZYLPIPERAZINE (MBZP) 2	86	63	10
194.261	163	6.03	1-METHYLAMINO-1-(3,4-METHYLENEDIOXYPHENYL) PROPANE 1	61	13	22
194.261	105.1	6.03	1-METHYLAMINO-1-(3,4-METHYLENEDIOXYPHENYL) PROPANE 2	61	33	16
230.937	188	8.52	2,3-DICHLOROPHENYLPIPERAZINE (DCPP) 1	91	27	24
230.937	152	8.52	2,3-DICHLOROPHENYLPIPERAZINE (DCPP) 2	91	45	20
206.062	188.1	7.43	2,3-DIMETHYLETHCATHINONE (2,3-DMEC) 1	91	17	24
206.062	158.1	7.43	2,3-DIMETHYLETHCATHINONE (2,3-DMEC) 2	91	39	20
192.202	174	7.02	2,3-DIMETHYLMETHCATHINONE (2,3-DMMC) 1	66	17	20
192.202	159.1	7.02	2,3-DIMETHYLMETHCATHINONE (2,3-DMMC) 2	66	27	20
222.247	174.1	5.43	2,3-ETHYLONE ISOMER 1	86	23	8
222.247	146.1	5.43	2,3-ETHYLONE ISOMER 2	86	35	8
194.351	135	5.69	2,3-MDMA 1	91	25	18
194.351	77	5.69	2,3-MDMA 2	91	53	12
276.236	135	7.57	2,3-MDPV 1	91	31	16
276.236	126.1	7.57	2,3-MDPV 2	91	37	14
226.297	209.1	6.18	2,4,5-TRIMETHOXYAMPHETAMINE 1	76	15	10
226.297	179.1	6.18	2,4,5-TRIMETHOXYAMPHETAMINE 2	76	35	10
192.19	174.1	7.46	2,4-DIMETHYLMETHCATHINONE (2,4-DMMC) 1	76	17	20
192.19	159	7.46	2,4-DIMETHYLMETHCATHINONE (2,4-DMMC) 2	76	27	18
206.063	188.1	7.92	2,4-DMEC 1	41	17	12
206.063	158.1	7.92	2,4-DMEC 2	41	47	20
210.264	151.1	6.71	2,5-DMMA 1	56	23	20
210.264	121.1	6.71	2,5-DMMA 2	56	35	16
368.124	243	10.15	25B-NBF 1	106	27	12
370.116	245	10.15	25B-NBF 2	131	27	12
324.164	199	9.89	25C-NBF 1	111	25	10
324.164	184	9.89	25C-NBF 2	111	37	10
322.138	199	9.72	25C-NBOH 1	101	27	24
322.138	77	9.72	25C-NBOH 2	101	85	12
336.16	121.1	10.25	25C-NBOMe 1	96	25	14
336.16	91.1	10.25	25C-NBOMe 2	96	59	12
316.169	91	10.44	25D-NBOMe 1	81	57	12
316.169	121	10.44	25D-NBOMe 2	81	25	16
330.231	91	11.26	25E-NBOMe 1	106	61	12
330.231	121.1	11.26	25E-NBOMe 2	106	27	16
330.142	91	11.04	25G-NBOMe 1	81	61	12
330.142	121.1	11.04	25G-NBOMe 2	81	27	14
302.346	91	9.40	25H-NBOMe 1	81	55	12
302.346	121.1	9.40	25H-NBOMe 2	81	23	18
428.183	91	10.88	25-I-NB2OMe 1	121	75	12
428.183	121	10.88	25-I-NB2OMe 2	121	27	16
428.176	121.1	10.82	25I-NB3OMe 1	131	33	14
428.176	91.1	10.82	25I-NB3OMe 2	131	75	12
428.177	121.1	10.75	25I-NB4OMe 1	91	21	16
428.177	78	10.75	25I-NB4OMe 2	91	113	10
416.016	290.8	10.58	25I-NBF 1	121	29	12
416.016	276	10.58	25I-NBF 2	121	43	14
442.154	135.1	10.71	25I-NBMD 1	116	31	16
442.154	77	10.71	25I-NBMD 2	116	93	12
414.121	291	10.42	25I-NBOH 1	101	31	12
414.121	307.9	10.42	25I-NBOH 2	101	23	14
347.2	91	9.05	25 *N*-NBOMe 1	86	59	12
347.2	121.1	9.05	25 *N*-NBOMe 2	86	23	16
362.264	91	10.77	25 T2-NBOMe 1	121	59	10

(*continued on next page*)

Table 1 (*continued*)

Precursor Ion (Q1)	Product Ion (Q3)	Retention time [min]	Analyte	Declustering potential (DP)	Collision energy (CE)	Cell exit potential (CXP)
362.264	121.1	10.77	25 T2-NBOMe 2	121	27	14
348.035	91.1	10.05	25 *T*-NBOMe 1	96	63	14
348.035	121.1	10.05	25 *T*-NBOMe 2	96	27	16
150.209	91	6.08	2-AMINO-1-PHENYLBUTANE 1	61	23	12
150.209	65	6.08	2-AMINO-1-PHENYLBUTANE 2	61	49	10
134.257	117.1	3.87	2-AMINOINDANE 1	51	19	14
134.257	115.1	3.87	2-AMINOINDANE 2	51	33	14
214.186	169	7.04	2-BROMOAMPHETAMINE 1	61	27	8
216.192	170.9	7.04	2-BROMOAMPHETAMINE 2	56	27	20
228.188	169	7.10	2-BROMOMETHAMPHETAMINE 1	71	29	20
230.177	171	7.10	2-BROMOMETHAMPHETAMINE 2	71	27	10
259.957	243	7.70	2C-B 1	51	17	12
259.957	227.9	7.70	2C-B 2	51	29	10
283.976	267	7.99	2C-B_FLY 1	106	21	12
283.976	188.1	7.99	2C-B_FLY 2	106	33	24
216.441	199	7.28	2C-C 1	76	15	24
216.441	184	7.28	2C-C 2	76	27	22
195.583	179	7.50	2C-D 1	71	15	24
195.583	164.1	7.50	2C-D 2	71	25	20
210.052	178	8.54	2C-G 1	76	23	22
210.052	163	8.54	2C-G 2	76	37	20
170.196	125	6.56	2-CHLOROAMPHETAMINE 1	61	25	16
170.196	89	6.56	2-CHLOROAMPHETAMINE 2	61	51	14
307.947	291	8.39	2C-I 1	66	19	12
307.947	276	8.39	2C-I 2	66	31	12
224.065	207.1	10.09	2C-P 1	66	15	10
224.065	192.1	10.09	2C-P 2	66	25	24
256.022	239.1	9.58	2C-T-7 1	71	17	10
256.022	91.1	9.58	2C-T-7 2	71	63	12
250.269	233.1	8.67	2C-TFM 1	91	17	10
250.269	218	8.67	2C-TFM 2	91	29	12
196.255	148.1	4.67	2-FEC 1	76	41	18
196.255	135.1	4.67	2-FEC 2	76	37	10
168.199	123.1	3.17	2-FIC 1	61	21	14
168.199	103.1	3.17	2-FIC 2	61	33	14
154.13	109	5.10	2-FLUOROAMPHETAMINE 1	61	23	14
154.13	137.1	5.10	2-FLUOROAMPHETAMINE 2	61	13	16
168.247	109.1	5.35	2-FLUOROMETHAMPHETAMINE (2-FMA) 1	61	25	12
168.247	83.1	5.35	2-FLUOROMETHAMPHETAMINE (2-FMA) 2	61	53	12
182.187	164.1	4.02	2-FLUOROMETHCATHINONE (2-FMC) 1	81	19	22
182.187	149	4.02	2-FLUOROMETHCATHINONE (2-FMC) 2	81	29	16
262.178	216.9	7.76	2-IODOAMPHETAMINE 1	81	27	12
262.178	90	7.76	2-IODOAMPHETAMINE 2	81	47	12
190.239	58	7.05	2-MAPB 1	51	19	8
190.239	91.1	7.05	2-MAPB 2	51	47	14
194.219	176.1	5.30	2-MeOMC 1	61	17	10
194.219	161.1	5.30	2-MeOMC 2	61	27	16
152.214	120.1	4.95	2-METHOXY-2-PHENYLETHYLAMINE 1	61	15	14
152.214	77	4.95	2-METHOXY-2-PHENYLETHYLAMINE 2	61	45	12
166.068	121.1	6.16	2-METHOXYAMPHETAMINE (2-MA) 1	56	21	16
166.068	149	6.16	2-METHOXYAMPHETAMINE (2-MA) 2	56	13	18
180.322	120.9	6.34	2-METHOXYMETHAMPHETAMINE (2-MeOMA) 1	66	23	14
180.322	91.1	6.34	2-METHOXYMETHAMPHETAMINE (2-MeOMA) 2	66	39	8
164.237	91	6.20	2-METHYLAMINO-1-PHENYLBUTANE 1	71	25	14
164.237	65	6.20	2-METHYLAMINO-1-PHENYLBUTANE 2	71	55	8
178.06	160.1	5.73	2-METHYLMETHCATHINONE (2-MMC) 1	76	17	22
178.06	145.1	5.73	2-METHYLMETHCATHINONE (2-MMC) 2	76	27	18
232.265	105.1	7.34	2-METHYL-PBP 1	116	33	12
232.265	91	7.34	2-METHYL-PBP 2	116	53	12
218.291	98.1	6.47	2-METHYL-PPP 1	116	31	16
218.291	119.1	6.47	2-METHYL-PPP 2	116	31	8
303.454	84.1	9.94	3,4-DICHLOROMETHYLPHENIDATE (3,4-CTMP) 1	121	27	12
303.454	56	9.94	3,4-DICHLOROMETHYLPHENIDATE (3,4-CTMP) 2	121	77	8
292.246	151	7.44	3,4-DIMETHOXY-ALPHA-PVP 1	116	35	22
292.246	126.1	7.44	3,4-DIMETHOXY-ALPHA-PVP 2	116	33	12
192.031	174.1	7.32	3,4-DIMETHYLMETHCATHINONE (3,4-DMMC) 1	81	17	20
192.031	159.2	7.32	3,4-DIMETHYLMETHCATHINONE (3,4-DMMC) 2	81	27	18
206.146	158.1	7.74	3,4-DMEC 1	86	43	14
206.146	115.1	7.74	3,4-DMEC 2	86	67	6
210.063	179.1	5.21	3,4-DMMA 1	61	17	22
210.063	151.1	5.21	3,4-DMMA 2	61	29	20
208.248	177.1	5.61	3,4-EDMA 1	61	19	10
208.248	149.1	5.61	3,4-EDMA 2	61	29	20
222.191	204	5.23	3,4-EDMC 1	61	19	10
222.191	189.1	5.23	3,4-EDMC 2	61	29	10

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Table 1 (*continued*)

Precursor Ion (Q1)	Product Ion (Q3)	Retention time [min]	Analyte	Declustering potential (DP)	Collision energy (CE)	Cell exit potential (CXP)
194.025	163.1	5.27	3,4-MDMA (ECSTAZY) 1	76	17	20
194.025	105.1	5.27	3,4-MDMA (ECSTAZY) 2	76	33	14
222.051	163	6.74	3,4-MDPA 1	81	19	20
222.051	105.1	6.74	3,4-MDPA 2	81	35	14
290.285	135.1	8.66	3,4-MDPHP 1	131	35	16
290.285	140.2	8.66	3,4-MDPHP 2	131	35	18
276.144	126.1	7.50	3,4-METHYLENDIOXYPYROVALERONE 1	76	31	12
276.144	135.1	7.50	3,4-METHYLENDIOXYPYROVALERONE 2	76	41	8
318.23	135.1	10.83	3,4-METHYLENEDIOXY_PV9 1	166	35	8
318.23	168.2	10.83	3,4-METHYLENEDIOXY_PV9 2	166	39	20
396.257	181.1	9.73	30C-NBOMe 1	61	23	10
396.257	148.1	9.73	30C-NBOMe 2	61	59	18
214.192	168.9	7.31	3-BROMOAMPHETAMINE 1	46	25	20
216.189	171.1	7.31	3-BROMOAMPHETAMINE 2	66	25	14
228.18	169	7.38	3-BROMOMETHAMPHETAMINE 1	86	27	22
230.202	170.9	7.38	3-BROMOMETHAMPHETAMINE 2	66	27	20
244.143	145	6.64	3-BROMOMETHCATHINONE (3-BMC) 1	86	23	20
242.128	145.1	6.64	3-BROMOMETHCATHINONE (3-BMC) 2	96	25	22
383.161	239	15.28	3-CAF 1	101	19	12
383.161	210	15.28	3-CAF 2	101	65	24
298.069	280.9	8.54	3C-B-FLY 1	66	21	12
300.079	283	8.54	3C-B-FLY 2	46	17	16
170.206	125.1	6.83	3-CHLOROAMPHETAMINE 1	66	25	14
170.206	89	6.83	3-CHLOROAMPHETAMINE 2	66	53	12
198.231	145.1	5.95	3-CHLOROMETHCATHINONE (3-CMC) 1	76	25	18
198.231	144.1	5.95	3-CHLOROMETHCATHINONE (3-CMC) 2	76	41	18
197.249	154.1	6.78	3-CHLOROPHENYLPIPERAZINE (mCPP) 1	101	27	18
197.249	118.1	6.78	3-CHLOROPHENYLPIPERAZINE (mCPP) 2	101	47	14
254.286	195.1	8.42	3C-P 1	56	19	10
254.286	107.1	8.42	3C-P 2	56	35	14
274.249	126.1	7.99	3-DESOXY-3,4-MDPV 1	126	31	18
274.249	133.1	7.99	3-DESOXY-3,4-MDPV 2	126	37	16
192.22	174.1	7.45	3-ETHYLMETHCATHINONE (3-EMC) 1	66	17	22
192.22	144.1	7.45	3-ETHYLMETHCATHINONE (3-EMC) 2	66	43	18
196.262	135.1	4.96	3-FEC 1	81	39	18
196.262	148.1	4.96	3-FEC 2	81	41	18
222.28	123.1	5.30	3-FLUORO-ALFA-PPP 1	86	31	12
222.28	98.1	5.30	3-FLUORO-ALFA-PPP 2	86	33	14
154.134	109	5.10	3-FLUOROAMPHETAMINE 1	76	25	14
154.134	137.1	5.10	3-FLUOROAMPHETAMINE 2	76	13	16
168.223	109.1	5.35	3-FLUOROMETHAMPHETAMINE (3-FMA) 1	76	27	18
168.223	83.1	5.35	3-FLUOROMETHAMPHETAMINE (3-FMA) 2	76	53	10
182.014	164.1	4.38	3-FLUOROMETHCATHINONE (3-FMC) 1	81	19	20
182.014	149.1	4.38	3-FLUOROMETHCATHINONE (3-FMC) 2	81	27	18
331.895	286.9	9.11	3-HYDROXYBROMAZEPAM 1	106	27	12
331.895	314.9	9.11	3-HYDROXYBROMAZEPAM 2	106	21	14
330.031	238	10.15	3-HYDROXYFLUNITRAZEPAM 1	96	43	12
330.031	284	10.15	3-HYDROXYFLUNITRAZEPAM 2	96	27	12
262.179	217	8.06	3-IODOAMPHETAMINE 1	66	25	10
262.179	117.1	8.06	3-IODOAMPHETAMINE 2	66	43	14
192.185	144.2	6.44	3-MEC 1	86	39	16
192.185	91.1	6.44	3-MEC 2	86	47	14
194.225	161.1	5.30	3-MeOMC 1	81	25	20
194.225	118.1	5.30	3-MeOMC 2	81	47	12
166.07	121.1	5.59	3-METHOXYAMPHETAMINE (3-MA) 1	41	21	16
166.07	91	5.59	3-METHOXYAMPHETAMINE (3-MA) 2	41	37	14
274.19	86.1	8.92	3-METHOXYPHENCYCLIDINE 1	46	17	10
274.19	121.1	8.92	3-METHOXYPHENCYCLIDINE 2	46	37	14
178.046	160.1	5.92	3-METHYLMETHCATHINONE (3-MMC) 1	86	17	20
178.046	145.1	5.92	3-METHYLMETHCATHINONE (3-MMC) 2	86	27	18
218.209	119.3	6.64	3-METHYL-PPP 1	116	31	6
218.209	91	6.64	3-METHYL-PPP 2	116	49	8
191.255	148.1	7.31	4,4′-DMAR 1	61	17	18
191.255	91	7.31	4,4′-DMAR 2	61	39	12
275.216	86	6.36	4-AcO-DET 1	81	23	12
275.216	160	6.36	4-AcO-DET 2	81	35	20
247.314	58.1	5.45	4-AcO-DMT 1	81	21	6
247.314	160.1	5.45	4-AcO-DMT 2	81	33	16
261.3	72	5.92	4-AcO-MET 1	76	21	10
261.3	160	5.92	4-AcO-MET 2	76	35	22
176.148	131.1	6.67	4-APB 1	66	25	16
176.148	91	6.67	4-APB 2	66	39	12
178.238	161.1	5.56	4-APDB 1	71	13	22
178.238	133.1	5.56	4-APDB 2	71	25	16
288.233	257	8.31	4-BROMO-2,5-DMMA 1	61	19	12

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Table 1 (*continued*)

Precursor Ion (Q1)	Product Ion (Q3)	Retention time [min]	Analyte	Declustering potential (DP)	Collision energy (CE)	Cell exit potential (CXP)
290.24	259	8.31	4-BROMO-2,5-DMMA 2	56	19	12
214.182	169	7.44	4-BROMOAMPHETAMINE 1	76	25	20
216.181	170.9	7.44	4-BROMOAMPHETAMINE 2	56	25	22
228.205	168.9	7.52	4-BROMOMETHAMPHETAMINE 1	91	29	20
230.2	170.9	7.52	4-BROMOMETHAMPHETAMINE 2	91	27	20
243.495	145.1	6.64	4-BROMOMETHCATHINONE (BREFEDRONE) 1	101	23	18
243.495	144.1	6.64	4-BROMOMETHCATHINONE (BREFEDRONE) 2	101	45	18
184.174	125.1	7.98	4-CAB 1	46	25	16
184.174	89	7.98	4-CAB 2	46	57	14
212.21	159.3	6.65	4-CEC 1	66	25	8
212.21	144.1	6.65	4-CEC 2	66	39	18
238.267	139.1	6.85	4-CHLORO-ALPHA-PPP 1	111	33	16
238.267	98.1	6.85	4-CHLORO-ALPHA-PPP 2	111	33	12
170.197	125	6.93	4-CHLOROAMPHETAMINE 1	51	25	12
170.197	89	6.93	4-CHLOROAMPHETAMINE 2	51	53	12
198	145.1	6.15	4-CHLOROMETHCATHINONE (4-CMC) 1	76	25	18
198.008	144.1	6.15	4-CHLOROMETHCATHINONE (4-CMC) 2	71	41	18
184.235	125.1	7.05	4-CMA 1	81	29	14
184.235	89	7.05	4-CMA 2	81	57	12
204.264	131.1	7.34	4-EAPB 1	76	29	10
204.264	91	7.34	4-EAPB 2	76	45	12
206.207	133.2	7.50	4-ETHYL-N,*N*-DMC 1	61	27	14
206.207	105.2	7.50	4-ETHYL-N,*N*-DMC 2	61	35	18
196.26	148.1	4.97	4-FEC 1	71	41	18
196.26	135.1	4.97	4-FEC 2	71	37	16
196.234	149.1	5.73	4-FLUORO BUPHEDRONE 1	76	31	18
196.234	148.1	5.73	4-FLUORO BUPHEDRONE 2	76	47	18
210.264	109	7.20	4-FLUORO PENTEDRONE 1	86	33	14
210.264	74	7.20	4-FLUORO PENTEDRONE 2	86	111	10
278.165	109	10.00	4-FLUORO PV8 1	126	33	16
278.165	95.1	10.00	4-FLUORO PV8 2	126	71	12
292.257	109.1	11.02	4-FLUORO PV9 1	116	35	14
292.257	95	11.02	4-FLUORO PV9 2	116	71	14
222.267	123.1	5.30	4-FLUORO-ALFA-PPP 1	86	31	8
222.267	98.1	5.30	4-FLUORO-ALFA-PPP 2	86	33	14
168.214	109.1	5.34	4-FLUOROMETHAMPHETAMINE (4-FMA) 1	81	27	12
168.214	137	5.34	4-FLUOROMETHAMPHETAMINE (4-FMA) 2	81	15	18
182.011	164.1	4.37	4-FLUOROMETHCATHINONE (4-FMC) 1	71	19	22
182.011	149	4.37	4-FLUOROMETHCATHINONE (4-FMC) 2	71	29	20
250.25	109	7.55	4F-PVP 1	91	31	12
250.25	126.1	7.55	4F-PVP 2	91	35	16
262.005	161.1	6.30	4-HYDROXY DiPT 1	171	31	20
262.005	114.1	6.30	4-HYDROXY DiPT 2	171	21	14
341.932	325	8.80	4-HYDROXYMIDAZOLAM 1	121	31	14
341.932	297	8.80	4-HYDROXYMIDAZOLAM 2	121	41	14
262.177	245	8.19	4-IODOAMPHETAMINE 1	56	15	12
262.177	216.9	8.19	4-IODOAMPHETAMINE 2	56	27	12
190.254	131.1	6.84	4-MAPB 1	76	27	18
190.254	91	6.84	4-MAPB 2	76	41	10
220.297	144.1	8.56	4-MEAP 1	66	43	18
220.297	105.1	8.56	4-MEAP 2	66	29	12
262.212	121.1	8.02	4-MEO-ALPHA-PVP 1	91	33	12
262.212	191.2	8.02	4-MEO-ALPHA-PVP 2	91	25	18
248.282	112.1	6.90	4-MeOPBP 1	101	31	14
248.282	121.1	6.90	4-MeOPBP 2	101	37	16
274.176	121.1	8.92	4-METHOXY PHENCYCLIDINE 1	61	39	14
274.176	189.1	8.92	4-METHOXY PHENCYCLIDINE 2	61	17	10
290.295	121.1	10.17	4-METHOXY PV8 1	126	35	16
290.295	154.2	10.17	4-METHOXY PV8 2	126	33	8
304.286	121.1	11.12	4-METHOXY PV9 1	101	35	14
304.286	168.2	11.12	4-METHOXY PV9 2	101	35	8
180.289	149	5.58	4-METHOXYMETHAMPHETAMINE (PMMA) 1	66	15	20
180.289	121.1	5.58	4-METHOXYMETHAMPHETAMINE (PMMA) 2	66	27	14
206.274	144.1	8.28	4-METHYL PENTEDRONE 1	86	47	18
206.274	105.1	8.28	4-METHYL PENTEDRONE 2	86	29	14
206.11	188.3	7.43	4-METHYL-ALPHA-ETHYLAMINOBUTIOPHENONE 1	56	19	22
206.11	144.2	7.43	4-METHYL-ALPHA-ETHYLAMINOBUTIOPHENONE 2	56	43	10
150.227	105.1	6.68	4-METHYLAMPHETAMINE 1	56	23	16
150.227	133.1	6.68	4-METHYLAMPHETAMINE 2	56	11	8
164.232	146.1	5.65	4-METHYLCATHINONE 1	71	15	18
164.232	131	5.65	4-METHYLCATHINONE 2	71	27	16
164.25	105.1	6.82	4-METHYLMETHAMPHETAMINE (4-MMA) 1	66	25	14
164.25	133.1	6.82	4-METHYLMETHAMPHETAMINE (4-MMA) 2	66	15	16
178.066	160.1	5.92	4-METHYLMETHCATHINONE (4-MMC) 1	71	17	20
178.066	145.1	5.92	4-METHYLMETHCATHINONE (4-MMC) 2	71	27	18

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Table 1 (*continued*)

Precursor Ion (Q1)	Product Ion (Q3)	Retention time [min]	Analyte	Declustering potential (DP)	Collision energy (CE)	Cell exit potential (CXP)
192.249	119.1	6.01	4-METHYL-N,*N*-DMC 1	101	27	16
192.249	72.1	6.01	4-METHYL-N,*N*-DMC 2	101	33	12
206.209	105	7.07	4-METHYL-*N*-METHYLBUPHEDRONE 1	51	29	16
206.209	90.9	7.07	4-METHYL-*N*-METHYLBUPHEDRONE 2	51	47	12
220.287	144.1	9.42	4-METHYL-*N*-METHYLHEXANOPHENONE 1	86	47	16
220.287	105.1	9.42	4-METHYL-*N*-METHYLHEXANOPHENONE 2	86	29	14
232.31	105.1	7.47	4-METHYL-PBP 1	81	33	14
232.31	91	7.47	4-METHYL-PBP 2	81	55	12
260.347	105.1	9.62	4-METHYL-PHP 1	131	33	14
260.347	91.1	9.62	4-METHYL-PHP 2	131	63	10
203.04	144.1	8.36	4-METHYL-α-ETHYLTRYPTAMINE 1	56	29	20
203.04	186	8.36	4-METHYL-α-ETHYLTRYPTAMINE 2	56	13	24
176.082	44	6.98	5-APB 1	46	23	8
176.082	91	6.98	5-APB 2	46	47	10
178.29	161	5.56	5-APDB 1	56	13	22
178.29	133.1	5.56	5-APDB 2	56	27	18
176.173	159.2	8.71	5-APDI 1	71	13	22
176.173	131.2	8.71	5-APDI 2	71	27	10
365.216	320.1	12.99	5-CHLORO AB-PINACA 1	91	21	14
367.248	322.2	12.99	5-CHLORO AB-PINACA 2	86	21	14
391.226	247.9	14.09	5-CHLORO-NNEI 1	86	31	12
391.226	144.1	14.09	5-CHLORO-NNEI 2	86	55	8
204.961	132.1	7.09	5-EAPB 1	86	29	16
204.961	131.6	7.09	5-EAPB 2	86	29	16
348.07	232.1	12.10	5F-ABICA 1	71	29	12
348.07	144.1	12.10	5F-ABICA 2	71	53	18
349.193	233.1	12.23	5F-AB-PINACA 1	86	33	10
349.193	304.1	12.23	5F-AB-PINACA 2	86	21	14
378.193	233.1	14.03	5F-ADB (5F-MDMB-PINACA) 1	116	33	10
378.193	318.2	14.03	5F-ADB (5F-MDMB-PINACA) 2	116	23	14
364.092	233.1	13.50	5F-AMB (5F-AMB-PINACA) 1	101	31	10
364.092	304.2	13.50	5F-AMB (5F-AMB-PINACA) 2	101	21	14
383.14	135.1	15.01	5F-APICA (STS-135) 1	156	39	16
383.14	77	15.01	5F-APICA (STS-135) 2	156	119	12
384.207	135.1	15.46	5F-APINACA (AKB-48-5F) 1	106	29	16
384.207	77.1	15.46	5F-APINACA (AKB-48-5F) 2	106	121	12
368.294	135.1	15.30	5-F-JWH-018 ADAMANTYL ANALOG 1	171	39	10
368.294	77	15.30	5-F-JWH-018 ADAMANTYL ANALOG 2	171	113	12
375.043	232.1	13.54	5-FLUORO MN-24 (5-FLUORO NNEI) 1	111	31	10
375.043	144.1	13.54	5-FLUORO MN-24 (5-FLUORO NNEI) 2	111	57	18
377.255	233.1	15.13	5-FLUORO THJ 1	91	29	12
377.255	145.1	15.13	5-FLUORO THJ 2	91	53	14
363.254	145.1	12.29	5-FLUORO-2-ADB-PINACA_ISOMER_2 1	116	47	10
363.254	318.1	12.29	5-FLUORO-2-ADB-PINACA_ISOMER_2 2	116	29	14
367.233	249.1	13.78	5-FLUORO-CUMYL-PICA 1	96	21	12
367.233	91	13.78	5-FLUORO-CUMYL-PICA 2	96	77	14
376.497	233.1	14.60	5-FLUORO-MN-18 1	126	23	10
376.497	145.1	14.60	5-FLUORO-MN-18 2	126	53	18
376.066	145.1	9.85	5-FLUORO-MN-21 (5-FLUORO-PCN) 1	201	55	18
376.066	117	9.85	5-FLUORO-MN-21 (5-FLUORO-PCN) 2	201	89	14
339.222	91	13.04	5-FLUORO-SDB-006 1	141	63	14
339.222	232	13.04	5-FLUORO-SDB-006 2	141	31	10
378.028	233.1	14.03	5F-NPB-22 1	81	23	10
378.028	145.1	14.03	5F-NPB-22 2	81	55	18
377.092	232.1	13.60	5F-PB-22 1	81	27	10
377.092	144.1	13.60	5F-PB-22 2	81	57	20
311.223	144.1	12.11	5-F-PENTYL-3-PYRIDINOYLINDOLE 1	136	51	18
311.223	89	12.11	5-F-PENTYL-3-PYRIDINOYLINDOLE 2	136	99	12
377.212	233.1	14.79	5F-SDB-005 1	121	15	10
377.212	145.1	14.79	5F-SDB-005 2	121	51	10
205.058	58.1	2.86	5-HYDROXY DMT 1	81	17	8
205.058	160.1	2.86	5-HYDROXY DMT 2	81	25	20
175.275	158.1	4.98	5-IT 1	61	13	18
175.275	130.1	4.98	5-IT 2	61	31	18
190.252	159.1	6.61	5-MAPB 1	56	15	16
190.252	131.1	6.61	5-MAPB 2	56	29	20
192.202	161.1	5.67	5-MAPDB 1	56	17	18
192.202	133.1	5.67	5-MAPDB 2	56	31	14
219.295	160.1	7.06	5-MeO-ALPHA-ET 1	71	27	18
219.295	117.1	7.06	5-MeO-ALPHA-ET 2	71	55	14
271.063	110.1	7.20	5-MeO-DALT 1	86	21	14
271.063	174.1	7.20	5-MeO-DALT 2	86	27	22
205.05	188	5.90	5-METHOXY AMT 1	56	15	24
205.05	147.1	5.90	5-METHOXY AMT 2	56	27	20
275.078	114.2	7.16	5-METHOXY DiPT 1	91	21	14

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Table 1 (*continued*)

Precursor Ion (Q1)	Product Ion (Q3)	Retention time [min]	Analyte	Declustering potential (DP)	Collision energy (CE)	Cell exit potential (CXP)
275.078	174.1	7.16	5-METHOXY DiPT 2	91	29	22
219.968	58.1	5.16	5-METHOXY DMT 1	146	21	8
219.968	175	5.16	5-METHOXY DMT 2	146	21	22
238.277	190.1	5.53	5-METHOXY METHYLONE 1	96	21	24
238.277	147.1	5.53	5-METHOXY METHYLONE 2	96	37	16
247.988	86.1	6.16	5-METHOXY MiPT 1	156	19	10
247.988	87.1	6.16	5-METHOXY MiPT 2	156	19	10
176.049	159.1	6.45	6-APB 1	66	13	20
176.049	131.1	6.45	6-APB 2	66	25	18
178.157	161	5.80	6-APDB 1	36	15	22
178.157	132.9	5.80	6-APDB 2	36	29	8
272.17	240.9	7.47	6-BROMO-MDMA 1	86	19	12
274.156	242.8	7.47	6-BROMO-MDMA 2	76	19	12
228.238	169	7.09	6-CHLORO-MDMA 1	61	29	12
228.238	77	7.09	6-CHLORO-MDMA 2	61	53	12
204.15	131.1	7.10	6-EAPB 1	56	29	16
204.15	159.1	7.10	6-EAPB 2	56	17	8
175.258	158.1	5.85	6-IT 1	51	15	8
175.258	130.1	5.85	6-IT 2	51	31	18
328.01	165	5.06	6-MAM 1	141	51	20
328.01	43	5.06	6-MAM 2	141	95	8
190.239	131.1	6.60	6-MAPB 1	71	27	10
190.239	91	6.60	6-MAPB 2	71	43	10
286.241	121.1	6.51	7-AMINOCLONAZEPAM 1	111	39	14
286.241	222.1	6.51	7-AMINOCLONAZEPAM 2	111	33	26
270.396	121.1	5.51	7-AMINODESMETHYLFLUNITRAZEPAM 1	146	37	14
270.396	77	5.51	7-AMINODESMETHYLFLUNITRAZEPAM 2	146	75	10
283.767	135.1	7.55	7-AMINOFLUNITRAZEPAM 1	121	37	18
283.767	77.1	7.55	7-AMINOFLUNITRAZEPAM 2	121	87	12
252.005	121.1	4.57	7-AMINONITRAZEPAM 1	111	35	16
252.005	77.1	4.57	7-AMINONITRAZEPAM 2	111	73	10
176.239	131.1	6.68	7-APB 1	46	25	14
176.239	77	6.68	7-APB 2	46	53	10
178.233	161.1	6.38	7-APDB 1	61	15	10
178.233	133.1	6.38	7-APDB 2	61	25	18
355.053	125.1	11.59	A-796260 1	106	27	16
355.053	114.1	11.59	A-796260 2	106	35	14
340.308	125.1	14.21	A-834735 1	156	29	16
340.308	55	14.21	A-834735 2	156	61	10
311.15	187.1	12.39	A-836339 1	101	23	12
311.15	125.2	12.39	A-836339 2	101	33	10
350.211	135.1	16.10	AB-001 1	146	39	16
350.211	77.1	16.10	AB-001 2	146	117	12
352.92	98.2	11.39	AB005 1	116	53	12
352.92	112.1	11.39	AB005 2	116	29	16
357.16	241.1	14.11	AB-CHMINACA 1	91	37	12
357.16	312.1	14.11	AB-CHMINACA 2	91	23	14
369.13	352	12.67	AB-FUBINACA 1	81	13	14
369.13	109.1	12.67	AB-FUBINACA 2	81	47	14
369.269	253	12.86	AB-FUBINACA 2-FLUOROBENZYL ISOMER 1	86	33	12
369.269	324.2	12.86	AB-FUBINACA 2-FLUOROBENZYL ISOMER 2	86	19	14
369.241	253	12.67	AB-FUBINACA 3-FLUOROBENZYL ISOMER 1	66	35	12
369.241	324.1	12.67	AB-FUBINACA 3-FLUOROBENZYL ISOMER 2	66	21	14
331.065	215.1	13.49	AB-PINACA 1	86	33	10
331.065	286.1	13.49	AB-PINACA 2	86	21	14
382.972	253	13.27	ADB-FUBINACA 1	101	33	12
382.972	109.1	13.27	ADB-FUBINACA 2	101	55	12
345.052	215	14.01	ADB-PINACA 1	91	35	10
345.052	328.2	14.01	ADB-PINACA 2	91	13	14
345.335	215.1	13.69	ADB-PINACA ISOMER_1 1	86	33	10
345.335	300.2	13.69	ADB-PINACA ISOMER_1 2	86	21	14
345.304	215.1	14.06	ADB-PINACA ISOMER_2 1	71	35	10
345.304	300.1	14.06	ADB-PINACA ISOMER_2 2	71	19	14
345.292	215.1	14.05	ADB-PINACA ISOMER_3 1	71	33	10
345.292	300.2	14.05	ADB-PINACA ISOMER_3 2	71	19	14
345.305	215.1	13.98	ADB-PINACA ISOMER_4 1	81	33	10
345.305	300.1	13.98	ADB-PINACA ISOMER_4 2	81	19	14
329.174	284	9.70	AH-7921 1	91	23	12
329.174	173	9.70	AH-7921 2	91	35	18
404.265	135.1	15.64	AKB48_N-(4-FLUOROBENZYL)_ANALOG 1	136	29	16
404.265	77	15.64	AKB48_N-(4-FLUOROBENZYL)_ANALOG 2	136	121	14
206.323	188.1	7.09	ALFA-ETHYLAMINOPENTIOPHENONE 1	86	17	22
206.323	91	7.09	ALFA-ETHYLAMINOPENTIOPHENONE 2	86	39	12
220.315	202.1	7.83	ALFA-PROPYLAMINOPENTIOPHENONE 1	91	19	10
220.315	91.1	7.83	ALFA-PROPYLAMINOPENTIOPHENONE 2	91	33	10

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Table 1 (*continued*)

Precursor Ion (Q1)	Product Ion (Q3)	Retention time [min]	Analyte	Declustering potential (DP)	Collision energy (CE)	Cell exit potential (CXP)
238.321	221.1	6.95	ALLYLESCALINE 1	51	13	10
238.321	77	6.95	ALLYLESCALINE 2	51	67	12
206.291	91.1	6.84	ALPHA-DIMETHYLAMINOPENTIOPHENONE 1	101	27	14
206.291	77.1	6.84	ALPHA-DIMETHYLAMINOPENTIOPHENONE 2	101	57	12
220.312	91	8.41	ALPHA-ETHYLAMINOHEXANOPHENONE 1	106	33	12
220.312	130.1	8.41	ALPHA-ETHYLAMINOHEXANOPHENONE 2	106	47	14
188.767	130.1	7.09	ALPHA-ETHYLTRYPTAMINE 1	76	27	16
188.767	172.1	7.09	ALPHA-ETHYLTRYPTAMINE 2	76	11	20
341.989	324	9.92	ALPHA-HYDROXYMIDAZOLAM 1	121	29	14
341.989	203	9.92	ALPHA-HYDROXYMIDAZOLAM 2	121	37	26
175.029	158.1	5.68	ALPHA-METHYLTRYPTAMINE 1	56	15	20
175.029	143.1	5.68	ALPHA-METHYLTRYPTAMINE 2	56	35	16
246.318	91	8.41	ALPHA-PHP 1	76	33	10
246.318	77	8.41	ALPHA-PHP 2	76	65	10
280.193	105.1	11.76	ALPHA-PHTALIMIDOPROPIOPHENONE 1	116	31	14
280.193	77	11.76	ALPHA-PHTALIMIDOPROPIOPHENONE 2	116	79	12
232.294	91.1	6.48	ALPHA-PIPBP 1	106	33	8
232.294	77	6.48	ALPHA-PIPBP 2	106	61	10
204.261	105.1	5.00	ALPHA-PPP 1	71	31	14
204.261	98.1	5.00	ALPHA-PPP 2	71	33	8
232.243	91.1	7.17	ALPHA-PVP 1	71	39	8
232.243	126.1	7.17	ALPHA-PVP 2	71	57	6
238.017	126.2	6.24	ALPHA-PVT 1	91	29	16
238.017	97	6.24	ALPHA-PVT 2	91	31	12
224.19	112.2	4.95	ALPHA-PYRROLIDINOBUTHIOPHENONE 1	81	29	12
224.19	97	4.95	ALPHA-PYRROLIDINOBUTHIOPHENONE 2	81	39	12
309.934	282	11.35	ALPRAZOLAM 1	171	37	12
309.934	206	11.35	ALPRAZOLAM 2	171	57	26
383.315	98	10.51	AM1220 1	101	49	14
383.315	112.1	10.51	AM1220 2	101	27	12
391.166	135.2	12.07	AM-1248 1	131	39	16
391.166	112.1	12.07	AM-1248 2	131	39	14
360.031	127.1	14.16	AM-2201 1	171	65	16
360.031	155.1	14.16	AM-2201 2	171	33	18
376.237	232.1	14.94	AM2201 8-QUINOLINYL CARBOXAMIDE 1	86	23	12
376.237	144.1	14.94	AM2201 8-QUINOLINYL CARBOXAMIDE 2	86	55	16
361.184	127.1	14.44	AM2201 BENZIMIDAZOLE ANALOG 1	131	73	16
361.184	155.1	14.44	AM2201 BENZIMIDAZOLE ANALOG 2	131	41	20
353.245	155.1	12.76	AM2232 1	131	31	18
353.245	127	12.76	AM2232 2	131	63	14
278.073	91	10.85	AMITRIPTYLINE 1	101	33	12
278.073	105.1	10.85	AMITRIPTYLINE 2	101	31	14
136.03	91	4.73	AMPHETAMINE 1	51	23	12
136.03	119.1	4.73	AMPHETAMINE 2	51	11	16
267.122	145.1	3.91	ATENOLOL 1	101	35	20
267.122	56.1	3.91	ATENOLOL 2	101	43	8
216.245	174	11.12	ATRAZYNA 1	126	23	24
216.245	104	11.12	ATRAZYNA 2	126	39	14
268.279	250.1	8.69	AZACYCLONOL 1	81	17	20
268.279	91	8.69	AZACYCLONOL 2	81	51	14
385.123	240.1	15.13	BB-22 1	101	19	16
385.123	144	15.13	BB-22 2	101	51	18
194.03	135	6.36	BDB 1	56	25	18
194.03	177	6.36	BDB 2	56	11	24
300.293	215.1	10.62	BENOCYCLIDINE 1	66	17	10
300.293	147	10.62	BENOCYCLIDINE 2	66	39	18
254.273	91.1	9.14	BENZEDRONE 1	111	31	12
254.273	65.1	9.14	BENZEDRONE 2	111	77	10
166.03	120	8.84	BENZOCAINE 1	71	25	16
166.03	94	8.84	BENZOCAINE 2	71	23	12
290.034	168.1	6.54	BENZOYLECGONINE 1	91	27	20
290.034	77	6.54	BENZOYLECGONINE 2	91	77	10
310.213	86.1	10.20	BENZYDAMINE 1	106	23	10
310.213	58.1	10.20	BENZYDAMINE 2	106	71	10
274.896	163	6.96	bk-2C-B 1	81	39	39
274.896	178.1	6.96	bk-2C-B 2	81	21	21
194.195	146	4.23	bk-MDA 1	56	19	14
194.195	118.1	4.23	bk-MDA 2	56	31	14
136.133	91	4.86	BMPEA 1	46	25	10
136.133	119.1	4.86	BMPEA 2	46	11	16
293.977	276.9	10.04	BROMO-DRAGON-FLY 1	71	15	42
296.128	278.9	10.04	BROMO-DRAGON-FLY 2	81	17	12
468.189	55	9.63	BUPRENORPHINE 1	116	95	12
468.189	152	9.63	BUPRENORPHINE 2	116	117	10
239.672	184	8.02	BUPROPION 1	66	17	24

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Table 1 (*continued*)

Precursor Ion (Q1)	Product Ion (Q3)	Retention time [min]	Analyte	Declustering potential (DP)	Collision energy (CE)	Cell exit potential (CXP)
239.672	131.1	8.02	BUPROPION 2	66	37	16
222.185	174.1	5.77	BUTYLONE (bk-MBDB) 1	66	25	20
222.185	204.1	5.77	BUTYLONE (bk-MBDB) 2	66	17	10
202.289	91	8.22	CAMFETAMINE 1	76	43	14
202.289	67	8.22	CAMFETAMINE 2	76	25	14
315.323	193	15.06	CANNABIDIOL 1	121	29	10
315.323	123	15.06	CANNABIDIOL 2	121	43	16
237.209	194.1	10.49	CARBAMAZEPINE 1	111	27	24
237.209	192.1	10.49	CARBAMAZEPINE 2	111	45	24
152.256	134.1	3.67	CATHINE 1	51	13	22
152.256	117.1	3.67	CATHINE 2	51	23	14
150.03	132.1	3.71	CATHINONE 1	56	17	18
150.03	117.1	3.71	CATHINONE 2	56	31	14
369.1	127	16.51	CB-13 1	151	61	20
369.1	170.7	16.51	CB-13 2	151	39	24
358.214	214.1	15.81	CBL-018 1	76	21	10
358.214	144.1	15.81	CBL-018 2	76	49	20
394.203	188.9	14.95	CI2201 1	151	37	24
396.214	191	14.95	CI2201 2	151	35	24
301.995	260	11.09	CLOBAZAM 1	151	29	12
301.995	225	11.09	CLOBAZAM 2	151	45	26
315.043	86.1	11.59	CLOMIPRAMINE 1	106	23	12
315.043	58	11.59	CLOMIPRAMINE 2	106	65	8
316.097	270.1	10.73	CLONAZEPAM 1	151	35	12
316.097	214.3	10.73	CLONAZEPAM 2	151	45	22
318.094	196.1	8.04	COCAETHYLENE 1	101	27	24
318.094	82	8.04	COCAETHYLENE 2	101	39	12
304.198	182.1	7.06	COCAINE 1	106	27	22
304.198	77.1	7.06	COCAINE 2	106	79	12
300.058	152	4.32	CODEINE 1	136	85	18
300.058	115.1	4.32	CODEINE 2	136	95	16
349.217	231.1	14.69	CUMYL-PICA 1	86	21	12
349.217	91	14.69	CUMYL-PICA 2	86	73	12
254.299	236.2	7.95	D2PM 1	81	19	12
254.299	130.1	7.95	D2PM 2	81	39	8
286.956	179.9	10.20	DEMOXEPAM 1	131	31	22
286.956	269	10.20	DEMOXEPAM 2	131	37	12
289.917	140	11.56	DESALKYLFLURAZEPAM 1	116	39	18
289.917	141	11.56	DESALKYLFLURAZEPAM 2	116	39	18
310.255	281	11.39	DESCHLOROETIZOLAM 1	151	33	12
310.255	256	11.39	DESCHLOROETIZOLAM 2	151	31	12
218.287	91	6.21	DESCHLORO-*N*-ETHYL-KETAMINE 1	96	39	10
218.287	145.1	6.21	DESCHLORO-*N*-ETHYL-KETAMINE 2	96	23	8
267.085	72.1	10.70	DESIPRAMINE 1	71	21	10
267.085	44.1	10.70	DESIPRAMINE 2	71	63	8
271.978	209.1	11.89	DESMETHYLDIAZEPAM (NORDIAZEPAM) 2	141	39	26
271.978	140	11.89	DESMETHYLDIAZEPAM (NORDIAZEPAM) 1	141	39	18
299.977	254.1	10.31	DESMETHYLFLUNITRAZEPAM 1	116	35	12
299.977	198	10.31	DESMETHYLFLUNITRAZEPAM 2	116	53	24
272.254	167.1	5.08	DESOMORPHINE 1	126	49	20
272.254	152.1	5.08	DESOMORPHINE 2	126	73	18
238.301	91	8.68	DESOXY-D2PM 1	101	33	12
238.301	117.1	8.68	DESOXY-D2PM 2	101	23	8
252.331	91.1	9.03	DESOXYPIPRADROL (2-DPMP) 1	91	49	12
252.331	65	9.03	DESOXYPIPRADROL (2-DPMP) 2	91	85	10
272.289	128.1	9.23	DEXTROMETHORPHAN 1	126	81	16
272.289	171	9.23	DEXTROMETHORPHAN 2	126	51	20
285.397	154	12.30	DIAZEPAM 1	166	37	20
285.397	193	12.30	DIAZEPAM 2	166	43	24
320.306	228	12.33	DICLAZEPAM 1	166	43	28
320.306	89	12.33	DICLAZEPAM 2	166	103	12
322.115	121.1	11.03	DICLOFENSINE 1	151	33	16
322.115	279	11.03	DICLOFENSINE 2	151	29	14
206.061	105.1	5.24	DIETHYLCATHINONE (AMFEPRAMONE) 1	81	31	12
206.061	100.1	5.24	DIETHYLCATHINONE (AMFEPRAMONE) 2	81	29	14
302.062	199	4.26	DIHYDROCODEINE 1	121	43	26
302.062	128.1	4.26	DIHYDROCODEINE 2	121	81	16
279.175	120.1	6.17	DIMETHOCAINE 1	106	31	14
279.175	65	6.17	DIMETHOCAINE 2	106	81	10
222.209	72.2	4.77	DIMETHYLONE (bk-MDDMA) 1	86	25	10
222.209	91	4.77	DIMETHYLONE (bk-MDDMA) 2	86	49	12
256.071	167.1	9.27	DIPHENHYDRAMINE 1	56	17	22
256.071	165.1	9.27	DIPHENHYDRAMINE 2	56	57	22
266.099	181.1	8.71	DIPHENIDINE 1	76	25	22
266.099	103.1	8.71	DIPHENIDINE 2	76	47	12

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Table 1 (*continued*)

Precursor Ion (Q1)	Product Ion (Q3)	Retention time [min]	Analyte	Declustering potential (DP)	Collision energy (CE)	Cell exit potential (CXP)
244.891	114.2	7.30	DiPT 1	81	21	14
244.891	144.1	7.30	DiPT 2	81	31	20
266.292	248.1	7.33	DL-4662 1	86	19	12
266.292	188	7.33	DL-4662 2	86	35	22
322.068	304.9	8.92	DOI 1	61	17	12
322.068	277	8.92	DOI 2	61	27	12
296.089	202	10.16	DOTHIEPIN 1	86	75	26
296.089	220.9	10.16	DOTHIEPIN 2	86	61	28
279.918	107.1	9.52	DOXEPIN 1	101	31	14
279.918	77	9.52	DOXEPIN 2	101	73	10
271.067	167.1	5.77	DOXYLAMINE 1	61	49	22
271.067	182	5.77	DOXYLAMINE 2	61	23	22
388.297	183.1	14.95	EAM-2201 1	81	35	10
388.297	153	14.95	EAM-2201 2	81	65	20
278.507	234.2	9.25	EDDP 1	86	41	10
278.507	249.1	9.25	EDDP 2	86	33	10
410.225	155	15.66	EG-2201 1	181	33	22
410.225	127.1	15.66	EG-2201 2	181	71	16
326.4	223.1	5.32	ERGOMETRINE 1	116	31	10
326.4	208.1	5.32	ERGOMETRINE 2	116	39	10
295.921	268	10.99	ESTAZOLAM 1	101	33	12
295.921	206	10.99	ESTAZOLAM 2	101	55	24
264.918	146.1	11.91	ETAQUALONE 1	116	37	18
264.918	77	11.91	ETAQUALONE 2	116	89	12
180.064	162.1	4.72	ETHCATHINONE METABOLITE 1	76	17	20
180.064	115.1	4.72	ETHCATHINONE METABOLITE 2	76	39	14
222.228	174.1	5.14	ETHYLONE (bk-MDEA) 1	71	25	20
222.228	204.1	5.14	ETHYLONE (bk-MDEA) 2	71	19	10
248.328	84.1	8.17	ETHYLPHENIDATE 1	111	25	12
248.328	56	8.17	ETHYLPHENIDATE 2	111	69	8
343.91	315	11.69	ETIZOLAM 1	121	35	14
343.91	224.1	11.69	ETIZOLAM 2	121	65	10
236.294	188.1	6.18	EUTYLONE (bk-EBDB) 1	96	25	24
236.294	189.1	6.18	EUTYLONE (bk-EBDB) 2	96	29	22
396.194	109.1	15.21	FDU-PB-22 1	96	47	12
396.194	252	15.21	FDU-PB-22 2	96	17	12
232.018	159	8.34	FENFLURAMINE 1	86	31	20
232.018	109	8.34	FENFLURAMINE 2	86	57	14
337.171	188	8.81	FENTANYL 1	131	29	10
337.171	105	8.81	FENTANYL 2	131	57	12
334.716	226.1	11.77	FLUBROMAZEPAM 1	161	39	10
334.716	186	11.77	FLUBROMAZEPAM 2	161	41	22
303.922	212	11.99	FLUDIAZEPAM 1	141	43	26
303.922	89	11.99	FLUDIAZEPAM 2	141	93	12
303.986	258.1	9.20	FLUMAZENIL 1	81	23	12
303.986	217	9.20	FLUMAZENIL 2	81	35	26
313.814	268	10.83	FLUNITRAZEPAM 1	136	35	12
313.814	239	10.83	FLUNITRAZEPAM 2	136	47	12
310.021	44.1	11.20	FLUOXETINE 1	51	43	8
310.021	148.1	11.20	FLUOXETINE 2	51	11	18
388.023	315	9.32	FLURAZEPAM 1	91	31	14
388.023	107	9.32	FLURAZEPAM 2	91	111	14
350.227	109.1	14.95	FUB-144 1	111	61	14
350.227	125.1	14.95	FUB-144 2	111	29	14
380.203	155.1	14.47	FUB-JWH-018 1	176	33	8
380.203	109	14.47	FUB-JWH-018 2	176	63	18
398.186	253	13.65	FUB-NPB-22 1	86	23	12
398.186	109.1	13.65	FUB-NPB-22 2	86	47	8
396.975	109.1	15.21	FUB-PB-22 1	116	45	14
396.975	253.1	15.21	FUB-PB-22 2	116	17	12
375.29	105.1	8.86	FURANYLFENTANYL (Fu-F) 1	136	55	14
375.29	188.1	8.86	FURANYLFENTANYL (Fu-F) 2	136	29	20
102.935	85	1.31	GHB 1	−75	−10	−12
102.935	57	1.31	GHB 2	−75	−10	−18
215.051	174	7.45	HARMALINE 1	61	29	10
215.051	171.9	7.45	HARMALINE 2	61	37	18
212.795	170.1	7.85	HARMINE 1	121	41	20
212.795	198	7.85	HARMINE 2	121	31	26
387.195	243.1	15.91	HU-210 1	146	25	12
387.195	43	15.91	HU-210 2	146	71	8
300.05	199	4.83	HYDROCODONE 1	131	39	24
300.05	128.1	4.83	HYDROCODONE 2	131	77	16
312.288	122.1	7.91	IBOGAINE 1	281	43	14
312.288	77	7.91	IBOGAINE 2	281	119	12
281.078	86.1	10.55	IMIPRAMINE 1	66	21	12

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Table 1 (*continued*)

Precursor Ion (Q1)	Product Ion (Q3)	Retention time [min]	Analyte	Declustering potential (DP)	Collision energy (CE)	Cell exit potential (CXP)
281.078	58.1	10.55	IMIPRAMINE 2	66	59	8
192.055	91	6.81	ISOPENTEDRONE 1	71	33	12
192.055	161	6.81	ISOPENTEDRONE 2	71	17	22
343.221	126.6	15.44	JWH 018 BENZIMIDAZOLE ANALOG 1	121	109	16
343.221	155.1	15.44	JWH 018 BENZIMIDAZOLE ANALOG 2	121	41	20
384.202	155.1	15.80	JWH-011 1	151	37	16
384.202	127.1	15.80	JWH-011 2	151	71	14
342.097	127.1	15.16	JWH-016 1	146	67	16
342.097	155.1	15.16	JWH-016 2	146	33	20
342.063	127.1	14.91	JWH-018 1	146	65	16
342.063	155	14.91	JWH-018 2	146	33	20
365.291	135.1	15.72	JWH-018 ADAMANTYL CARBOXAMIDE 1	156	37	20
365.291	77	15.72	JWH-018 ADAMANTYL CARBOXAMIDE 2	156	109	12
370.197	127.1	15.90	JWH-020 1	156	67	16
370.197	155	15.90	JWH-020 2	156	35	20
340.223	155.1	14.75	JWH-022 1	136	31	8
340.223	127.1	14.75	JWH-022 2	136	61	16
306.155	127.1	14.85	JWH-031 1	131	51	8
306.155	76.9	14.85	JWH-031 2	131	95	6
300.22	127.1	13.63	JWH-071 1	111	57	16
300.22	155.1	13.63	JWH-071 2	111	29	8
328.077	127.1	14.71	JWH-073 1	131	63	16
328.077	155.1	14.71	JWH-073 2	131	31	20
358.107	185	14.96	JWH-080 1	61	33	24
358.107	127.1	14.96	JWH-080 2	61	69	16
372.132	185.1	15.37	JWH-081 1	156	35	24
372.132	114.1	15.37	JWH-081 2	156	93	14
386.111	185	15.50	JWH-098 1	146	35	22
386.111	114.1	15.50	JWH-098 2	146	101	14
370.219	155.2	15.65	JWH-116 1	121	33	16
370.219	127.1	15.65	JWH-116 2	121	69	6
356.234	169.1	15.53	JWH-122 1	126	33	20
356.234	115.1	15.53	JWH-122 2	126	91	14
367.929	154.8	15.59	JWH-145 1	91	35	22
367.929	127.1	15.59	JWH-145 2	91	69	18
396.312	155.1	16.20	JWH-146 1	141	27	18
396.312	127	16.20	JWH-146 2	141	71	22
382.164	155	15.91	JWH-147 1	136	27	20
382.164	127.1	15.91	JWH-147 2	136	69	16
370.172	169.1	15.65	JWH-149 1	156	35	26
370.172	115.2	15.65	JWH-149 2	156	95	14
306.156	91.1	14.55	JWH-167 1	86	31	12
306.156	214.2	14.55	JWH-167 2	86	35	30
328.281	141.1	16.76	JWH-175 1	106	29	18
328.281	115.1	16.76	JWH-175 2	106	83	14
384.268	197	16.06	JWH-182 1	196	33	10
384.268	141	16.06	JWH-182 2	196	61	14
399.123	169.1	11.73	JWH-193 1	116	31	10
399.123	115	11.73	JWH-193 2	116	97	6
415.117	185.1	11.51	JWH-198 1	181	33	22
415.117	114.2	11.51	JWH-198 2	181	35	10
385.076	155.1	10.92	JWH-200 1	121	29	20
385.076	127.1	10.92	JWH-200 2	121	71	16
336.263	121.1	14.46	JWH-201 1	151	35	16
336.263	77	14.46	JWH-201 2	151	77	10
384.326	183.1	15.91	JWH-213 1	181	35	22
384.326	153.1	15.91	JWH-213 2	181	61	18
386.153	155	15.47	JWH-307 1	66	27	24
386.153	127.1	15.47	JWH-307 2	66	81	16
418.325	155	16.09	JWH-309 1	141	29	20
418.325	127.1	16.09	JWH-309 2	141	77	16
386.132	155.1	15.59	JWH-368 1	106	29	20
386.132	127	15.59	JWH-368 2	106	69	16
402.279	155.1	15.69	JWH-369 1	126	29	20
402.279	127	15.69	JWH-369 2	126	65	18
360.213	173	15.41	JWH-412 1	161	33	10
360.213	145.1	15.41	JWH-412 2	161	63	18
422.179	235	14.95	JWH-424 1	131	37	12
420.174	233	14.95	JWH-424 2	111	37	12
238.083	125	6.41	KETAMINE 1	61	37	16
238.083	89	6.41	KETAMINE 2	61	73	12
324.164	223	8.19	LAMPA 1	116	33	28
324.164	208	8.19	LAMPA 2	116	41	26
235.081	86.1	5.70	LIDOCAINE 1	126	23	10
235.081	58.1	5.70	LIDOCAINE 2	126	51	10

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Table 1 (*continued*)

Precursor Ion (Q1)	Product Ion (Q3)	Retention time [min]	Analyte	Declustering potential (DP)	Collision energy (CE)	Cell exit potential (CXP)
464.983	252	9.21	LOPRAZOLAM 1	126	57	12
464.983	111.1	9.21	LOPRAZOLAM 2	126	35	14
321.924	275.9	11.33	LORAZEPAM 1	111	29	12
321.924	303.9	11.33	LORAZEPAM 2	111	21	14
335.939	289.9	11.79	LORMETAZEPAM 1	86	29	14
335.939	177.9	11.79	LORMETAZEPAM 2	86	45	12
324.277	223	8.02	LSD 1	101	33	28
324.277	207	8.02	LSD 2	101	57	26
374.126	169	14.60	MAM-2201 1	126	35	22
374.126	115.1	14.60	MAM-2201 2	126	97	14
278.114	191	10.71	MAPROTILINE 1	116	47	24
278.114	189	10.71	MAPROTILINE 2	116	83	22
208.04	135	6.39	MBDB 1	51	27	18
208.04	77	6.39	MBDB 2	51	55	10
192.204	175.1	5.49	MDAT 1	66	15	10
192.204	117.1	5.49	MDAT 2	66	35	8
221.272	135	2.36	MDBP 1	61	23	10
221.272	77	2.36	MDBP 2	61	53	12
208.054	163	5.80	MDEA 1	66	19	20
208.054	105	5.80	MDEA 2	66	35	14
385.124	240.1	15.12	MDMB-CHMICA (MMB-CHMINACA) 1	81	27	12
385.124	144	15.12	MDMB-CHMICA (MMB-CHMINACA) 2	81	53	18
386.303	241.1	15.49	MDMB-CHMINACA 1	156	33	12
386.303	145	15.49	MDMB-CHMINACA 2	156	57	18
262.024	161	6.30	MDPBP 1	86	31	20
262.024	112.1	6.30	MDPBP 2	86	35	14
329.969	284	11.40	MECLONAZEPAM 1	91	37	14
329.969	238	11.40	MECLONAZEPAM 2	91	57	12
271.019	206.9	9.31	MEDAZEPAM 1	126	37	26
271.019	165.1	9.31	MEDAZEPAM 2	126	61	20
180.261	163.2	9.37	MEMANITINE 1	56	19	8
180.261	107.2	9.37	MEMANITINE 2	56	33	10
248.14	220.1	7.50	MEPERIDINE 1	121	31	20
248.14	91.1	7.50	MEPERIDINE 2	121	59	8
190.139	44	5.33	MEPHTETRAMINE (MTTA) 1	101	31	8
190.139	147.1	5.33	MEPHTETRAMINE (MTTA) 2	101	13	18
314.241	214.1	10.12	MEPIRAPIM 1	66	21	10
314.241	144.1	10.12	MEPIRAPIM 2	66	47	8
219.029	158.1	8.76	MEPROBAMATE 1	66	11	20
219.029	55.1	8.76	MEPROBAMATE 2	66	31	8
212.183	195.1	5.11	MESCALINE 1	76	13	24
212.183	77	5.11	MESCALINE 2	76	63	12
310.094	265.1	10.75	METHADONE 1	66	21	12
310.094	105	10.75	METHADONE 2	66	35	14
150.063	91	4.96	METHAMPHETAMINE 1	51	25	12
150.063	119.1	4.96	METHAMPHETAMINE 2	51	15	16
301.06	121.2	12.42	METHANDIENONE 1	131	35	14
301.06	149.1	12.42	METHANDIENONE 2	131	21	18
251.007	132.1	11.03	METHAQUALONE 1	131	37	18
251.007	91	11.03	METHAQUALONE 2	131	57	12
164.056	131.1	4.07	METHCATHINONE 1	61	27	18
164.056	130.1	4.07	METHCATHINONE 2	61	41	16
193.998	176	5.29	METHEDRONE (bk-PMMA) 1	56	15	10
193.998	161	5.29	METHEDRONE (bk-PMMA) 2	56	31	6
263.072	221	11.80	METHOHEXITAL 1	116	19	10
263.072	77.1	11.80	METHOHEXITAL 2	116	67	10
248.059	121.1	7.08	METHOXETAMINE 1	76	37	16
248.059	203	7.08	METHOXETAMINE 2	76	19	26
297.324	129.1	9.25	METHOXPHENIDINE 1	101	27	16
297.324	117.1	9.25	METHOXPHENIDINE 2	101	31	14
116.066	57	5.74	METHYLHEXANAMINE 1	71	17	8
116.066	41.1	5.74	METHYLHEXANAMINE 2	71	31	6
208.272	160	4.56	METHYLONE (bk-MDMA) 1	86	25	20
208.272	132.1	4.56	METHYLONE (bk-MDMA) 2	86	37	14
234.3	84.1	7.11	METHYLPHENIDATE 1	71	23	10
234.3	56	7.11	METHYLPHENIDATE 2	71	65	8
208.3	91	6.34	MEXEDRONE 1	76	47	16
208.3	119	6.34	MEXEDRONE 2	76	29	6
265.493	208.1	9.27	MIANSERIN 1	146	29	24
265.493	58.1	9.27	MIANSERIN 2	146	45	10
326.065	291.1	9.28	MIDAZOLAM 1	136	37	12
326.065	248.9	9.28	MIDAZOLAM 2	136	51	30
399.094	174	9.16	MITRAGYNINE 1	136	41	22
399.094	159.1	9.16	MITRAGYNINE 2	136	63	20
178.131	161	6.85	MMAI 1	61	15	22

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Table 1 (*continued*)

Precursor Ion (Q1)	Product Ion (Q3)	Retention time [min]	Analyte	Declustering potential (DP)	Collision energy (CE)	Cell exit potential (CXP)
178.131	103	6.85	MMAI 2	61	53	14
345.251	214.1	14.15	MMB018 1	66	19	10
345.251	144	14.15	MMB018 2	66	51	20
363.251	232.1	13.10	MMB2201 1	81	21	10
363.251	144.1	13.10	MMB2201 2	81	53	16
358.061	215.1	15.53	MN-18 1	126	25	10
358.061	145	15.53	MN-18 2	126	49	18
440.336	114.1	12.76	MN-25 1	141	41	12
440.336	261.1	12.76	MN-25 2	141	33	12
454.347	114.1	13.18	MN-25–2-METHYL DERIVATIVE 1	151	41	18
454.347	275.1	13.18	MN-25–2-METHYL DERIVATIVE 2	151	31	14
387.261	241.1	15.46	MO-CHMINACA 1	121	27	22
387.261	145.1	15.46	MO-CHMINACA 2	121	47	8
286.043	152.1	2.36	MORPHINE 1	176	79	20
286.043	128.1	2.36	MORPHINE 2	176	77	16
232.059	105.1	7.46	MPBP 1	116	33	14
232.059	91.1	7.46	MPBP 2	116	57	12
349.38	181	10.78	MT-45 1	176	37	24
349.38	77	10.78	MT-45 2	176	93	12
191.273	105.1	3.89	N-(3-METHYLBENZYL)PIPERAZINE 1	81	27	14
191.273	77	3.89	N-(3-METHYLBENZYL)PIPERAZINE 2	81	55	10
178.273	105.1	5.31	N,*N*-DIETHYLPHENETHYLAMINE 1	101	25	10
178.273	77	5.31	N,*N*-DIETHYLPHENETHYLAMINE 2	101	55	12
250.302	100.1	7.20	N,*N*-DIMETHYLPENTYLONE (bk-DMBDP) 1	101	27	12
250.302	135	7.20	N,*N*-DIMETHYLPENTYLONE (bk-DMBDP) 2	101	31	14
189.572	58	4.73	N,*N*-DMT 1	116	19	8
189.572	144.1	4.73	N,*N*-DMT 2	116	23	18
250.245	208.1	9.24	*N*-ACETYL-3,4-MDMC 1	76	19	22
250.245	160.1	9.24	*N*-ACETYL-3,4-MDMC 2	76	35	18
282.065	140.9	10.07	NAPHYRONE 1	51	37	10
282.065	127	10.07	NAPHYRONE 2	51	59	24
282.125	127	9.59	NAPHYRONE-1-NAPHTYL ISOMER 1	51	57	22
282.125	141	9.59	NAPHYRONE-1-NAPHTYL ISOMER 2	51	37	10
298.241	91.1	8.71	*N*-BENZYLNORBUTYLONE 1	96	41	14
298.241	65	8.71	*N*-BENZYLNORBUTYLONE 2	96	91	16
194.253	121	6.10	*N*-ETHYL-4-METHOXYAMPHETAMNE 1	66	29	16
194.253	91	6.10	*N*-ETHYL-4-METHOXYAMPHETAMNE 2	66	45	14
192.296	130.1	5.78	*N*-ETHYLBUPHEDRONE 1	66	39	10
192.296	91	5.78	*N*-ETHYLBUPHEDRONE 2	66	35	14
192.099	105	4.85	*N*-ETHYL-*N*-METHYLCATHINONE 1	76	29	6
192.099	77.2	4.85	*N*-ETHYL-*N*-METHYLCATHINONE 2	76	57	14
299.364	165.1	12.84	*N*-ETHYLNORDAZEPAM 1	216	59	20
299.364	77	12.84	*N*-ETHYLNORDAZEPAM 2	216	89	10
252.18	125	7.10	*N*-ETHYLNORKETAMINE 1	71	41	16
252.18	89.1	7.10	*N*-ETHYLNORKETAMINE 2	71	75	14
315.994	270	12.19	*N*-ETHYLOXAZEPAM 1	116	29	12
315.994	242	12.19	*N*-ETHYLOXAZEPAM 2	116	47	12
250.269	232.2	7.42	*N*-ETHYLPENTYLONE 1	71	21	22
250.269	202	7.42	*N*-ETHYLPENTYLONE 2	71	27	12
296.187	250.1	10.91	NIMETAZEPAM 1	171	35	12
296.187	221	10.91	NIMETAZEPAM 2	171	45	26
309.822	92	7.76	NITRACAINE 1	216	57	12
309.822	76	7.76	NITRACAINE 2	216	91	12
281.974	236	10.55	NITRAZEPAM 1	141	33	30
281.974	180.1	10.55	NITRAZEPAM 2	141	51	24
376.276	232	14.93	NM2201 1	131	21	12
376.276	144.1	14.93	NM2201 2	131	51	18
148.043	117.1	4.24	*N*-METHYL-2AI 1	81	23	14
148.043	115.1	4.24	*N*-METHYL-2AI 2	81	37	14
136.182	105.1	3.68	*N*-METHYL-PEA 1	51	19	18
136.182	77	3.68	*N*-METHYL-PEA 2	51	43	12
175.508	144.1	4.73	*N*-METHYLTRYPTAMINE 1	66	17	18
175.508	117.1	4.73	*N*-METHYLTRYPTAMINE 2	66	37	14
178.233	105	4.29	NN-DMC 1	91	29	14
178.233	72.1	4.29	NN-DMC 2	91	29	10
357.005	214.2	14.48	NNEI 1	81	29	10
357.005	144	14.48	NNEI 2	81	53	20
286.954	245.1	10.65	NORCLOBAZAM 1	141	27	12
286.954	210	10.65	NORCLOBAZAM 2	141	43	26
301.026	72.1	11.72	NORCLOMIPRAMINE 1	101	21	10
301.026	44.1	11.72	NORCLOMIPRAMINE 2	101	65	8
224.176	125.1	6.37	NORKETAMINE 1	51	13	12
224.176	207.2	6.37	NORKETAMINE 2	51	21	12
264.066	91.1	10.99	NORTRIPTYLINE 1	81	29	12
264.066	105.1	10.99	NORTRIPTYLINE 2	81	27	14

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Table 1 (*continued*)

Precursor Ion (Q1)	Product Ion (Q3)	Retention time [min]	Analyte	Declustering potential (DP)	Collision energy (CE)	Cell exit potential (CXP)
178.103	119.1	6.64	*N*-PROPYLAMPHETAMINE 1	86	17	16
178.103	65	6.64	*N*-PROPYLAMPHETAMINE 2	86	61	10
242.25	181.1	9.83	NRG-3 1	81	35	8
242.25	180.1	9.83	NRG-3 2	81	53	16
197.229	154.1	6.76	o-CPP 1	121	27	20
197.229	118.1	6.76	o-CPP 2	121	45	8
235.279	100.1	6.08	OCTACAINE 1	81	23	14
235.279	72.1	6.08	OCTACAINE 2	81	51	10
384.309	270.2	11.55	ORG-28611 1	71	25	12
384.309	174	11.55	ORG-28611 2	71	47	22
288.031	242.1	11.31	OXAZEPAM 1	91	31	12
288.031	269.9	11.31	OXAZEPAM 2	91	21	12
302.251	284	2.59	OXYMORPHONE 1	151	25	14
302.251	227.1	2.59	OXYMORPHONE 2	151	37	12
152.016	110	3.78	PARACETAMOL 1	81	21	14
152.016	65	3.78	PARACETAMOL 2	81	39	10
330.014	70	10.51	PAROXETINE 1	111	49	10
330.014	44.1	10.51	PAROXETINE 2	111	71	8
359.081	214.2	14.60	PB-22 1	71	21	10
359.081	144.1	14.60	PB-22 2	71	51	16
248.346	91	9.17	PCEEA 1	56	45	12
248.346	90.1	9.17	PCEEA 2	56	13	12
248.342	91	8.94	PCMPA 1	66	43	14
248.342	90.1	8.94	PCMPA 2	66	15	12
218.345	91	9.07	PCPr 1	46	39	6
218.345	159.1	9.07	PCPr 2	46	15	22
192.062	91	6.81	PENTEDRONE 1	81	31	12
192.062	132.1	6.81	PENTEDRONE 2	81	25	16
194.308	176.1	6.88	PENTEDRONE METABOLITE 1	81	17	22
194.308	91	6.88	PENTEDRONE METABOLITE 2	81	43	12
235.658	188.1	7.12	PENTYLONE (bk-MBDP) 1	136	25	24
235.658	218.1	7.12	PENTYLONE (bk-MBDP) 2	136	19	10
350.845	206	12.06	PHENAZEPAM 1	131	49	26
350.845	179	12.06	PHENAZEPAM 2	131	63	22
244.103	86.1	8.43	PHENCYCLIDINE (PCP) 1	56	17	12
244.103	91	8.43	PHENCYCLIDINE (PCP) 2	56	43	12
231.014	42	8.46	PHENOBARBITAL 1	−100	−10	−44
231.014	188	8.46	PHENOBARBITAL 2	−100	−10	−14
150.067	91	5.93	PHENTERMINE 1	41	27	12
150.067	133.1	5.93	PHENTERMINE 2	41	13	16
253.004	182.1	10.17	PHENYTOIN 1	116	25	24
253.004	104.1	10.17	PHENYTOIN 2	116	45	12
379.06	135.1	10.20	PRAVADOLINE 1	76	23	14
379.06	77.1	10.20	PRAVADOLINE 2	76	89	12
325.365	271	13.48	PRAZEPAM 1	126	31	12
325.365	140	13.48	PRAZEPAM 2	126	49	18
160.078	142.1	4.61	PREGABALIN 1	116	15	18
160.078	55	4.61	PREGABALIN 2	116	29	8
237.063	100.1	4.01	PROCAINE 1	81	21	12
237.063	120.1	4.01	PROCAINE 2	81	37	14
218.162	91.1	7.95	PROLINTANE 1	86	33	12
218.162	72.1	7.95	PROLINTANE 2	86	23	10
285.029	86.1	10.13	PROMETHAZINE 1	76	21	12
285.029	71.1	10.13	PROMETHAZINE 2	76	63	10
342.045	116.1	10.65	PROPAFENONE 1	86	29	14
342.045	72.1	10.65	PROPAFENONE 2	86	47	10
260.069	56	9.06	PROPRANOLOL 1	86	45	8
260.069	58.1	9.06	PROPRANOLOL 2	86	45	10
155.882	69.1	7.99	PROPYLHEXEDRINE 1	81	23	10
155.882	55	7.99	PROPYLHEXEDRINE 2	81	37	8
367.248	259.1	15.96	PSB-SB-1202 1	121	23	12
367.248	121.1	15.96	PSB-SB-1202 2	121	23	8
356.299	283	12.52	PTI-1 1	106	29	14
356.299	213.1	12.52	PTI-1 2	106	47	10
400.341	283	12.77	PTI-2 1	116	31	14
400.341	213.1	12.77	PTI-2 2	116	51	10
260.116	91.1	9.63	PV-8 1	96	33	12
260.116	77.1	9.63	PV-8 2	96	73	10
274.307	91	10.68	PV9 1	126	33	12
274.307	77	10.68	PV9 2	126	73	12
396.09	144	12.62	PX-1 1	76	59	18
396.09	231.9	12.62	PX-1 2	76	31	10
397.253	233	12.76	PX-2 1	86	33	12
397.253	352.2	12.76	PX-2 2	86	21	14
353.943	167.1	9.35	PYRAZOLAM 1	151	47	20

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Table 1 (*continued*)

Precursor Ion (Q1)	Product Ion (Q3)	Retention time [min]	Analyte	Declustering potential (DP)	Collision energy (CE)	Cell exit potential (CXP)
353.943	206	9.35	PYRAZOLAM 2	151	41	26
384.09	253.1	9.53	QUETIAPINE 1	116	31	12
384.09	221	9.53	QUETIAPINE 2	116	51	28
322.05	135.1	14.62	RCS-4 1	136	31	16
322.05	77	14.62	RCS-4 2	136	73	10
326.3	121.1	8.12	RH-34 1	91	25	14
326.3	91.1	8.12	RH-34 2	91	57	10
236.144	188.2	6.86	R-MMC 1	61	25	10
236.144	218.1	6.86	R-MMC 2	61	17	18
303.805	138.1	4.73	SCOPOLAMINE 1	96	29	18
303.805	156.1	4.73	SCOPOLAMINE 2	96	23	20
359.177	215.2	15.57	SDB-005 1	51	21	10
359.177	145	15.57	SDB-005 2	51	45	20
321.153	91	14.09	SDB-006 1	171	61	12
321.153	214.1	14.09	SDB-006 2	171	29	10
306.988	276	11.51	SERTRALINE 1	66	17	12
306.988	159	11.51	SERTRALINE 2	66	37	20
475.047	58.1	10.22	SILDENAFIL 1	91	103	10
475.047	100.1	10.22	SILDENAFIL 2	91	35	12
329.138	81.1	13.96	STANOZOLOL 1	241	79	12
329.138	95.1	13.96	STANOZOLOL 2	241	51	12
222.343	107.1	7.32	TAPENTADOL 1	86	35	14
222.343	77	7.32	TAPENTADOL 2	86	63	12
301.993	256	11.62	TEMAZEPAM 1	116	31	12
301.993	284.1	11.62	TEMAZEPAM 2	116	19	12
265.226	176.1	9.01	TETRACAINE 1	96	21	18
265.226	72	9.01	TETRACAINE 2	96	37	10
315.093	193.1	15.93	THC 1	106	31	24
315.093	123	15.93	THC 2	106	43	16
345.2	299.2	14.97	THCCOOH 1	106	23	10
345.2	193.1	14.97	THCCOOH 2	120	45	10
142.098	125	3.73	THIOPROPAMINE 1	51	13	8
142.098	97	3.73	THIOPROPAMINE 2	51	25	12
359.247	215.2	15.98	THJ 1	121	29	10
359.247	145	15.98	THJ 2	121	49	16
343.076	215.1	15.53	THJ-018 1	136	25	10
343.076	145.1	15.53	THJ-018 2	136	45	18
361.067	233.1	14.62	THJ-2201 (5-FLUORO THJ-018) 1	131	25	10
361.067	145.1	14.62	THJ-2201 (5-FLUORO THJ-018) 2	131	49	18
224.246	179	5.68	TILETAMINE 1	51	13	10
224.246	151.1	5.68	TILETAMINE 2	51	23	18
264.304	58.1	6.88	TRAMADOL 1	96	47	8
264.304	42.1	6.88	TRAMADOL 2	96	113	8
372.082	176	8.24	TRAZODONE 1	126	33	24
372.082	148	8.24	TRAZODONE 2	126	45	20
343.99	309.1	11.35	TRIAZOLAM 1	106	37	14
343.99	239.9	11.35	TRIAZOLAM 2	106	57	30
294.788	100.2	10.95	TRIMIPRAMINE 1	81	23	12
294.788	58.1	10.95	TRIMIPRAMINE 2	81	61	8
329.037	284	9.09	U-47700 1	56	25	14
331.017	286	9.09	U-47700 2	96	25	14
312.107	125.1	15.56	UR-144 1	96	29	16
312.107	214	15.56	UR-144 2	96	33	10
328.092	125.1	13.77	UR-144 metabolite 1	96	27	16
328.092	230.1	13.77	UR-144 metabolite 2	96	33	10
377.154	105.1	13.30	W-15 1	141	33	16
379.165	105.2	13.30	W-15 2	166	33	12
457.176	135.1	12.36	WIN 54,461 1	126	29	12
457.176	77	12.36	WIN 54,461 2	126	95	12
427.117	155.1	13.63	WIN 55,212–2 1	161	33	18
427.117	127.2	13.63	WIN 55,212–2 2	161	75	12
330.293	125.1	14.69	XLR-11 1	116	31	16
330.293	232.1	14.69	XLR-11 2	116	33	10
352.216	125.1	14.79	XLR12 1	141	31	8
352.216	254	14.79	XLR12 2	141	35	12
259.148	161	11.88	YANGONIN 1	121	29	22
259.148	89	11.88	YANGONIN 2	121	93	10
305.911	264	9.91	ZALEPLON 1	141	31	12
305.911	236.1	9.91	ZALEPLON 2	141	37	10
308.323	235.1	7.76	ZOLPIDEM 1	111	47	10
308.323	236	7.76	ZOLPIDEM 2	111	37	30
389.014	244.9	6.70	ZOPICLONE 1	81	23	12
389.014	112	6.70	ZOPICLONE 2	81	79	16
401.024	221	12.12	ZUCLOPENTHIXOL 1	101	73	26
401.024	231	12.12	ZUCLOPENTHIXOL 2	101	49	28

(10.000 RCF, 1 min). In the last step, 50 μL of blood extract and 450 μL of mobile phase (A:B; 90:10, v/v/) were placed in an autosampler vials. The injection volume was 20 μL.

2.6. Validation

The developed method was validated according to the SWGTOX validation guidelines for whole blood and urine [21]. The parameters such as selectivity, specificity, linearity, precision, BIAS, recovery, reproducibility, LOD and LOQ were designated.

The analysis of pure blood samples and samples fortified with all analytes by adding small amounts of a mixture of all analytes was used to determine selectivity and specificity. The samples were subjected to the preparation and analysis process in accordance with the developed method in order to exclude the presence of exogenous analytes affecting the analysis result of live samples.

Analysis of six repetitions of the curve in a matrix made of pure blood fortified with a mix of analytes with concentrations ranging from 0.05 to 50 ng/mL for each analyte made it possible to determine the linearity range of the method for individual analytes. Calibration curves were generated by plotting the peak area ratio (PAR) versus the spiked analyte concentration. Blank matrix and blank matrix containing only IS was analyzed with each batch but not included in the calibration curves. The correlation coefficient (R^2) was calculated and deemed acceptable for R^2 values >0.99.

Precision and BIAS was calculated by running six replicates of calibration standards for five concentrations (1-only for THC, 2, 10, 200, 400, 500 and 1000 ng/mL). For precision and BIAS, accuracy limit of ± 20 % was selected. The six repetitions were also used to determine the mean recovery.

The LOD value was determined as the lowest calibration standard which exhibited as S/N ratio ≥ 3, while the LOQ was determined to be the lowest calibration standard which exhibited as S/N ratio ≥ 10. Meanwhile, the reproducibility of the analytical method has been verified by proficiency tests.

The matrix effects could be eliminated using matrix-matched calibration curve. Due to, the obtained results for the given calibration points take into account the matrix's influence on their analysis.

3. Results and discussion

3.1. Experimental conditions for HPLC and MS

The analytical standards of the psychoactive substances selected for the study were subjected to individual optimization in order to select the best possible work parameters of the mass spectrometer. Parameters such as the ionization mode, Q1, Q3, declustering potential (DP), entrance potential (EP), collision energy (CE), collision cell exit potential (CXP) were determined for each of substance, with The Analyst 1.6.3 software used for this optimization. For all analytes positive ionization mode turned out to be better, except for GHB and Phenobarbital, which should be analyzed in negative ionization mode. Entrance potential (EP) for all analytes was 10. The MRM pairs and values DP, CE, CXP for each analyte are collected in Table 1. The MRM transitions for each analyte were monitored only in specific detection windows that were defined as ± 0.5 min from the expected retention time. Subsequently, the chromatographic conditions were optimized to allow the best possible separation of the 522 optimized analytes. In addition, full chemical name, its abbreviation, full chemical structure and precursor ion were included in the supplementary data as Table S1. The gradient elution was performed with 2 mM ammonium formate with 0.1 % formic acid in water (**A**), and with 2 mM ammonium formate with 0.1 % formic acid in methanol (**B**). Acetonitrile was also tested as phase **B**; however, it did not significantly change the obtained chromatogram, so due to its expensive nature and the amount of harmful waste generated during the analysis, it was not used for further studies. The content of ammonium formate in mobile phases was also modified. The values of 2 mM and 5 mM were tested, but similarly to the case of acetonitrile, it did not improve the separation of analytes either. The gradient was run at a flow rate of 0.5 mL/min starting at 5 % **B** for 1 min, then increasing to 95 % **B** over 15 min and run isocratic elution at those conditions for 6 min. The gradient was then changed to the starting conditions over 6 min and kept constant for 3 min to re-equilibrate the system. The total run time was 30 min. The selected chromatographic conditions were checked on three columns: Kinetex C18 column (Phenomenex, 3.0 × 100 mm; 2.6 μm), Kinetex Biphenyl (Phenomenex, 3.0 × 100 mm; 2.6 μm) and Kinetex Phenyl-Hexyl (Phenomenex, 3.0 × 100 mm; 2.6 μm). The best separation was obtained for the Kinetex C18 column (Phenomenex, 3.0 × 100 mm; 2.6 μm), so it was selected for further analysis. Fig. S2 shows the chromatogram obtained for this column. This gradient method allowed separation of all compounds except 3-MMC and 4-MMC within a 30-min run time. The retention times of all compounds were from 1.38 to 16.76 min and are presented in Table 2.

3.2. Procedure for isolating psychoactive substances

The solid phase extraction (SPE) method was used for the first attempts to isolate psychoactive substances from blood samples. However, this method did not yield satisfactory results. The large number of analytes from different study groups contributed to this: to obtain valuable results, several types of columns should be used for each analysis, which significantly extends the analysis time, increases its cost and requires a larger amount of material for testing. In order to enable quick isolation of all compounds contained in the developed procedure, liquid–liquid extraction (LLE) with cold acetonitrile (2 mM ammonium formate, 0.1 % (v/v) formic acid) (0.5 mL) was used. Atrazine (IS) solution was used to verify the extraction process. This solution of the same concentration was added to each sample. In the sample preparation procedure described above, samples are frozen only once. In the course of the research, re-freezing before the last centrifugation was also tested. However, the results showed that freezing at that point had no effect on the percentage of analyte recovery from the sample so it was removed from the procedure.

3.3. Validation

The developed method of isolating and determining psychoactive compounds, drugs and their metabolites from blood samples was validated according to the SWGTOX guidelines. Only 2 from 522 validated compounds failed the validation criteria and were not included in the routine analysis of blood samples. The range of linearity is from 0.05 to 50 ng/mL, and the range of quantification of the analytes depends on the group of compounds to which they belong. In the case of cannabinoids and synthetic cannabinoids it is 2–200 ng/mL (THC, 1–200 ng/mL), while for other compounds it is 10–1000 ng/mL. Differences in these values occur due to legal regulations and standards required in the labeling of these substances. The exceptions found during the validation are 25 *T*-NBOMe (1–400 ng/mL), 2C-I and 4-hydroxymidazolam (10–500 ng/mL), 3-Methylmethcathinone (10–500 ng/mL), 4-AcO-MET (200–1000 ng/mL), 4-CAB, 4-EAPB, 4-fluoro PV9, 6-APB, 6-bromo-MDMA, 7-APB, Benzedrone, D2PM, MMAI and RH-34 (10–400 ng/mL), Nitracaine (200–1000 ng/mL) and THCCOOH (10–200 ng/mL). The correlation coefficient (R^2) was calculated and deemed acceptable for R^2 values >0.99. The use of this type of standard curve allowed elimination of the influence of the matrix effect in real samples. The method was found to be selective for the tested compounds. The only exception were 3-MMC and 4-MMC, which did not separate during the analysis. Drug-free blood samples showed no evidence of interference. The lowest recovery value (43.37 %) was obtained for 2-FIC and the highest (119.97 %) for Quetiapine. For precision and bias accuracy, the limit of ± 20 % was used. The values of precision and bias ranged from 1.12 % to 24.08 % and −56.63 % to 19.97 % respectively. The

Table 2
Summary of the results of validation of the developed analytical method.

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
1-(2-METHOXYPHENYL)PIPERAZINE	5.33	10	82.66	9.70	11.74	−17.34	10
		400	86.68	4.92	5.67	−13.32	
		1000	97.20	11.93	12.28	−2.80	
1-(3-TRIFLUOROMETHYLPHENYL)PIPERAZINE (TFMPP)	7.98	10	81.70	7.10	8.70	−18.30	10
		200	95.74	3.42	3.58	−4.26	
		500	105.76	16.93	16.01	5.76	
		1000	92.61	9.34	10.09	−7.39	
1-(4-CHLOROPHENYL)PIPERAZINE (pCPP)	6.24	10	88.00	10.40	11.80	−12.00	10
		200	88.34	7.09	8.03	−11.66	
		500	102.16	8.51	8.33	2.16	
		1000	100.92	4.83	4.79	0.92	
1-(4-FLUOROPHENYL)PIPERAZINE (FPP)	4.74	10	92.67	15.45	16.67	−7.33	10
		200	93.91	6.63	7.06	−6.09	
		500	103.79	9.20	8.86	3.79	
		1000	93.31	5.09	5.46	−6.69	
1.4-DIBENZYLPIPERAZINE (DBZP)	7.80	10	104.77	8.71	8.32	4.77	10
		200	113.13	5.81	5.14	13.13	
		500	109.00	7.80	7.20	9.00	
		1000	93.40	3.66	3.92	−6.60	
1-AMINOINDAN	3.88	10	83.37	16.34	19.60	−16.63	10
		200	86.83	5.49	6.32	−13.17	
		500	113.24	3.23	2.85	13.24	
		1000	96.29	5.83	6.05	−3.71	
1-METHYL-4-BENZYLPIPERAZINE (MBZP)	3.24	10	104.80	15.02	14.33	4.80	10
		200	112.40	8.60	7.70	12.40	
		500	104.27	6.68	6.40	4.27	
		1000	110.50	2.20	2.00	10.50	
1-METHYLAMINO-1-(3.4-METHYLENEDIOXYPHENYL) PROPANE	6.06	10	91.79	16.72	18.22	−8.21	10
		400	81.43	4.03	4.95	−18.57	
		1000	87.74	10.52	11.99	−12.26	
2.3-DICHLOROPHENYLPIPERAZINE (DCPP)	8.58	10	80.18	8.73	10.89	−19.83	10
		200	108.09	10.91	10.09	8.09	
		500	115.26	13.80	11.97	15.26	
		1000	80.69	7.68	9.51	−19.31	
2.3-DIMETHYLETHCATHINONE (2.3-DMEC)	7.50	10	118.80	4.41	3.40	18.80	10
		200	95.78	9.71	10.14	−4.22	
		500	118.28	8.31	7.02	18.28	
		1000	90.64	2.20	2.43	−9.36	
2.3-DIMETHYLMETHCATHINONE (2.3-DMMC)	7.07	10	90.50	11.79	13.03	−9.50	10
		200	97.47	4.24	4.35	−2.53	
		500	111.13	6.47	5.82	11.13	
		1000	90.39	5.57	6.16	−9.61	
2.3-ETHYLONE ISOMER	5.46	10	88.36	10.62	12.02	−11.65	10
		400	87.43	11.12	12.72	−12.57	
		1000	93.11	9.79	10.52	−6.89	
2.3-MDMA	5.77	10	110.00	6.60	6.00	10.00	10
		200	99.66	5.56	5.58	−0.34	
		500	112.45	9.06	8.06	12.45	
		1000	93.63	3.14	3.36	−6.37	
2.3-MDPV	7.61	10	98.11	5.12	5.21	−1.89	10
		400	88.11	5.62	6.38	−11.89	
		1000	91.43	6.07	6.64	−8.57	
2.4.5-TRIMETHOXYAMPHETAMINE	6.19	10	102.57	14.17	13.81	2.57	10
		400	94.80	7.12	7.51	−5.20	
		1000	102.65	6.52	6.35	2.65	
2.4-DIMETHYLMETHCATHINONE (2.4-DMMC)	7.52	10	100.35	12.00	11.96	0.35	10
		200	112.30	8.50	7.50	12.30	
		500	112.90	4.20	3.70	12.90	
		1000	82.00	1.70	2.10	−18.00	
2.4-DMEC	7.95	10	93.33	13.76	14.74	−6.67	10
		400	89.37	7.04	7.88	−10.63	
		1000	90.58	6.28	6.93	−9.42	
2.5-DMMA	6.73	10	96.38	8.70	9.02	−3.62	10
		400	91.70	8.63	9.41	−8.30	
		1000	89.84	6.12	6.81	−10.16	
25B-NBF	10.17	10	88.69	8.46	9.54	−11.31	10
		400	102.45	5.59	5.45	2.45	
		1000	90.51	4.41	4.88	−9.49	
25C-NBF	9.90	10	97.86	8.54	8.73	−2.14	10
		400	101.38	7.40	7.30	1.38	
		1000	94.91	5.34	5.63	−5.09	
25C-NBOH	9.78	10	88.50	9.30	10.50	−11.50	10

(*continued on next page*)

Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
		200	97.63	6.01	6.15	−2.37	
		500	116.10	9.20	7.90	16.10	
		1000	92.59	8.07	8.72	−7.41	
25C-NBOMe	10.32	10	92.44	8.72	9.43	−7.56	10
		200	114.03	6.76	5.93	14.03	
		500	111.37	10.04	9.01	11.37	
		1000	93.20	3.98	4.27	−6.80	
25D-NBOMe	10.51	10	102.96	13.34	12.96	2.96	10
		200	112.11	6.19	5.52	12.11	
		500	114.62	9.11	7.95	14.62	
		1000	91.04	1.68	1.85	−8.96	
25E-NBOMe	11.33	10	98.72	14.55	14.74	−1.28	10
		200	117.07	12.25	10.47	17.07	
		500	98.76	8.26	8.36	−1.24	
		1000	93.36	2.21	2.37	−6.64	
25G-NBOMe	11.05	10	100.47	8.08	8.05	0.47	10
		400	97.71	4.63	4.74	−2.29	
		1000	85.53	2.10	2.45	−14.47	
25H-NBOMe	9.49	10	96.08	10.19	10.60	−3.92	10
		200	116.01	11.20	9.65	16.01	
		500	115.30	10.00	8.70	15.30	
		1000	91.95	4.70	5.11	−8.05	
25-I-NB2OMe	10.90	10	103.42	7.23	6.99	3.42	10
		400	99.95	5.06	5.07	−0.05	
		1000	92.70	7.22	7.79	−7.30	
25I-NB3OMe	10.84	10	81.38	7.12	8.75	−18.62	10
		400	85.42	4.97	5.82	−14.58	
		1000	86.75	8.61	9.93	−13.25	
25I-NB4OMe	10.76	10	86.55	2.54	2.93	−13.45	10
		400	93.99	6.78	7.21	−6.01	
		1000	88.75	9.41	10.61	−11.25	
25I-NBF	10.60	10	95.69	6.29	6.58	−4.31	10
		400	112.79	4.17	3.69	12.79	
		1000	115.79	8.11	7.01	15.79	
25I-NBMD	10.72	10	83.65	9.74	11.64	−16.35	10
		400	98.92	9.93	10.04	−1.08	
		1000	94.43	8.85	9.37	−5.57	
25I-NBOH	10.49	10	84.74	11.50	13.57	−15.26	10
		200	94.24	7.37	7.82	−5.76	
		500	108.00	9.85	9.12	8.00	
		1000	85.44	2.05	2.40	−14.56	
25 *N*-NBOMe	9.14	10	102.32	7.24	7.08	2.32	10
		200	108.84	10.37	9.52	8.84	
		500	108.00	9.90	9.10	8.00	
		1000	91.97	3.49	3.79	−8.03	
25 T2-NBOMe	10.78	10	96.78	6.18	6.39	−3.22	10
		400	88.45	5.27	5.96	−11.55	
		1000	69.87	2.15	3.07	−30.13	
25 *T*-NBOMe	10.13	10	92.86	10.90	11.74	−7.15	10
		200	101.63	4.83	4.75	1.63	
		500	114.49	9.61	8.39	14.49	
		1000	94.24	3.72	3.95	−5.76	
2-AMINO-1-PHENYLBUTANE	6.11	10	90.10	10.70	11.87	−9.90	10
		400	80.68	9.34	11.57	−19.32	
		1000	86.08	8.31	9.65	−13.92	
2-AMINOINDANE	3.89	10	90.54	10.93	12.07	−9.46	10
		200	81.66	9.43	11.55	−18.34	
		500	92.90	4.60	5.00	−7.10	
		1000	85.63	6.87	8.03	−14.37	
2-BROMOAMPHETAMINE	7.06	10	84.49	9.79	11.59	−15.51	10
		400	84.26	12.40	14.71	−15.74	
		1000	82.16	6.41	7.80	−17.84	
2-BROMOMETHAMPHETAMINE	7.20	10	94.75	7.92	8.36	−5.25	10
		200	108.15	13.54	12.52	8.15	
		500	114.04	17.05	14.95	14.04	
		1000	99.25	4.07	4.10	−0.75	
2C-B	7.75	10	95.20	13.63	14.32	−4.80	10
		200	95.24	10.28	10.80	−4.76	
		500	105.84	10.03	9.48	5.84	
		1000	89.58	3.85	4.30	−10.42	
2C-B_FLY	8.05	10	109.90	21.45	19.52	9.90	10
		200	91.43	8.17	8.93	−8.57	
		500	107.97	12.06	11.17	7.97	
		1000	85.22	6.44	7.56	−14.78	

(*continued on next page*)

Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
2C-C	7.27	10	119.30	11.00	9.20	19.30	10
		200	81.60	14.86	18.21	−18.40	
		500	90.57	9.66	10.67	−9.43	
		1000	82.00	3.70	4.60	−18.00	
2C-D	7.54	10	106.50	11.60	10.90	6.50	10
		200	106.48	8.18	7.68	6.48	
		500	118.37	9.15	7.73	18.37	
		1000	85.68	4.13	4.82	−14.32	
2C-G	8.58	10	103.69	10.00	9.64	3.69	10
		200	106.82	7.68	7.19	6.82	
		500	115.13	11.41	9.91	15.13	
		1000	91.52	4.01	4.38	−8.48	
2-CHLOROAMPHETAMINE	6.60	10	100.46	13.28	13.22	0.46	10
		400	88.32	13.85	15.69	−11.68	
		1000	96.85	11.29	11.66	−3.15	
2C-I	8.44	10	99.10	13.27	13.39	−0.90	10
		200	96.47	9.30	9.64	−3.53	
		500	114.60	9.70	8.40	14.60	
2C-P	10.13	10	98.74	16.42	16.63	−1.26	10
		200	105.68	10.68	10.11	5.68	
		500	108.05	12.77	11.82	8.05	
		1000	100.46	4.66	4.63	0.46	
2C-T-7	9.63	10	95.75	6.17	6.44	−4.25	10
		200	99.22	5.64	5.69	−0.78	
		500	114.49	10.63	9.29	14.49	
		1000	89.31	3.69	4.14	−10.69	
2C-TFM	8.69	10	102.97	11.89	11.54	2.97	10
		400	91.98	9.74	10.59	−8.02	
		1000	93.43	9.74	10.42	−6.57	
2-FEC	4.71	10	80.52	5.14	6.39	−19.48	10
		400	84.11	4.77	5.67	−15.89	
		1000	93.65	4.17	4.45	−6.35	
2-FIC	3.20	10	81.89	8.86	10.82	−18.11	10
		400	43.37	2.53	5.83	−56.63	
		1000	80.23	10.98	13.68	−19.77	
2-FLUOROAMPHETAMINE	5.13	10	102.94	14.30	13.89	2.94	10
		200	103.77	9.91	9.55	3.77	
		500	111.42	8.50	7.63	11.42	
		1000	95.70	5.21	5.45	−4.30	
2-FLUOROMETHAMPHETAMINE (2-FMA)	5.39	10	115.82	9.61	8.30	15.82	10
		200	111.57	5.57	5.00	11.57	
		500	119.69	9.54	7.97	19.69	
		1000	89.56	3.47	3.88	−10.44	
2-FLUOROMETHCATHINONE (2-FMC)	4.09	10	84.86	6.33	7.46	−15.15	10
		200	91.58	6.15	6.72	−8.42	
		500	115.65	6.69	5.78	15.65	
		1000	93.53	4.07	4.35	−6.47	
2-IODOAMPHETAMINE	7.78	10	91.46	8.83	9.66	−8.54	10
		400	103.78	10.06	9.70	3.78	
		1000	99.29	11.88	11.96	−0.71	
2-MAPB	7.07	10	93.26	8.78	9.41	−6.74	10
		400	85.87	5.04	5.87	−14.13	
		1000	86.52	6.75	7.80	−13.48	
2-MeOMC	5.33	10	96.82	11.26	11.63	−3.18	10
		400	91.00	3.75	4.12	−9.00	
		1000	92.63	5.19	5.60	−7.37	
2-METHOXY-2-PHENYLETHYLAMINE	4.98	10	92.92	7.33	7.89	−7.08	10
		400	88.07	5.24	5.95	−11.93	
		1000	96.53	10.56	10.94	−3.47	
2-METHOXYAMPHETAMINE (2-MA)	6.20	10	100.26	9.96	9.94	0.26	10
		200	101.45	5.81	5.73	1.45	
		500	114.25	13.68	11.98	14.25	
		1000	94.03	5.59	5.94	−5.97	
2-METHOXYMETHAMPHETAMINE (2-MeOMA)	6.40	10	99.78	7.09	7.11	−0.22	10
		200	106.55	5.39	5.06	6.55	
		500	115.10	15.00	13.10	15.10	
		1000	93.65	3.16	3.38	−6.35	
2-METHYLAMINO-1-PHENYLBUTANE	6.24	10	82.88	10.06	12.13	−17.12	10
		400	81.41	3.92	4.81	−18.59	
		1000	87.49	6.22	7.10	−12.51	
2-METHYLMETHCATHINONE (2-MMC)	6.00	10	81.29	11.90	14.64	−18.72	10
		200	102.38	10.54	10.29	2.38	
		500	110.00	13.90	12.60	10.00	
		1000	95.27	5.60	5.88	−4.73	

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Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
2-METHYL-PBP	7.27	10	93.41	7.06	7.55	−6.59	10
		400	89.45	11.02	12.32	−10.55	
		1000	99.18	6.68	6.74	−0.82	
2-METHYL-PPP	6.51	10	90.06	10.99	12.21	−9.94	10
		400	107.46	7.78	7.24	7.46	
		1000	116.89	7.93	6.79	16.89	
3.4-DICHLOROMETHYLPHENIDATE (3.4-CTMP)	9.99	10	84.68	8.72	10.29	−15.32	10
		200	95.15	6.20	6.52	−4.85	
		500	119.74	8.00	6.68	19.74	
		1000	96.94	2.19	2.26	−3.06	
3.4-DIMETHOXY-ALPHA-PVP	7.45	10	106.69	6.99	6.55	6.69	10
		400	97.77	10.40	10.64	−2.23	
		1000	102.76	5.83	5.68	2.76	
3.4-DIMETHYLMETHCATHINONE (3.4-DMMC)	7.38	10	111.45	17.15	15.39	11.45	10
		200	105.77	6.59	6.23	5.77	
		500	103.80	9.00	8.70	3.80	
		1000	91.41	3.92	4.29	−8.59	
3.4-DMEC	7.76	10	99.22	13.84	13.94	−0.78	10
		400	95.05	6.19	6.51	−4.95	
		1000	90.37	13.10	14.50	−9.63	
3.4-DMMA	5.33	10	112.58	16.67	14.81	12.58	10
		200	114.55	12.84	11.21	14.55	
		500	114.20	10.60	9.30	14.20	
		1000	98.48	4.24	4.30	−1.52	
3.4-EDMA	5.63	10	103.83	12.94	12.46	3.83	10
		400	98.40	7.59	7.71	−1.60	
		1000	99.73	7.11	7.13	−0.27	
3.4-EDMC	5.25	10	105.75	14.60	13.81	5.75	10
		400	95.80	9.69	10.12	−4.20	
		1000	98.14	12.85	13.09	−1.86	
3.4-MDMA (ECSTAZY)	5.35	10	105.42	7.74	7.34	5.42	10
		200	113.89	11.91	10.46	13.89	
		500	111.46	12.45	11.17	11.46	
		1000	98.05	2.57	2.62	−1.95	
3.4-MDPA	6.80	10	106.14	15.62	14.71	6.14	10
		200	103.93	7.72	7.43	3.93	
		500	113.82	3.77	3.31	13.82	
		1000	94.21	3.20	3.40	−5.79	
3.4-MDPHP	8.68	10	89.07	8.22	9.23	−10.93	10
		400	87.27	9.82	11.25	−12.73	
		1000	92.81	9.06	9.77	−7.19	
3.4-METHYLENDIOXYPYROVALERONE	7.55	10	92.57	11.08	11.97	−7.43	10
		400	87.48	6.31	7.22	−12.52	
		1000	93.41	8.10	8.68	−6.59	
3.4-METHYLENEDIOXY_PV9	10.84	10	105.32	6.47	6.14	5.32	10
		400	103.02	9.34	9.07	3.02	
		1000	89.42	4.00	4.47	−10.58	
30C-NBOMe	9.75	10	97.00	11.75	12.11	−3.00	10
		400	89.87	10.31	11.47	−10.13	
		1000	90.71	6.46	7.12	−9.29	
3-BROMOAMPHETAMINE	7.32	10	94.34	10.44	11.06	−5.66	10
		200	97.83	11.15	11.39	−2.17	
		500	116.33	10.00	8.60	16.33	
		1000	87.66	2.92	3.34	−12.34	
3-BROMOMETHAMPHETAMINE	7.30	10	90.26	15.75	17.44	−9.74	10
		200	101.45	6.53	6.43	1.45	
		500	108.30	11.50	10.60	8.30	
		1000	92.49	7.34	7.94	−7.51	
3-BROMOMETHCATHINONE (3-BMC)	6.70	10	98.22	18.23	18.56	−1.78	10
		200	96.90	6.35	6.56	−3.10	
		500	114.85	14.83	12.91	14.85	
		1000	96.61	7.12	7.37	−3.39	
3-CAF	15.29	2	101.28	7.11	7.02	1.28	2
		200	101.34	6.67	6.58	1.34	
3C-B-FLY	8.56	10	86.86	11.52	13.27	−13.14	10
		400	80.26	6.39	7.96	−19.74	
		1000	80.99	5.50	6.80	−19.01	
3-CHLOROAMPHETAMINE	6.85	10	86.23	16.47	19.10	−13.77	10
		400	83.96	7.03	8.37	−16.04	
		1000	91.04	10.00	10.99	−8.96	
3-CHLOROMETHCATHINONE (3-CMC)	6.02	10	92.66	11.44	12.35	−7.34	10
		200	103.27	10.00	9.68	3.27	
		500	115.33	7.18	6.22	15.33	
		1000	90.56	3.78	4.17	−9.44	

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Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
3-CHLOROPHENYLPIPERAZINE (mCPP)	6.78	10	86.50	6.40	7.40	−13.50	10
		200	100.74	2.88	2.85	0.74	
		500	107.33	7.17	6.68	7.33	
		1000	84.39	3.50	4.15	−15.61	
3C-P	8.43	10	95.84	11.01	11.49	−4.16	10
		400	98.98	11.21	11.32	−1.02	
		1000	103.40	6.44	6.23	3.40	
3-DESOXY-3.4-MDPV	8.00	10	105.00	13.06	12.44	4.99	10
		400	99.72	8.18	8.20	−0.28	
		1000	103.03	8.42	8.17	3.03	
3-ETHYLMETHCATHINONE (3-EMC)	7.52	10	114.37	21.54	18.84	14.37	10
		200	111.10	7.70	6.90	11.10	
		500	115.78	7.33	6.33	15.78	
		1000	102.50	9.90	9.70	2.50	
3-FEC	4.88	10	91.30	9.34	10.23	−8.71	10
		400	87.24	3.01	3.45	−12.76	
		1000	97.95	6.01	6.13	−2.05	
3-FLUORO-ALFA-PPP	5.35	10	92.48	3.42	3.70	−7.52	10
		400	89.04	4.21	4.73	−10.96	
		1000	94.58	7.65	8.09	−5.42	
3-FLUOROAMPHETAMINE	5.13	10	92.17	7.17	7.78	−7.83	10
		200	101.72	6.16	6.06	1.72	
		500	112.91	6.72	5.95	12.91	
		1000	96.15	3.66	3.81	−3.85	
3-FLUOROMETHAMPHETAMINE (3-FMA)	5.39	10	108.43	12.58	11.60	8.43	10
		200	116.02	8.90	7.67	16.02	
		500	113.22	12.50	11.04	13.22	
		1000	83.18	2.27	2.73	−16.82	
3-FLUOROMETHCATHINONE (3-FMC)	4.42	10	100.32	18.87	18.81	0.32	10
		200	102.13	5.71	5.59	2.13	
		500	113.63	19.30	16.99	13.63	
		1000	99.94	3.27	3.27	−0.06	
3-HYDROXYBROMAZEPAM	9.17	10	85.19	20.26	23.78	−14.81	10
		200	88.28	2.43	2.75	−11.72	
		500	108.76	13.90	12.78	8.76	
		1000	90.03	3.22	3.58	−9.97	
3-HYDROXYFLUNITRAZEPAM	10.21	10	111.96	9.32	8.32	11.96	10
		200	118.80	6.30	5.30	18.80	
		500	108.88	7.61	6.99	8.88	
		1000	88.12	3.30	3.74	−11.88	
3-IODOAMPHETAMINE	8.07	10	92.39	11.26	12.19	−7.61	10
		400	96.34	5.46	5.67	−3.66	
		1000	95.26	9.68	10.16	−4.74	
3-MEC	6.47	10	99.34	7.17	7.21	−0.67	10
		400	84.30	3.45	4.09	−15.70	
		1000	104.61	11.81	11.28	4.61	
3-MeOMC	5.33	10	91.89	12.89	14.03	−8.11	10
		400	95.83	4.03	4.21	−4.17	
		1000	97.77	5.51	5.64	−2.23	
3-METHOXYAMPHETAMINE (3-MA)	5.66	10	95.86	12.36	12.90	−4.14	10
		200	108.20	12.70	11.80	8.20	
		500	117.29	11.39	9.71	17.29	
		1000	96.59	9.39	9.72	−3.41	
3-METHOXYPHENCYCLIDINE	8.94	10	99.46	4.15	4.17	−0.55	10
		400	91.70	10.42	11.36	−8.30	
		1000	96.03	4.31	4.49	−3.97	
3-METHYLMETHCATHINONE (3-MMC)	6.00	10	108.44	11.94	11.01	8.44	10
		200	108.80	8.31	7.64	8.80	
		500	117.60	6.20	5.30	17.60	
3-METHYL-PBP	7.51	10	113.33	13.49	11.90	13.33	10
		400	93.65	10.28	10.97	−6.35	
		1000	91.70	5.41	5.90	−8.30	
3-METHYL-PPP	6.67	10	96.09	12.60	13.11	−3.91	10
		400	99.81	11.18	11.20	−0.19	
		1000	100.14	7.83	7.81	0.14	
4.4′-DMAR	7.37	10	91.92	6.32	6.88	−8.08	10
		200	109.31	4.47	4.09	9.31	
		500	118.50	4.10	3.50	18.50	
		1000	91.11	4.49	4.93	−8.89	
4-AcO-DET	6.38	10	80.10	12.37	15.44	−19.90	10
		400	89.64	13.33	14.87	−10.36	
		1000	95.89	8.95	9.33	−4.11	
4-AcO-DMT	5.47	10	88.82	11.90	13.40	−11.18	10
		400	102.79	5.26	5.12	2.79	

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Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
		1000	119.60	7.12	5.95	19.60	
4-AcO-MET	5.98	200	103.93	12.29	11.83	3.93	200
		500	108.39	13.17	12.15	8.39	
		1000	98.59	4.33	4.39	−1.41	
4-APB	6.71	10	92.02	8.55	9.29	−7.98	10
		400	86.69	6.36	7.34	−13.31	
		1000	104.74	7.87	7.51	4.74	
4-APDB	5.57	10	84.42	11.23	13.31	−15.58	10
		400	83.69	9.51	11.36	−16.31	
		1000	101.62	13.89	13.67	1.62	
4-BROMO-2.5-DMMA	8.37	10	92.32	14.14	15.32	−7.68	10
		200	107.51	11.46	10.66	7.51	
		500	118.50	11.20	9.50	18.50	
		1000	91.03	6.62	7.27	−8.97	
4-BROMOAMPHETAMINE	7.46	10	84.70	13.90	16.40	−15.30	10
		200	99.46	8.47	8.52	−0.54	
		500	113.77	6.16	5.41	13.77	
		1000	91.16	6.04	6.62	−8.84	
4-BROMOMETHAMPHETAMINE	7.41	10	85.10	12.70	14.90	−14.90	10
		200	85.10	12.70	14.90	−14.90	
		500	114.93	13.12	11.42	14.93	
		1000	89.53	4.54	5.07	−10.47	
4-BROMOMETHCATHINONE (BREFEDRONE)	6.69	10	115.62	14.26	12.34	15.62	10
		200	107.91	7.08	6.56	7.91	
		500	110.16	11.08	10.06	10.16	
		1000	88.88	1.92	2.16	−11.12	
4-CAB	8.00	10	80.55	4.92	6.10	−19.45	10
		400	81.18	5.81	7.16	−18.82	
		1000	79.33	6.52	8.22	−20.67	
4-CEC	6.68	10	95.82	23.07	24.08	−4.18	10
		400	82.61	7.76	9.39	−17.39	
		1000	94.72	10.50	11.09	−5.28	
4-CHLORO-ALPHA-PPP	6.89	10	85.73	6.80	7.93	−14.27	10
		400	92.89	11.63	12.52	−7.11	
		1000	99.37	8.63	8.69	−0.63	
4-CHLOROAMPHETAMINE	6.96	10	85.62	10.06	11.75	−14.38	10
		400	82.61	3.56	4.31	−17.39	
		1000	93.40	11.81	12.64	−6.60	
4-CHLOROMETHCATHINONE (4-CMC)	6.20	10	85.47	13.76	16.10	−14.53	10
		200	96.39	5.52	5.72	−3.61	
		500	107.30	7.50	7.00	7.30	
		1000	92.73	6.65	7.17	−7.27	
4-CMA	7.08	10	100.57	4.41	4.38	0.57	10
		400	83.64	8.18	9.78	−16.36	
		1000	86.04	8.20	9.53	−13.96	
4-EAPB	7.36	10	91.53	7.28	7.96	−8.47	10
		400	83.53	9.13	10.93	−16.47	
		1000	85.27	7.54	8.84	−14.73	
4-ETHYL-N.*N*-DMC	7.53	10	91.92	9.61	10.45	−8.08	10
		400	89.69	12.26	13.67	−10.31	
		1000	90.45	4.96	5.48	−9.55	
4-FEC	5.00	10	93.59	7.88	8.42	−6.41	10
		400	86.43	6.01	6.96	−13.57	
		1000	96.42	2.29	2.38	−3.58	
4-FLUORO BUPHEDRONE	5.77	10	93.43	13.30	14.24	−6.57	10
		400	83.21	5.70	6.84	−16.79	
		1000	98.76	2.74	2.78	−1.24	
4-FLUORO PENTEDRONE	7.22	10	97.79	8.80	9.00	−2.21	10
		400	85.21	9.27	10.88	−14.79	
		1000	87.56	7.55	8.62	−12.44	
4-FLUORO PV8	10.02	10	103.42	5.58	5.39	3.42	10
		400	99.36	6.75	6.79	−0.64	
		1000	101.30	8.85	8.74	1.30	
4-FLUORO PV9	11.04	10	98.17	6.38	6.50	−1.83	10
		400	87.86	4.89	5.56	−12.14	
		1000	75.27	3.07	4.08	−24.73	
4-FLUORO-ALFA-PPP	5.36	10	95.12	8.06	8.47	−4.88	10
		400	89.68	5.11	5.70	−10.32	
		1000	97.01	7.72	7.96	−2.99	
4-FLUOROMETHAMPHETAMINE (4-FMA)	5.38	10	85.40	4.50	5.30	−14.60	10
		200	101.12	6.98	6.90	1.12	
		500	106.98	8.94	8.36	6.98	
		1000	95.29	3.28	3.44	−4.71	
4-FLUOROMETHCATHINONE (4-FMC)	4.42	10	110.24	16.19	14.69	10.24	10

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Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
		200	99.70	5.95	5.97	−0.30	
		500	112.96	13.98	12.37	12.96	
		1000	92.71	5.36	5.78	−7.29	
4F-PVP	7.63	10	99.80	9.50	9.52	−0.20	10
		200	111.16	7.46	6.71	11.16	
		500	114.20	8.80	7.70	14.20	
		1000	102.91	3.35	3.26	2.91	
4-HYDROXY DiPT	6.46	10	86.86	4.95	5.70	−13.14	10
		200	86.74	4.61	5.32	−13.26	
		500	104.78	5.37	5.12	4.78	
		1000	87.17	4.93	5.65	−12.83	
4-HYDROXYMIDAZOLAM	8.88	10	92.86	14.18	15.28	−7.14	10
		200	101.81	3.88	3.81	1.81	
		500	117.40	11.80	10.10	17.40	
4-IODOAMPHETAMINE	8.22	10	84.23	11.87	14.09	−15.77	10
		400	87.08	11.32	12.99	−12.92	
		1000	94.91	6.51	6.86	−5.09	
4-MAPB	6.87	10	89.51	8.10	9.05	−10.49	10
		400	88.05	6.60	7.49	−11.95	
		1000	91.47	2.99	3.27	−8.53	
4-MEAP	8.58	10	91.82	12.12	13.20	−8.18	10
		400	90.34	6.33	7.01	−9.66	
		1000	95.19	7.30	7.66	−4.81	
4-MEO-ALPHA-PVP	8.05	10	97.04	9.05	9.33	−2.96	10
		400	91.76	6.27	6.84	−8.24	
		1000	97.93	7.56	7.72	−2.07	
4-MeOPBP	6.92	10	96.77	8.31	8.59	−3.23	10
		400	88.08	11.79	13.38	−11.92	
		1000	97.11	10.21	10.52	−2.89	
4-METHOXY PHENCYCLIDINE	8.94	10	105.66	10.20	9.65	5.66	10
		400	95.94	6.96	7.25	−4.06	
		1000	97.57	7.19	7.37	−2.43	
4-METHOXY PV8	10.19	10	100.43	8.52	8.48	0.43	10
		400	94.83	6.40	6.74	−5.17	
		1000	91.15	6.77	7.43	−8.85	
4-METHOXY PV9	11.14	10	105.86	6.70	6.33	5.86	10
		400	97.59	6.67	6.83	−2.41	
		1000	90.63	3.83	4.23	−9.37	
4-METHOXYMETHAMPHETAMINE (PMMA)	5.67	10	117.31	18.12	15.45	17.31	10
		200	112.53	4.13	3.67	12.53	
		500	116.22	9.76	8.40	16.22	
		1000	100.84	5.28	5.24	0.84	
4-METHYL PENTEDRONE	8.30	10	99.96	8.04	8.04	−0.04	10
		400	87.25	3.46	3.97	−12.75	
		1000	96.23	9.15	9.51	−3.77	
4-METHYL-ALPHA-ETHYLAMINOBUTIOPHENONE	7.44	10	101.56	7.20	7.09	1.56	10
		400	86.28	5.96	6.91	−13.72	
		1000	90.67	6.63	7.32	−9.33	
4-METHYLAMPHETAMINE	6.72	10	86.01	15.75	18.32	−14.00	10
		400	81.62	9.54	11.69	−18.38	
		1000	95.91	6.31	6.58	−4.09	
4-METHYLCATHINONE	5.70	10	110.08	17.39	15.80	10.08	10
		200	102.56	5.10	4.97	2.56	
		500	115.60	12.20	10.60	15.60	
		1000	88.45	3.44	3.89	−11.55	
4-METHYLMETHAMPHETAMINE (4-MMA)	6.87	10	95.20	18.00	18.90	−4.80	10
		200	91.61	11.15	12.17	−8.39	
		500	105.25	11.10	10.54	5.25	
		1000	95.41	7.43	7.79	−4.59	
4-METHYLMETHCATHINONE (4-MMC)	6.00	10	106.39	12.19	11.46	6.39	10
		200	92.10	8.40	9.10	−7.90	
		500	117.80	6.90	5.90	17.80	
		1000	91.30	6.20	6.80	−8.70	
4-METHYL-N.*N*-DMC	6.04	10	81.17	8.64	10.65	−18.83	10
		400	87.09	5.37	6.17	−12.91	
		1000	94.37	12.84	13.60	−5.63	
4-METHYL-*N*-METHYLBUPHEDRONE	7.10	10	98.21	13.20	13.44	−1.80	10
		400	84.18	8.39	9.97	−15.82	
		1000	93.50	11.45	12.25	−6.50	
4-METHYL-*N*-METHYLHEXANOPHENONE	9.44	10	92.73	11.74	12.67	−7.27	10
		400	92.36	3.82	4.14	−7.64	
		1000	94.79	8.44	8.90	−5.21	
4-METHYL-PHP	9.63	10	101.66	5.94	5.84	1.65	10
		400	94.85	9.22	9.72	−5.15	

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Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
		1000	91.34	8.35	9.14	−8.66	
4-METHYL-α-ETHYLTRYPTAMINE	8.40	10	82.50	7.80	9.50	−17.50	10
		200	101.70	6.79	6.68	1.70	
		500	117.30	12.00	10.20	17.30	
		1000	92.15	9.89	10.73	−7.85	
5-APB	7.02	10	81.90	6.30	7.70	−18.10	10
		200	91.35	7.05	7.71	−8.65	
		500	105.18	5.94	5.65	5.18	
		1000	86.93	5.87	6.76	−13.07	
5-APDB	5.65	10	101.64	13.21	13.00	1.64	10
		200	112.18	12.00	10.70	12.18	
		500	106.24	6.36	5.99	6.24	
		1000	105.36	2.55	2.42	5.36	
5-APDI	8.75	10	82.04	15.88	19.36	−17.96	10
		400	96.37	5.67	5.89	−3.63	
		1000	98.63	11.90	12.06	−1.37	
5-CHLORO AB-PINACA	13.00	2	112.17	12.76	11.37	12.17	2
		200	82.70	10.00	12.09	−17.30	
5-CHLORO-NNEI	14.10	2	89.76	14.37	16.01	−10.24	2
		200	117.12	17.94	15.32	17.12	
5-EAPB	7.21	10	113.21	21.04	18.59	13.21	10
		200	95.33	6.58	6.90	−4.67	
		500	105.70	17.71	16.76	5.70	
		1000	89.86	4.51	5.02	−10.14	
5F-ABICA	12.12	2	108.78	13.25	12.18	8.77	2
		200	95.03	5.02	5.28	−4.98	
5F-AB-PINACA	12.30	2	94.98	16.18	17.04	−5.02	2
		200	87.03	4.37	5.03	−12.97	
5F-ADB (5F-MDMB-PINACA)	14.07	2	115.00	12.25	10.65	15.00	2
		200	119.71	7.88	6.58	19.71	
5F-AMB (5F-AMB-PINACA)	13.55	2	115.09	10.98	9.54	15.09	2
		200	92.69	1.68	1.81	−7.31	
5F-APICA (STS-135)	15.03	2	118.31	8.63	7.29	18.31	2
		200	117.78	4.31	3.66	17.78	
5F-APINACA (AKB-48-5F)	15.49	2	119.35	7.18	6.02	19.35	2
		200	109.20	6.09	5.58	9.20	
5-F-JWH-018 ADAMANTYL ANALOG	15.30	2	116.50	12.06	10.35	16.50	2
		200	85.39	4.10	4.80	−14.61	
5-FLUORO MN-24 (5-FLUORO NNEI)	13.59	2	107.61	11.99	11.14	7.61	2
		200	84.68	3.76	4.43	−15.32	
5-FLUORO THJ	15.13	2	84.99	11.52	13.55	−15.01	2
		200	96.44	8.41	8.72	−3.56	
5-FLUORO-2-ADB-PINACA_ISOMER_2	12.31	2	102.77	13.88	13.51	2.77	2
		200	94.10	4.98	5.30	−5.90	
5-FLUORO-CUMYL-PICA	13.79	2	83.42	5.73	6.87	−16.58	2
		200	103.22	12.97	12.56	3.22	
5-FLUORO-MN-18	14.64	2	119.64	19.01	15.89	19.64	2
		200	119.82	4.02	3.35	19.82	
5-FLUORO-MN-21 (5-FLUORO-PCN)	9.94	2	96.11	10.28	10.70	−3.89	2
		200	96.15	12.38	12.88	−3.85	
5-FLUORO-SDB-006	13.05	2	99.27	11.93	12.02	−0.73	2
		200	96.89	4.65	4.80	−3.11	
5F-NPB-22	14.06	2	117.00	6.71	5.73	17.00	2
		200	116.77	6.94	5.95	16.77	
5F-PB-22	13.66	2	112.74	12.26	10.87	12.74	2
		200	93.46	3.05	3.26	−6.54	
5-F-PENTYL-3-PYRIDINOYLINDOLE	12.13	2	96.76	11.89	12.28	−3.24	2
		200	95.33	8.03	8.42	−4.67	
5F-SDB-005	14.79	2	109.65	14.88	13.57	9.65	2
		200	103.60	10.45	10.08	3.60	
5-HYDROXY DMT	2.95	10	80.64	8.15	10.10	−19.36	10
		200	92.90	8.60	9.20	−7.10	
		500	114.80	6.40	5.60	14.80	
		1000	87.30	3.70	4.20	−12.70	
5-IT	5.06	10	94.21	16.91	17.95	−5.79	10
		200	101.69	3.53	3.47	1.69	
		500	107.98	10.36	9.59	7.98	
		1000	87.71	5.53	6.30	−12.29	
5-MAPB	6.69	10	104.99	17.13	16.32	4.99	10
		200	109.30	5.14	4.71	9.30	
		500	114.91	12.88	11.21	14.91	
		1000	91.75	3.98	4.34	−8.25	
5-MAPDB	5.70	10	88.72	12.63	14.24	−11.28	10
		400	86.49	5.27	6.09	−13.51	

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Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
		1000	97.36	11.44	11.75	−2.64	
5-MeO-ALPHA-ET	7.08	10	93.97	14.10	15.01	−6.03	10
		400	92.59	7.55	8.16	−7.41	
		1000	96.26	9.30	9.66	−3.74	
5-MeO-DALT	7.31	10	93.52	11.50	12.30	−6.49	10
		200	91.86	6.62	7.21	−8.14	
		500	117.29	5.75	4.90	17.29	
		1000	88.50	4.46	5.04	−11.50	
5-METHOXY AMT	5.99	10	99.11	13.29	13.41	−0.89	10
		200	101.24	7.35	7.26	1.24	
		500	115.72	7.32	6.33	15.72	
		1000	87.36	2.57	2.94	−12.64	
5-METHOXY DiPT	7.30	10	105.80	5.89	5.56	5.80	10
		200	101.69	7.91	7.78	1.69	
		500	117.02	8.73	7.46	17.02	
		1000	91.24	1.78	1.96	−8.76	
5-METHOXY DMT	5.31	10	93.05	10.08	10.83	−6.96	10
		200	91.93	12.66	13.78	−8.07	
		500	114.23	11.86	10.38	14.23	
		1000	90.83	5.17	5.70	−9.17	
5-METHOXY METHYLONE	5.56	10	101.47	9.23	9.09	1.47	10
		400	92.19	7.41	8.03	−7.81	
		1000	100.93	8.21	8.13	0.93	
5-METHOXY MiPT	6.31	10	91.85	18.16	19.78	−8.15	10
		200	91.71	6.49	7.08	−8.29	
		500	118.10	2.20	1.90	18.10	
		1000	95.19	6.83	7.18	−4.81	
6-APB	6.50	10	80.81	9.86	12.21	−19.20	10
		200	110.34	10.31	9.35	10.34	
		500	112.25	10.05	8.95	12.25	
		1000	106.34	10.88	10.23	6.34	
6-APDB	5.82	10	88.26	19.76	22.39	−11.74	10
		400	86.35	11.23	13.00	−13.65	
		1000	87.59	10.90	12.44	−12.41	
6-BROMO-MDMA	7.50	10	93.83	15.58	16.61	−6.17	10
		400	87.92	10.04	11.42	−12.08	
		1000	82.73	5.31	6.41	−17.27	
6-CHLORO-MDMA	7.09	10	86.81	8.97	10.34	−13.19	10
		400	84.98	4.28	5.04	−15.02	
		1000	86.92	7.99	9.20	−13.08	
6-EAPB	7.08	10	87.65	15.21	17.36	−12.35	10
		400	93.66	9.56	10.21	−6.34	
		1000	93.94	8.06	8.58	−6.06	
6-IT	5.88	10	92.18	15.82	17.16	−7.82	10
		400	82.48	6.98	8.47	−17.52	
		1000	81.27	8.33	10.25	−18.73	
6-MAM	5.18	10	90.61	15.28	16.86	−9.39	10
		200	94.69	7.56	7.98	−5.31	
		500	115.10	4.40	3.90	15.10	
		1000	89.85	1.03	1.15	−10.15	
6-MAPB	6.59	10	85.98	17.42	20.26	−14.02	10
		400	82.92	6.40	7.72	−17.08	
		1000	91.90	7.09	7.71	−8.10	
7-AMINOCLONAZEPAM	6.64	10	109.83	21.10	19.21	9.83	10
		200	99.71	8.35	8.38	−0.29	
		500	93.60	8.78	9.38	−6.40	
		1000	89.81	6.94	7.73	−10.19	
7-AMINODESMETHYLFLUNITRAZEPAM	5.65	10	112.18	17.38	15.49	12.18	10
		200	102.75	7.84	7.63	2.75	
		500	98.16	11.66	11.88	−1.84	
		1000	94.60	6.00	6.34	−5.40	
7-AMINOFLUNITRAZEPAM	7.67	10	92.14	3.40	3.70	−7.86	10
		200	90.72	8.68	9.56	−9.28	
		500	107.07	12.04	11.24	7.07	
		1000	94.59	10.97	11.60	−5.41	
7-AMINONITRAZEPAM	4.69	10	103.06	11.42	11.08	3.06	10
		200	87.37	6.66	7.62	−12.63	
		500	97.94	8.71	8.89	−2.06	
		1000	86.55	5.04	5.82	−13.45	
7-APB	6.69	10	108.06	15.83	14.65	8.06	10
		400	105.41	7.30	6.93	5.41	
		1000	81.60	6.97	8.54	−18.40	
7-APDB	7.45	10	110.14	16.34	14.84	10.14	10
		400	96.21	7.80	8.11	−3.79	

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Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
		1000	109.03	3.34	3.06	9.03	
A-796260	11.67	2	97.78	15.23	15.58	−2.22	2
		200	86.49	5.11	5.91	−13.51	
A-834735	14.21	2	104.88	8.16	7.78	4.88	2
		200	118.38	4.91	4.14	18.38	
A-836339	12.49	2	102.20	9.94	9.72	2.20	2
		200	90.10	2.76	3.07	−9.90	
AB-001	16.12	2	87.38	7.18	8.22	−12.62	2
		200	87.19	2.65	3.04	−12.81	
AB005	11.45	2	90.95	17.18	18.89	−9.05	2
		200	82.47	8.83	10.71	−17.53	
AB-CHMINACA	14.15	2	89.17	17.15	19.24	−10.83	2
		200	118.82	5.11	4.30	18.82	
AB-FUBINACA	12.68	2	83.41	8.26	9.90	−16.59	2
		200	92.23	7.31	7.93	−7.77	
AB-FUBINACA 2-FLUOROBENZYL ISOMER	12.86	2	92.77	7.79	8.40	−7.23	2
		200	94.68	4.69	4.95	−5.32	
		2	93.13	15.23	16.36	−6.88	2
		200	93.86	2.89	3.08	−6.14	
AB-PINACA	13.54	2	112.32	11.50	10.24	12.32	2
		200	101.65	3.14	3.09	1.65	
ADB-FUBINACA	13.32	2	112.99	20.65	18.28	12.99	2
		200	87.59	4.15	4.74	−12.41	
ADB-PINACA	14.09	2	95.11	10.10	10.62	−4.89	2
		200	117.39	6.70	5.71	17.39	
ADB-PINACA ISOMER_1	13.69	2	98.16	10.31	10.51	−1.84	2
		200	102.34	9.59	9.37	2.34	
ADB-PINACA ISOMER_2	13.99	2	118.47	20.43	17.24	18.47	2
		200	111.55	6.11	5.48	11.55	
ADB-PINACA ISOMER_3	14.09	2	92.92	8.16	8.79	−7.08	2
		200	111.86	7.19	6.43	11.86	
ADB-PINACA ISOMER_4	14.00	2	98.22	10.19	10.37	−1.78	2
		200	111.55	6.11	5.48	11.55	
AH-7921	9.77	10	81.00	8.90	11.00	−19.00	10
		200	93.12	8.10	8.70	−6.88	
		500	118.10	13.90	11.80	18.10	
		1000	89.61	3.21	3.58	−10.39	
AKB48_N-(4-FLUOROBENZYL)_ANALOG	15.66	2	91.24	15.57	17.07	−8.76	2
		200	86.73	7.08	8.17	−13.27	
ALFA-ETHYLAMINOPENTIOPHENONE	7.14	10	99.74	14.92	14.96	−0.26	10
		200	95.38	8.19	8.59	−4.62	
		500	113.70	6.00	5.30	13.70	
		1000	95.78	6.07	6.34	−4.22	
ALFA-PROPYLAMINOPENTIOPHENONE	7.88	10	104.60	19.41	18.56	4.60	10
		200	93.96	7.97	8.48	−6.04	
		500	104.59	10.55	10.09	4.59	
		1000	95.56	5.71	5.97	−4.44	
ALLYLESCALINE	6.96	10	87.18	15.71	18.02	−12.82	10
		400	87.11	6.24	7.16	−12.89	
		1000	101.26	12.86	12.70	1.26	
ALPHA-DIMETHYLAMINOPENTIOPHENONE	6.87	10	107.73	8.09	7.51	7.73	10
		400	88.53	7.36	8.32	−11.47	
		1000	85.68	11.11	12.96	−14.32	
ALPHA-ETHYLAMINOHEXANOPHENONE	8.42	10	96.99	10.03	10.34	−3.01	10
		400	90.49	9.97	11.02	−9.51	
		1000	94.97	9.18	9.66	−5.03	
ALPHA-ETHYLTRYPTAMINE	7.15	10	91.42	11.90	13.01	−8.58	10
		200	101.11	9.20	9.09	1.11	
		500	111.72	12.34	11.04	11.72	
		1000	90.23	5.37	5.96	−9.77	
ALPHA-METHYLTRYPTAMINE	5.74	10	96.01	11.55	12.03	−3.99	10
		200	100.82	9.87	9.79	0.82	
		500	118.10	14.10	11.90	18.10	
		1000	94.35	6.04	6.40	−5.65	
ALPHA-PHP	8.44	10	106.39	8.70	8.18	6.39	10
		400	96.38	6.03	6.26	−3.62	
		1000	98.09	6.69	6.82	−1.91	
ALPHA-PHTALIMIDOPROPIOPHENONE	11.77	10	114.12	7.19	6.30	14.12	10
		400	90.07	5.29	5.87	−9.93	
		1000	82.69	3.94	4.77	−17.31	
ALPHA-PIPBP	6.52	10	90.50	8.24	9.10	−9.50	10
		400	83.38	7.92	9.50	−16.62	
		1000	94.09	9.69	10.30	−5.91	
ALPHA-PPP	5.05	10	90.85	7.64	8.41	−9.15	10

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Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
		400	84.54	2.96	3.50	−15.46	
		1000	98.35	4.17	4.24	−1.65	
ALPHA-PVP	7.27	10	106.21	20.58	19.37	6.21	10
		200	97.61	7.06	7.24	−2.39	
		500	111.42	11.95	10.73	11.42	
		1000	96.68	6.69	6.92	−3.32	
ALPHA-PVT	6.38	10	96.81	13.63	14.08	−3.20	10
		200	96.55	6.67	6.91	−3.45	
		500	118.20	8.50	7.20	18.20	
		1000	94.62	3.22	3.40	−5.38	
ALPHA-PYRROLIDINOBUTHIOPHENONE	5.00	10	96.45	4.73	4.90	−3.55	10
		400	91.87	3.41	3.71	−8.13	
		1000	102.37	6.27	6.12	2.37	
ALPRAZOLAM	11.44	10	82.34	12.47	15.15	−17.67	10
		200	88.80	5.49	6.18	−11.20	
		500	99.71	8.15	8.18	−0.29	
		1000	84.63	3.69	4.36	−15.37	
AM1220	10.52	2	102.44	9.62	9.39	2.44	2
		200	81.35	6.29	7.73	−18.65	
AM-1248	12.14	2	96.27	12.28	12.76	−3.73	2
		200	90.02	5.99	6.66	−9.98	
AM-2201	14.21	2	83.11	7.94	9.56	−16.89	2
		200	119.43	6.38	5.34	19.43	
AM2201 8-QUINOLINYL CARBOXAMIDE	15.00	2	104.32	15.01	14.39	4.32	2
		200	90.20	4.91	5.44	−9.80	
AM2201 BENZIMIDAZOLE ANALOG	14.45	2	119.33	8.74	7.33	19.33	2
		200	117.57	7.04	5.99	17.57	
AM2232	12.76	2	93.92	8.73	9.29	−6.08	2
		200	93.06	11.06	11.88	−6.94	
AMITRIPTYLINE	10.92	10	89.10	10.50	11.70	−10.90	10
		200	96.33	9.20	9.55	−3.67	
		500	108.03	7.78	7.20	8.03	
		1000	90.48	8.09	8.94	−9.52	
AMPHETAMINE	4.76	10	91.50	17.07	18.66	−8.50	10
		200	111.48	8.63	7.74	11.48	
		500	103.38	8.49	8.21	3.38	
		1000	104.11	8.58	8.24	4.11	
ATENOLOL	3.99	10	104.20	16.92	16.24	4.20	10
		200	108.80	7.40	6.80	8.80	
		500	99.30	4.67	4.71	−0.70	
		1000	100.30	13.20	13.10	0.30	
AZACYCLONOL	8.71	10	98.88	12.62	12.77	−1.13	10
		400	97.96	3.43	3.50	−2.04	
		1000	91.14	4.24	4.65	−8.86	
BB-22	15.12	2	112.55	20.45	18.17	12.55	2
		200	97.84	2.60	2.66	−2.16	
BDB	6.10	10	95.00	15.03	15.82	−5.00	10
		200	115.36	12.38	10.73	15.36	
		500	118.27	9.82	8.31	18.27	
		1000	92.12	6.19	6.71	−7.88	
BENOCYCLIDINE	10.63	10	80.52	4.69	5.82	−19.48	10
		400	81.71	3.42	4.19	−18.29	
		1000	91.05	5.12	5.62	−8.95	
BENZEDRONE	9.16	10	93.77	10.64	11.35	−6.23	10
		400	81.98	6.02	7.35	−18.02	
		1000	75.94	3.57	4.70	−24.06	
BENZOCAINE	8.92	10	103.92	10.74	10.34	3.92	10
		200	110.12	5.25	4.77	10.12	
		500	99.72	5.83	5.84	−0.28	
		1000	100.08	5.49	5.48	0.08	
BENZOYLECGONINE	6.69	10	119.61	15.19	12.70	19.61	10
		200	108.61	5.38	4.95	8.61	
		500	106.12	10.94	10.31	6.12	
		1000	89.18	5.67	6.35	−10.82	
BENZYDAMINE	10.28	10	88.98	9.14	10.27	−11.02	10
		200	109.10	6.10	5.59	9.10	
		500	114.23	9.32	8.15	14.23	
		1000	94.85	3.95	4.16	−5.15	
bk-2C-B	7.37	10	92.20	12.94	14.03	−7.80	10
		200	92.31	8.82	9.55	−7.69	
		500	114.90	18.30	16.00	14.90	
		1000	90.35	9.36	10.36	−9.65	
bk-MDA	4.26	10	87.47	9.24	10.57	−12.54	10
		400	90.62	4.47	4.93	−9.38	

(*continued on next page*)

Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
		1000	99.48	5.69	5.71	−0.52	
BMPEA	4.89	10	100.45	13.35	13.29	0.45	10
		400	82.77	6.44	7.78	−17.23	
		1000	88.15	4.46	5.06	−11.85	
BROMO-DRAGON-FLY	10.05	10	97.56	15.67	16.06	−2.44	10
		400	98.81	5.21	5.27	−1.19	
		1000	94.73	6.77	7.15	−5.27	
BUPRENORPHINE	9.65	10	97.69	16.93	17.33	−2.31	10
		400	85.48	2.54	2.97	−14.52	
		1000	94.25	8.99	9.54	−5.75	
BUPROPION	8.08	10	96.88	10.68	11.02	−3.12	10
		200	102.23	11.13	10.88	2.23	
		500	119.10	7.72	6.49	19.10	
		1000	94.33	7.90	8.38	−5.67	
BUTYLONE (bk-MBDB)	5.86	10	104.99	12.63	12.03	4.99	10
		200	109.66	8.01	7.31	9.66	
		500	117.80	3.50	3.00	17.80	
		1000	95.56	4.06	4.25	−4.44	
CAMFETAMINE	8.23	10	95.84	5.51	5.74	−4.16	10
		400	90.92	9.31	10.24	−9.08	
		1000	99.64	15.84	15.90	−0.36	
CANNABIDIOL	15.07	2	115.46	20.14	17.44	15.46	2
		200	94.45	11.32	11.98	−5.55	
CARBAMAZEPINE	10.56	10	118.12	15.29	12.95	18.12	10
		200	117.40	7.20	6.10	17.40	
		500	113.46	11.74	10.35	13.46	
		1000	85.25	1.84	2.15	−14.75	
CATHINE	3.65	10	86.04	15.24	17.71	−13.96	10
		200	89.53	7.40	8.26	−10.47	
		500	103.09	1.37	1.33	3.09	
		1000	88.69	2.90	3.27	−11.31	
CATHINONE	3.74	10	92.69	11.29	12.18	−7.31	10
		200	91.15	7.08	7.77	−8.85	
		500	109.58	2.20	2.01	9.58	
		1000	89.86	2.55	2.84	−10.14	
CB-13	16.51	2	81.43	13.46	16.53	−18.58	2
		200	89.63	9.67	10.79	−10.37	
CBL-018	15.81	2	99.66	9.22	9.25	−0.34	2
		200	81.04	6.35	7.83	−18.96	
CI2201	14.97	10	112.01	11.01	9.83	12.01	10
		400	87.87	11.13	12.67	−12.13	
		1000	82.73	5.39	6.51	−17.27	
CLOBAZAM	11.16	10	94.90	14.59	15.38	−5.10	10
		200	97.69	6.16	6.31	−2.31	
		500	113.80	14.38	12.63	13.80	
		1000	102.82	4.37	4.25	2.82	
CLOMIPRAMINE	11.65	10	80.90	3.90	4.90	−19.10	10
		200	101.08	8.82	8.73	1.08	
		500	111.39	8.61	7.73	11.39	
		1000	86.50	2.89	3.34	−13.50	
CLONAZEPAM	10.79	10	85.46	3.95	4.62	−14.55	10
		200	93.28	3.19	3.42	−6.72	
		500	110.44	11.14	10.08	10.44	
		1000	84.60	3.46	4.09	−15.40	
COCAETHYLENE	8.15	10	103.96	13.76	13.24	3.96	10
		200	110.37	7.10	6.43	10.37	
		500	117.10	9.20	7.80	17.10	
		1000	103.22	3.77	3.66	3.22	
COCAINE	7.19	10	117.87	13.29	11.28	17.87	10
		200	110.60	4.30	3.89	10.60	
		500	119.80	12.50	10.40	19.80	
		1000	97.75	6.61	6.77	−2.25	
CODEINE	4.45	10	119.15	23.28	19.54	19.15	10
		200	99.03	8.75	8.84	−0.97	
		500	99.40	8.90	9.00	−0.60	
		1000	93.75	4.11	4.38	−6.25	
CUMYL-PICA	14.70	2	117.77	13.73	11.66	17.77	2
		200	119.56	4.13	3.45	19.56	
D2PM	7.98	10	84.47	6.59	7.80	−15.53	10
		400	82.67	11.96	14.46	−17.33	
		1000	80.79	2.14	2.65	−19.21	
DEMOXEPAM	10.25	10	93.44	13.40	14.34	−6.56	10
		200	102.36	3.77	3.68	2.36	
		500	109.50	8.85	8.08	9.50	

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Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
		1000	91.97	2.66	2.89	−8.03	
DESALKYLFLURAZEPAM	11.64	10	80.21	13.19	16.44	−19.79	10
		200	105.72	12.38	11.71	5.72	
		500	104.46	12.79	12.24	4.46	
		1000	88.22	6.65	7.54	−11.78	
DESCHLOROETIZOLAM	11.50	10	96.49	7.10	7.36	−3.52	10
		200	103.97	6.83	6.57	3.97	
		500	105.08	9.28	8.83	5.08	
		1000	96.76	6.97	7.20	−3.24	
DESCHLORO-*N*-ETHYL-KETAMINE	6.23	10	92.71	8.69	9.38	−7.29	10
		400	80.21	5.98	7.46	−19.79	
		1000	89.25	9.27	10.39	−10.75	
DESIPRAMINE	10.75	10	87.76	12.08	13.76	−12.24	10
		200	112.04	11.14	9.95	12.04	
		500	109.52	5.13	4.68	9.52	
		1000	86.88	5.43	6.25	−13.12	
DESMETHYLDIAZEPAM (NORDIAZEPAM)	11.95	10	96.60	12.83	13.28	−3.40	10
		200	93.20	3.13	3.36	−6.80	
		500	97.90	6.63	6.77	−2.10	
		1000	85.82	3.88	4.53	−14.18	
DESMETHYLFLUNITRAZEPAM	10.38	10	84.40	7.90	9.30	−15.60	10
		200	97.39	4.09	4.20	−2.61	
		500	115.18	13.46	11.69	15.18	
		1000	88.40	2.79	3.16	−11.60	
DESOMORPHINE	5.21	10	98.99	18.81	19.01	−1.01	10
		200	92.87	6.70	7.22	−7.13	
		500	114.18	12.27	10.75	14.18	
		1000	88.72	6.37	7.18	−11.28	
DESOXY-D2PM	8.70	10	95.98	9.85	10.26	−4.02	10
		400	94.15	8.28	8.79	−5.85	
		1000	96.56	7.01	7.26	−3.44	
DESOXYPIPRADROL (2-DPMP)	9.09	10	112.74	21.76	19.30	12.74	10
		200	100.20	4.35	4.34	0.20	
		500	119.12	9.72	8.16	19.12	
		1000	88.90	3.75	4.22	−11.10	
DEXTROMETHORPHAN	9.31	10	84.85	15.24	17.97	−15.15	10
		200	101.78	8.50	8.35	1.78	
		500	117.80	7.60	6.50	17.80	
		1000	93.77	5.15	5.49	−6.23	
DIAZEPAM	12.36	10	97.22	11.66	11.99	−2.78	10
		200	95.89	3.63	3.79	−4.11	
		500	92.77	9.37	10.10	−7.23	
		1000	101.34	5.16	5.09	1.34	
DICLAZEPAM	12.38	10	97.70	14.30	14.63	−2.30	10
		200	95.48	5.52	5.78	−4.52	
		500	88.96	7.11	8.00	−11.04	
		1000	101.04	4.19	4.14	1.04	
DICLOFENSINE	11.05	10	86.61	7.66	8.84	−13.39	10
		400	83.84	7.78	9.28	−16.16	
		1000	85.67	8.01	9.35	−14.33	
DIETHYLCATHINONE (AMFEPRAMONE)	5.40	10	89.47	9.80	10.95	−10.53	10
		200	92.86	5.03	5.41	−7.14	
		500	115.28	13.79	11.96	15.28	
		1000	95.10	4.77	5.02	−4.90	
DIHYDROCODEINE	4.38	10	101.27	13.48	13.32	1.27	10
		200	97.23	7.86	8.09	−2.77	
		500	117.59	18.63	15.84	17.59	
		1000	92.37	4.62	5.00	−7.63	
DIMETHOCAINE	6.33	10	83.33	13.43	16.11	−16.67	10
		200	105.44	6.55	6.22	5.44	
		500	112.80	7.00	6.20	12.80	
		1000	94.09	4.49	4.77	−5.91	
DIMETHYLONE (bk-MDDMA)	4.90	10	92.32	11.48	12.43	−7.68	10
		200	99.81	11.14	11.16	−0.19	
		500	117.60	9.60	8.10	17.60	
		1000	101.11	3.15	3.12	1.11	
DIPHENHYDRAMINE	9.34	10	90.88	8.49	9.35	−9.12	10
		200	105.42	3.54	3.36	5.42	
		500	118.64	9.82	8.28	18.64	
		1000	98.28	5.30	5.39	−1.72	
DIPHENIDINE	8.79	10	100.88	11.34	11.24	0.88	10
		200	111.13	2.40	2.16	11.13	
		500	118.40	6.30	5.30	18.40	
		1000	96.42	2.12	2.20	−3.58	

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Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
DiPT	7.77	10	96.63	10.47	10.84	−3.37	10
		200	101.61	5.48	5.39	1.61	
		500	114.29	10.37	9.08	14.29	
		1000	95.04	6.61	6.96	−4.96	
DL-4662	7.34	10	114.55	21.64	18.89	14.55	10
		400	95.17	15.44	16.22	−4.83	
		1000	100.02	4.54	4.54	0.02	
DOI	8.97	10	95.89	8.39	8.75	−4.11	10
		200	98.35	7.46	7.58	−1.65	
		500	112.11	13.18	11.76	12.11	
		1000	84.68	4.04	4.77	−15.32	
DOTHIEPIN	10.22	10	88.29	10.89	12.34	−11.71	10
		200	104.97	4.05	3.85	4.97	
		500	112.70	7.12	6.32	12.70	
		1000	96.05	4.72	4.91	−3.95	
DOXEPIN	9.58	10	103.73	10.53	10.16	3.73	10
		200	94.29	8.04	8.53	−5.71	
		500	100.85	10.69	10.60	0.85	
		1000	94.05	3.97	4.22	−5.95	
DOXYLAMINE	6.00	10	95.71	15.24	15.92	−4.29	10
		200	112.29	14.56	12.96	12.29	
		500	107.88	4.28	3.97	7.88	
		1000	119.11	5.24	4.40	19.11	
EAM-2201	14.95	2	111.51	18.40	16.50	11.51	2
		200	88.23	8.54	9.68	−11.77	
EDDP	9.40	10	90.96	10.31	11.34	−9.04	10
		200	108.24	11.89	10.98	8.24	
		500	118.10	11.00	9.30	18.10	
		1000	111.92	5.47	4.88	11.92	
EG-2201	15.66	2	119.17	13.51	11.34	19.17	2
		200	87.71	5.05	5.76	−12.29	
ERGOMETRINE	5.33	10	81.56	5.58	6.84	−18.44	10
		400	81.22	4.93	6.07	−18.78	
		1000	85.98	7.34	8.54	−14.02	
ESTAZOLAM	11.08	10	102.01	20.82	20.41	2.01	10
		200	104.28	12.94	12.41	4.28	
		500	111.97	11.86	10.59	11.97	
		1000	97.20	6.80	7.00	−2.80	
ETAQUALONE	11.97	10	94.40	15.84	16.77	−5.60	10
		200	105.28	5.84	5.55	5.28	
		500	92.05	8.96	9.73	−7.95	
		1000	94.72	6.41	6.76	−5.28	
ETHCATHINONE METABOLITE	4.76	10	103.15	12.62	12.23	3.15	10
		200	98.34	8.26	8.39	−1.66	
		500	113.93	6.29	5.52	13.93	
		1000	90.75	3.89	4.28	−9.25	
ETHYLONE (bk-MDEA)	5.25	10	107.34	9.84	9.17	7.34	10
		200	109.02	5.68	5.21	9.02	
		500	116.14	12.61	10.85	16.14	
		1000	99.27	4.12	4.16	−0.73	
ETHYLPHENIDATE	8.21	10	110.59	7.75	7.01	10.59	10
		200	114.31	6.14	5.37	14.31	
		500	115.10	12.40	10.80	15.10	
		1000	86.68	1.79	2.06	−13.32	
ETIZOLAM	11.80	10	97.91	15.87	16.20	−2.09	10
		200	94.94	8.66	9.12	−5.06	
		500	108.00	17.02	15.76	8.00	
		1000	97.53	4.56	4.67	−2.47	
EUTYLONE (bk-EBDB)	6.28	10	98.15	15.10	15.39	−1.85	10
		200	100.41	6.82	6.80	0.41	
		500	118.42	14.48	12.23	18.42	
		1000	96.84	3.83	3.96	−3.16	
FDU-PB-22	15.25	2	85.20	4.02	4.72	−14.80	2
		200	87.03	5.47	6.29	−12.97	
FENFLURAMINE	8.37	10	110.15	18.56	16.85	10.15	10
		200	112.75	12.95	11.49	12.75	
		500	115.57	6.25	5.41	15.57	
		1000	85.10	3.06	3.60	−14.90	
FENTANYL	8.82	10	86.58	6.67	7.71	−13.42	10
		400	88.80	7.33	8.25	−11.20	
		1000	92.18	3.51	3.81	−7.82	
FLUBROMAZEPAM	11.84	10	89.68	16.21	18.08	−10.32	10
		200	99.06	5.06	5.11	−0.94	
		500	99.74	10.55	10.57	−0.26	

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Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
		1000	94.59	2.78	2.94	−5.41	
FLUDIAZEPAM	12.06	10	86.56	16.47	19.02	−13.44	10
		200	104.58	6.76	6.46	4.58	
		500	110.31	5.08	4.60	10.31	
		1000	99.52	6.75	6.78	−0.48	
FLUMAZENIL	9.30	10	105.88	8.48	8.01	5.88	10
		200	106.79	3.79	3.55	6.79	
		500	118.57	14.48	12.21	18.57	
		1000	89.71	2.85	3.18	−10.29	
FLUNITRAZEPAM	10.90	10	97.23	18.00	18.51	−2.77	10
		200	98.21	4.50	4.58	−1.79	
		500	107.56	5.88	5.46	7.56	
		1000	92.03	5.76	6.26	−7.97	
FLUOXETINE	11.24	10	81.33	8.29	10.20	−18.68	10
		200	100.21	6.64	6.63	0.21	
		500	115.10	8.30	7.20	15.10	
		1000	89.38	3.41	3.82	−10.62	
FLURAZEPAM	9.41	10	104.54	12.93	12.36	4.54	10
		200	103.08	7.30	7.08	3.08	
		500	119.70	9.20	7.70	19.70	
		1000	92.38	2.74	2.96	−7.62	
FUB-144	14.96	2	93.69	16.24	17.34	−6.31	2
		200	82.07	4.11	5.00	−17.93	
FUB-JWH-018	14.47	2	119.08	12.94	10.87	19.08	2
		200	114.38	5.15	4.50	14.38	
FUB-NPB-22	13.66	2	105.43	13.10	12.43	5.43	2
		200	101.05	9.43	9.33	1.05	
FUB-PB-22	15.26	2	96.47	10.91	11.31	−3.53	2
		200	93.28	4.45	4.77	−6.72	
FURANYLFENTANYL (Fu-F)	8.93	10	101.66	15.74	15.48	1.66	10
		200	111.42	8.18	7.34	11.42	
		500	107.89	7.07	6.55	7.89	
		1000	98.18	1.88	1.92	−1.82	
GHB	1.38	10	109.30	6.40	5.90	9.30	10
		500	88.68	14.54	16.40	−11.32	
		1000	81.36	6.08	7.48	−18.64	
HARMALINE	7.45	10	109.95	18.05	16.42	9.95	10
		400	113.46	9.21	8.11	13.46	
		1000	106.30	7.97	7.49	6.30	
HARMINE	8.01	10	95.61	9.80	10.25	−4.40	10
		200	109.10	10.07	9.23	9.10	
		500	115.72	11.30	9.76	15.72	
		1000	89.09	4.56	5.12	−10.91	
HU-210	15.92	2	89.13	9.04	10.14	−10.88	2
		200	89.78	3.14	3.50	−10.22	
HYDROCODONE	4.97	10	110.28	13.92	12.62	10.28	10
		200	92.26	9.54	10.34	−7.74	
		500	119.30	7.40	6.20	19.30	
		1000	92.87	6.98	7.52	−7.13	
IBOGAINE	8.04	10	99.52	12.57	12.63	−0.48	10
		200	87.56	8.53	9.74	−12.44	
		500	108.42	14.35	13.23	8.42	
		1000	90.34	6.56	7.26	−9.66	
IMIPRAMINE	10.61	10	93.85	10.62	11.32	−6.15	10
		200	112.10	4.95	4.42	12.10	
		500	113.11	12.79	11.31	13.11	
		1000	92.13	2.63	2.86	−7.87	
ISOPENTEDRONE	6.85	10	93.27	8.54	9.15	−6.73	10
		200	107.23	4.80	4.48	7.23	
		500	117.20	1.80	1.50	17.20	
		1000	89.78	7.03	7.83	−10.22	
JWH 018 BENZIMIDAZOLE ANALOG	15.45	2	97.03	16.98	17.50	−2.98	2
		200	80.07	7.54	9.41	−19.93	
JWH-011	15.81	2	89.28	16.33	18.30	−10.72	2
		200	84.45	6.23	7.37	−15.55	
JWH-016	15.20	2	91.59	6.69	7.30	−8.41	2
		200	101.24	1.71	1.69	1.24	
JWH-018	14.95	2	99.32	6.33	6.37	−0.68	2
		200	104.43	4.80	4.60	4.43	
JWH-018 ADAMANTYL CARBOXAMIDE	15.73	2	98.18	8.11	8.26	−1.82	2
		200	89.01	6.39	7.18	−10.99	
JWH-020	15.93	2	92.79	8.84	9.53	−7.21	2
		200	83.92	6.03	7.18	−16.08	
JWH-022	14.75	2	111.87	11.29	10.10	11.87	2

(*continued on next page*)

Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
		200	91.28	6.61	7.24	−8.72	
JWH-031	14.86	2	112.37	16.34	14.55	12.37	2
		200	85.55	6.76	7.91	−14.45	
JWH-071	13.64	2	98.68	7.54	7.64	−1.32	2
		200	94.63	7.64	8.07	−5.37	
JWH-073	14.75	2	106.01	7.76	7.32	6.01	2
		200	104.94	5.02	4.78	4.94	
JWH-080	14.97	2	113.10	17.69	15.64	13.10	2
		200	80.04	1.93	2.41	−19.96	
JWH-081	15.41	2	100.48	8.80	8.76	0.47	2
		200	97.49	3.00	3.08	−2.51	
JWH-098	15.54	2	109.13	7.87	7.21	9.13	2
		200	103.15	5.81	5.64	3.15	
JWH-116	15.66	2	94.93	18.36	19.34	−5.07	2
		200	92.26	5.97	6.47	−7.74	
JWH-122	15.56	2	96.76	4.27	4.42	−3.24	2
		200	94.70	3.74	3.95	−5.30	
JWH-145	15.58	2	99.72	13.52	13.56	−0.28	2
		200	81.67	3.10	3.79	−18.33	
JWH-146	16.21	2	87.94	13.72	15.60	−12.06	2
		200	92.31	8.42	9.12	−7.69	
JWH-147	15.94	2	96.96	10.81	11.15	−3.04	2
		200	88.59	3.81	4.30	−11.41	
JWH-149	15.66	2	82.36	14.75	17.91	−17.64	2
		200	82.14	2.29	2.79	−17.86	
JWH-167	14.55	2	118.04	4.31	3.65	18.04	2
		200	110.07	5.38	4.88	10.07	
JWH-175	16.76	2	97.20	7.40	7.62	−2.80	2
		200	87.12	4.14	4.75	−12.88	
JWH-182	16.07	2	94.72	12.21	12.89	−5.28	2
		200	96.15	7.73	8.04	−3.85	
JWH-193	11.81	2	99.18	12.77	12.88	−0.82	2
		200	89.33	5.72	6.40	−10.67	
JWH-198	11.59	2	101.63	10.45	10.28	1.63	2
		200	86.02	6.49	7.55	−13.98	
JWH-200	11.05	2	117.07	20.34	17.37	17.07	2
		200	92.57	10.16	10.97	−7.43	
JWH-201	14.47	2	119.97	16.18	13.49	19.97	2
		200	115.93	2.47	2.13	15.93	
JWH-213	15.91	2	84.09	10.76	12.79	−15.91	2
		200	97.59	6.18	6.34	−2.41	
JWH-307	15.47	2	87.49	15.28	17.47	−12.51	2
		200	81.36	11.38	13.98	−18.64	
JWH-309	16.09	2	90.45	7.67	8.48	−9.55	2
		200	93.39	4.73	5.06	−6.61	
JWH-368	15.59	2	116.21	6.96	5.99	16.21	2
		200	92.04	7.56	8.21	−7.96	
JWH-369	15.69	2	91.34	11.04	12.09	−8.66	2
		200	90.99	8.35	9.18	−9.01	
JWH-412	15.42	2	97.00	8.42	8.68	−3.00	2
		200	97.85	9.21	9.41	−2.15	
JWH-424	14.97	2	108.76	16.53	15.20	8.76	2
		200	96.71	6.96	7.20	−3.29	
KETAMINE	6.50	10	100.54	12.54	12.48	0.54	10
		200	116.08	2.03	1.75	16.08	
		500	111.40	5.40	4.90	11.40	
		1000	101.85	5.15	5.06	1.85	
LAMPA	8.30	10	91.60	6.50	7.10	−8.40	10
		200	88.59	6.38	7.20	−11.41	
		500	117.50	13.10	11.10	17.50	
		1000	96.26	10.41	10.81	−3.74	
LIDOCAINE	5.75	10	112.46	9.54	8.49	12.46	10
		200	100.58	5.66	5.63	0.58	
		500	118.53	7.84	6.61	18.53	
		1000	88.95	4.44	4.99	−11.05	
LOPRAZOLAM	9.29	10	107.41	17.54	16.33	7.41	10
		200	95.40	8.20	8.60	−4.60	
		500	118.12	14.59	12.35	18.12	
		1000	83.80	4.20	5.00	−16.20	
LORAZEPAM	11.38	10	111.88	17.58	15.72	11.88	10
		200	88.93	7.79	8.75	−11.07	
		500	98.70	4.69	4.75	−1.30	
		1000	89.21	6.50	7.28	−10.79	
LORMETAZEPAM	11.86	10	94.97	15.31	16.13	−5.04	10

(*continued on next page*)

Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
		200	99.68	11.62	11.66	−0.32	
		500	109.87	14.68	13.36	9.87	
		1000	92.01	7.65	8.31	−7.99	
LSD	8.14	10	91.49	15.47	16.91	−8.51	10
		200	88.87	7.91	8.90	−11.13	
		500	111.70	11.74	10.51	11.70	
		1000	85.49	2.72	3.18	−14.51	
MAM-2201	14.64	2	118.22	7.43	6.28	18.22	2
		200	119.69	7.72	6.45	19.69	
MAPROTILINE	10.75	10	96.93	16.45	16.97	−3.08	10
		200	100.52	6.89	6.85	0.52	
		500	110.02	6.37	5.79	10.02	
		1000	90.19	6.84	7.59	−9.81	
MBDB	6.46	10	104.60	7.10	6.80	4.60	10
		200	113.79	7.58	6.66	13.79	
		500	111.66	7.28	6.52	11.66	
		1000	89.95	2.24	2.49	−10.05	
MDAT	5.39	10	98.14	11.71	11.93	−1.86	10
		400	91.58	6.88	7.52	−8.42	
		1000	104.69	10.72	10.24	4.69	
MDBP	2.47	10	91.78	2.57	2.80	−8.22	10
		400	65.83	2.43	3.70	−34.17	
		1000	104.40	5.21	4.99	4.40	
MDEA	5.88	10	97.39	14.00	14.37	−2.61	10
		200	106.58	5.98	5.61	6.58	
		500	118.60	7.60	6.40	18.60	
		1000	90.89	4.40	4.84	−9.11	
MDMB-CHMICA (MMB-CHMINACA)	15.15	2	114.80	7.36	6.41	14.80	2
		200	113.42	3.00	2.64	13.42	
MDMB-CHMINACA	15.49	2	104.68	16.49	15.75	4.68	2
		200	97.41	9.44	9.69	−2.59	
MDPBP	6.45	10	86.48	12.71	14.70	−13.52	10
		200	83.39	5.12	6.14	−16.61	
		500	103.63	8.51	8.21	3.63	
		1000	86.56	4.65	5.37	−13.44	
MECLONAZEPAM	11.42	10	101.39	11.11	10.95	1.39	10
		400	88.70	4.56	5.15	−11.30	
		1000	92.20	8.32	9.02	−7.80	
MEDAZEPAM	9.44	10	81.40	5.60	6.90	−18.60	10
		200	85.15	3.44	4.04	−14.85	
		500	118.30	5.90	5.00	18.30	
		1000	103.51	6.69	6.47	3.51	
MEMANITINE	9.39	10	98.23	9.15	9.31	−1.77	10
		400	95.46	4.84	5.07	−4.54	
		1000	99.73	8.14	8.16	−0.27	
MEPERIDINE	7.53	10	101.07	12.86	12.73	1.07	10
		400	109.23	9.96	9.11	9.23	
		1000	114.34	11.67	10.21	14.34	
MEPHTETRAMINE (MTTA)	5.42	10	90.30	4.70	5.20	−9.70	10
		200	92.72	6.89	7.43	−7.28	
		500	119.80	16.41	13.70	19.80	
		1000	96.23	6.54	6.79	−3.77	
MEPIRAPIM	10.14	2	117.19	10.76	9.18	17.19	2
		200	88.90	5.47	6.15	−11.10	
MEPROBAMATE	8.81	10	93.91	9.79	10.43	−6.09	10
		200	109.09	4.60	4.22	9.09	
		500	107.08	5.03	4.70	7.08	
		1000	103.28	6.19	5.99	3.28	
MESCALINE	5.22	10	99.50	12.30	12.40	−0.50	10
		200	111.40	8.16	7.33	11.40	
		500	115.80	14.30	12.30	15.80	
		1000	105.51	6.56	6.22	5.51	
METHADONE	10.82	10	104.64	8.41	8.04	4.64	10
		200	117.57	4.87	4.15	17.57	
		500	112.59	11.66	10.36	12.59	
		1000	92.02	4.18	4.54	−7.98	
METHAMPHETAMINE	5.05	10	94.10	18.11	19.25	−5.90	10
		200	92.00	4.20	4.57	−8.00	
		500	117.90	8.90	7.60	17.90	
		1000	91.02	3.42	3.76	−8.98	
METHANDIENONE	12.51	10	103.63	10.01	9.66	3.63	10
		200	91.39	4.91	5.38	−8.61	
		500	93.52	4.13	4.41	−6.48	
		1000	89.37	6.10	6.83	−10.63	

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Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
METHAQUALONE	11.10	10	113.10	9.53	8.43	13.10	10
		200	118.22	8.52	7.20	18.22	
		500	115.64	11.42	9.87	15.64	
		1000	101.70	5.67	5.57	1.70	
METHCATHINONE	4.12	10	111.43	8.21	7.37	11.43	10
		200	91.28	6.63	7.26	−8.72	
		500	113.16	8.90	7.86	13.16	
		1000	90.09	2.04	2.27	−9.91	
METHEDRONE (bk-PMMA)	5.32	10	93.75	9.93	10.59	−6.25	10
		400	82.00	5.08	6.20	−18.00	
		1000	84.05	8.09	9.63	−15.95	
METHOHEXITAL	11.78	10	106.13	17.96	16.93	6.13	10
		200	96.42	7.13	7.39	−3.58	
		500	91.66	5.64	6.16	−8.34	
		1000	94.10	4.32	4.60	−5.90	
METHOXETAMINE	7.15	10	111.96	15.04	13.43	11.96	10
		200	109.61	11.51	10.50	9.61	
		500	108.64	5.09	4.69	8.64	
		1000	97.43	1.51	1.55	−2.57	
METHOXPHENIDINE	9.34	10	82.32	11.94	14.51	−17.68	10
		200	99.01	3.67	3.70	−0.99	
		500	114.40	9.00	7.80	14.40	
		1000	91.78	2.89	3.15	−8.22	
METHYLHEXANAMINE	5.89	10	94.60	10.00	10.60	−5.40	10
		200	108.80	9.10	8.40	8.80	
		500	115.52	15.17	13.13	15.52	
		1000	101.59	4.25	4.18	1.59	
METHYLONE (bk-MDMA)	4.67	10	109.92	11.80	10.74	9.92	10
		200	100.14	4.41	4.41	0.14	
		500	117.40	6.90	5.90	17.40	
		1000	97.73	3.56	3.64	−2.27	
METHYLPHENIDATE	7.15	10	114.59	9.26	8.08	14.59	10
		200	112.24	5.49	4.89	12.24	
		500	116.32	11.82	10.16	16.32	
		1000	86.09	2.13	2.48	−13.91	
MEXEDRONE	6.37	10	83.22	10.75	12.92	−16.78	10
		400	83.40	5.39	6.46	−16.60	
		1000	87.56	7.86	8.98	−12.44	
MIANSERIN	9.33	10	99.99	19.55	19.55	−0.01	10
		200	105.11	11.88	11.31	5.11	
		500	115.33	12.54	10.88	15.33	
		1000	105.44	6.93	6.57	5.44	
MIDAZOLAM	9.38	10	81.82	7.04	8.61	−18.18	10
		200	101.63	4.97	4.89	1.63	
		500	119.20	9.55	8.01	19.20	
		1000	96.01	2.12	2.20	−3.99	
MITRAGYNINE	9.25	10	85.99	16.28	18.94	−14.01	10
		200	80.10	6.20	7.70	−19.90	
		500	119.40	14.00	11.70	19.40	
		1000	85.56	3.74	4.38	−14.44	
MMAI	6.87	10	96.27	4.70	4.88	−3.73	10
		400	93.04	7.71	8.28	−6.96	
		1000	96.55	15.67	16.23	−3.45	
MMB018	14.16	2	110.38	12.71	11.52	10.38	2
		200	118.92	12.67	10.66	18.92	
MMB2201	13.10	2	100.38	9.37	9.33	0.38	2
		200	111.32	12.39	11.13	11.32	
MN-18	15.57	2	99.04	10.06	10.16	−0.96	2
		200	98.44	2.18	2.22	−1.56	
MN-25	12.52	2	86.65	9.86	11.38	−13.35	2
		200	87.62	7.51	8.58	−12.38	
MN-25–2-METHYL DERIVATIVE	13.25	2	89.72	13.46	15.00	−10.28	2
		200	90.25	7.06	7.82	−9.75	
MO-CHMINACA	15.47	2	90.52	13.27	14.66	−9.48	2
		200	105.16	8.20	7.80	5.16	
MORPHINE	2.42	10	100.20	11.90	11.80	0.20	10
		200	118.87	12.72	10.70	18.87	
		500	99.60	7.20	7.30	−0.40	
		1000	96.20	6.20	6.40	−3.80	
MPBP	7.58	10	95.67	7.61	7.95	−4.33	10
		200	106.75	7.37	6.90	6.75	
		500	111.91	3.96	3.54	11.91	
		1000	101.01	2.64	2.62	1.01	
MT-45	10.84	10	87.23	2.57	2.95	−12.78	10

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Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
		200	108.79	10.87	9.99	8.79	
		500	115.27	12.25	10.63	15.27	
		1000	98.79	2.57	2.60	−1.21	
N-(3-METHYLBENZYL)PIPERAZINE	4.02	10	92.38	4.16	4.50	−7.62	10
		400	91.66	3.96	4.32	−8.34	
		1000	104.01	5.50	5.29	4.01	
N.*N*-DIETHYLPHENETHYLAMINE	5.38	10	88.79	6.77	7.63	−11.22	10
		400	83.58	6.08	7.28	−16.42	
		1000	99.18	7.34	7.40	−0.82	
N.*N*-DIMETHYLPENTYLONE (bk-DMBDP)	7.30	10	108.13	19.01	17.58	8.13	10
		200	108.32	7.42	6.85	8.32	
		500	106.98	8.76	8.19	6.98	
		1000	101.48	5.68	5.59	1.48	
N.*N*-DMT	4.86	10	102.10	15.10	14.80	2.10	10
		200	93.65	7.11	7.60	−6.35	
		500	107.94	7.06	6.54	7.94	
		1000	95.91	3.11	3.24	−4.09	
N-ACETYL-3.4-MDMC	9.24	10	114.19	8.19	7.17	14.19	10
		400	93.27	10.48	11.23	−6.73	
		1000	91.45	6.98	7.63	−8.55	
NAPHYRONE	10.08	10	103.04	12.25	11.89	3.04	10
		400	99.08	7.12	7.19	−0.92	
		1000	105.40	10.55	10.01	5.40	
NAPHYRONE-1-NAPHTYL ISOMER	9.61	10	90.45	8.19	9.06	−9.55	10
		400	96.03	7.16	7.45	−3.97	
		1000	96.07	9.91	10.31	−3.93	
N-BENZYLNORBUTYLONE	8.72	10	106.87	6.50	6.09	6.87	10
		400	103.76	6.35	6.12	3.76	
		1000	93.86	3.04	3.24	−6.14	
N-ETHYL-4-METHOXYAMPHETAMNE	6.12	10	93.61	12.83	13.71	−6.39	10
		400	79.97	6.94	8.68	−20.03	
		1000	80.57	6.07	7.53	−19.43	
N-ETHYLBUPHEDRONE	5.82	10	95.78	15.11	15.78	−4.22	10
		400	84.39	3.99	4.72	−15.61	
		1000	96.08	6.20	6.45	−3.92	
N-ETHYL-*N*-METHYLCATHINONE	4.91	10	90.14	8.48	9.41	−9.86	10
		400	83.51	3.17	3.79	−16.49	
		1000	88.53	2.93	3.31	−11.47	
N-ETHYLNORDAZEPAM	12.89	10	88.21	7.56	8.57	−11.80	10
		200	91.88	4.79	5.22	−8.12	
		500	107.54	8.99	8.36	7.54	
		1000	92.79	4.77	5.14	−7.21	
N-ETHYLNORKETAMINE	7.12	10	97.16	14.68	15.11	−2.84	10
		400	87.49	8.69	9.93	−12.51	
		1000	89.93	6.50	7.22	−10.07	
N-ETHYLOXAZEPAM	12.25	10	97.99	18.37	18.74	−2.01	10
		200	89.75	2.47	2.76	−10.25	
		500	100.17	10.53	10.51	0.17	
		1000	94.07	6.93	7.37	−5.93	
N-ETHYLPENTYLONE	7.49	10	112.24	13.71	12.21	12.24	10
		200	104.48	9.09	8.70	4.48	
		500	118.50	7.30	6.20	18.50	
		1000	89.85	5.15	5.74	−10.15	
NIMETAZEPAM	10.98	10	99.50	12.48	12.54	−0.50	10
		200	111.97	6.60	5.89	11.97	
		500	115.00	13.20	11.50	15.00	
		1000	92.23	2.03	2.21	−7.77	
NITRACAINE	8.09	200	98.50	16.32	16.57	−1.50	200
		500	113.16	5.86	5.18	13.16	
		1000	100.90	4.84	4.79	0.90	
NITRAZEPAM	10.60	10	85.10	9.30	11.00	−14.90	10
		200	97.70	3.47	3.55	−2.30	
		500	102.45	10.25	10.01	2.45	
		1000	86.15	3.41	3.96	−13.85	
NM2201	14.96	2	92.02	12.99	14.12	−7.98	2
		200	87.29	4.45	5.10	−12.71	
N-METHYL-2AI	4.29	10	86.50	8.62	9.97	−13.50	10
		200	99.35	4.52	4.55	−0.65	
		500	114.86	13.33	11.60	14.86	
		1000	97.61	6.01	6.16	−2.39	
N-METHYL-PEA	3.73	10	88.46	4.39	4.97	−11.55	10
		400	87.44	3.36	3.84	−12.56	
		1000	95.02	6.16	6.48	−4.98	
N-METHYLTRYPTAMINE	4.82	10	115.46	21.12	18.29	15.46	10

(*continued on next page*)

Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
		200	81.20	2.40	2.90	−18.80	
		500	100.17	7.50	7.48	0.17	
		1000	84.30	7.40	8.70	−15.70	
NN-DMC	4.33	10	91.73	8.32	9.08	−8.27	10
		400	85.74	2.91	3.40	−14.26	
		1000	92.90	14.82	15.95	−7.10	
NNEI	14.51	2	115.61	5.88	5.09	15.61	2
		200	119.44	2.50	2.09	19.44	
NORCLOBAZAM	10.70	10	117.51	15.63	13.30	17.51	10
		200	101.92	4.39	4.31	1.92	
		500	102.76	9.35	9.10	2.76	
		1000	94.03	2.79	2.97	−5.97	
NORCLOMIPRAMINE	11.77	10	84.96	10.85	12.77	−15.04	10
		200	107.03	9.70	9.06	7.03	
		500	97.68	7.99	8.18	−2.32	
		1000	96.77	3.50	3.62	−3.23	
NORKETAMINE	6.44	10	101.96	17.09	16.76	1.96	10
		200	111.02	7.34	6.61	11.02	
		500	105.63	9.98	9.45	5.63	
		1000	97.99	5.33	5.44	−2.01	
NORTRIPTYLINE	11.05	10	83.93	9.84	11.72	−16.07	10
		200	95.18	5.95	6.25	−4.82	
		500	104.75	10.75	10.26	4.75	
		1000	81.79	6.81	8.32	−18.21	
N-PROPYLAMPHETAMINE	6.67	10	106.11	20.90	19.69	6.11	10
		200	104.69	6.29	6.01	4.69	
		500	113.16	12.99	11.48	13.16	
		1000	104.69	4.84	4.62	4.69	
NRG-3	9.85	10	95.87	9.63	10.04	−4.13	10
		400	95.10	7.31	7.68	−4.90	
		1000	94.54	11.27	11.92	−5.46	
o-CPP	6.80	10	88.46	4.15	4.70	−11.54	10
		400	100.43	6.06	6.03	0.43	
		1000	119.20	5.26	4.41	19.20	
OCTACAINE	6.11	10	86.02	8.85	10.29	−13.98	10
		400	86.51	5.84	6.75	−13.49	
		1000	86.16	5.84	6.78	−13.84	
ORG-28611	11.57	2	104.46	12.99	12.44	4.46	2
		200	86.25	4.48	5.20	−13.75	
OXAZEPAM	11.36	10	99.80	18.35	18.38	−0.20	10
		200	94.30	7.02	7.44	−5.70	
		500	103.84	11.62	11.19	3.84	
		1000	85.40	5.60	6.56	−14.60	
OXYMORPHONE	2.80	10	111.28	15.01	13.49	11.28	10
		400	97.13	9.03	9.29	−2.87	
		1000	111.26	11.18	10.05	11.26	
PARACETAMOL	3.90	10	108.80	6.90	6.30	8.80	10
		200	95.99	7.46	7.78	−4.01	
		500	107.47	4.42	4.11	7.47	
		1000	87.48	1.47	1.68	−12.52	
PAROXETINE	10.57	10	82.60	9.50	11.50	−17.40	10
		200	95.16	6.89	7.25	−4.84	
		500	110.00	10.61	9.64	10.00	
		1000	85.75	3.98	4.64	−14.25	
PB-22	14.65	2	118.55	10.46	8.82	18.55	2
		200	116.22	4.28	3.69	16.22	
PCEEA	9.19	10	96.75	9.08	9.38	−3.25	10
		400	96.29	5.08	5.28	−3.71	
		1000	96.47	9.39	9.73	−3.53	
PCMPA	8.96	10	90.18	10.75	11.92	−9.82	10
		400	86.43	11.24	13.00	−13.57	
		1000	88.48	6.81	7.69	−11.52	
PCPr	9.09	10	112.66	8.23	7.31	12.66	10
		400	91.98	7.39	8.04	−8.02	
		1000	99.31	11.20	11.28	−0.69	
PENTEDRONE	6.84	10	99.57	13.78	13.84	−0.43	10
		200	105.09	4.08	3.88	5.09	
		500	116.62	5.85	5.02	16.62	
		1000	89.82	3.67	4.09	−10.18	
PENTEDRONE METABOLITE	6.89	10	109.59	18.08	16.50	9.59	10
		200	110.45	9.57	8.66	10.45	
		500	117.90	7.70	6.50	17.90	
		1000	91.38	1.88	2.06	−8.62	
PENTYLONE (bk-MBDP)	7.19	10	99.85	6.20	6.21	−0.15	10

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Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
		200	99.84	11.34	11.36	−0.16	
		500	104.06	9.37	9.01	4.06	
		1000	91.03	6.19	6.80	−8.97	
PHENAZEPAM	12.12	10	87.20	3.00	3.40	−12.80	10
		200	92.85	4.10	4.42	−7.15	
		500	99.84	4.95	4.96	−0.16	
		1000	92.04	4.02	4.37	−7.96	
PHENCYCLIDINE (PCP)	8.54	10	83.30	4.10	4.90	−16.70	10
		200	107.58	6.99	6.50	7.58	
		500	109.40	8.80	8.10	9.40	
		1000	101.29	3.04	3.00	1.29	
PHENOBARBITAL	8.14	10	109.90	10.80	9.90	9.90	10
		200	80.27	9.65	12.02	−19.73	
		500	81.06	11.78	14.53	−18.94	
		1000	88.20	10.40	11.79	−11.80	
PHENTERMINE	5.96	10	113.89	17.94	15.75	13.89	10
		200	102.00	10.99	10.77	2.00	
		500	111.76	7.97	7.13	11.76	
		1000	103.35	7.70	7.45	3.35	
PHENYTOIN	10.20	10	91.03	12.65	13.90	−8.97	10
		200	97.29	4.79	4.93	−2.71	
		500	119.60	13.20	11.00	19.60	
		1000	91.43	4.07	4.46	−8.57	
PRAVADOLINE	10.26	10	95.01	10.83	11.40	−4.99	10
		400	89.46	7.11	7.94	−10.54	
		1000	96.60	9.43	9.76	−3.40	
PRAZEPAM	13.52	10	100.78	8.55	8.49	0.78	10
		200	100.47	2.38	2.37	0.47	
		500	82.20	7.20	8.70	−17.80	
		1000	87.71	4.49	5.12	−12.29	
PREGABALIN	4.63	10	100.10	11.62	11.61	0.10	10
		200	93.65	8.42	9.00	−6.35	
		500	108.93	6.63	6.08	8.93	
		1000	90.03	3.64	4.04	−9.97	
PROCAINE	4.18	10	81.70	7.00	8.60	−18.30	10
		200	94.57	6.13	6.48	−5.43	
		500	108.08	8.31	7.69	8.08	
		1000	94.61	4.14	4.38	−5.39	
PROLINTANE	8.04	10	88.60	16.62	18.76	−11.40	10
		200	97.06	6.69	6.89	−2.94	
		500	110.70	10.80	9.80	10.70	
		1000	101.38	7.88	7.77	1.38	
PROMETHAZINE	10.21	10	83.80	6.30	7.50	−16.20	10
		200	81.10	3.70	4.60	−18.90	
		500	85.09	6.58	7.73	−14.91	
		1000	82.80	3.30	4.00	−17.20	
PROPAFENONE	10.71	10	89.53	10.83	12.10	−10.47	10
		200	111.71	8.24	7.38	11.71	
		500	118.84	8.97	7.55	18.84	
		1000	97.09	5.35	5.51	−2.91	
PROPRANOLOL	9.11	10	84.78	9.90	11.68	−15.22	10
		200	94.66	4.34	4.59	−5.34	
		500	116.54	10.36	8.89	16.54	
		1000	88.83	4.85	5.46	−11.17	
PROPYLHEXEDRINE	8.04	10	84.40	10.56	12.52	−15.60	10
		200	99.46	5.99	6.02	−0.54	
		500	118.30	9.50	8.00	18.30	
		1000	103.20	4.47	4.33	3.20	
PSB-SB-1202	15.97	2	104.35	7.39	7.08	4.35	2
		200	91.99	7.68	8.35	−8.01	
PTI-1	12.54	2	93.76	5.59	5.96	−6.24	2
		200	86.37	6.25	7.24	−13.63	
PTI-2	12.78	2	104.91	7.60	7.25	4.91	2
		200	81.54	2.21	2.70	−18.46	
PV-8	9.70	10	91.80	10.71	11.67	−8.20	10
		200	103.55	4.79	4.63	3.55	
		500	113.14	5.66	5.01	13.14	
		1000	99.32	2.77	2.79	−0.68	
PV9	10.70	10	99.94	7.55	7.56	−0.06	10
		400	92.78	5.11	5.51	−7.22	
		1000	92.19	3.67	3.98	−7.81	
PX-1	12.68	2	112.66	19.78	17.55	12.66	2
		200	81.68	2.28	2.79	−18.32	
PX-2	12.76	2	99.58	13.09	13.14	−0.42	2

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Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
		200	85.41	5.04	5.91	−14.59	
PYRAZOLAM	9.47	10	87.22	12.56	14.40	−12.78	10
		200	94.57	4.12	4.36	−5.43	
		500	119.79	8.53	7.12	19.79	
		1000	98.99	6.46	6.52	−1.01	
QUETIAPINE	9.60	10	104.88	8.38	7.99	4.88	10
		200	105.25	6.67	6.33	5.25	
		500	119.89	10.10	8.42	19.89	
		1000	92.33	3.01	3.26	−7.67	
RCS-4	14.67	2	116.72	6.47	5.55	16.72	2
		200	110.96	5.74	5.18	10.96	
RH-34	8.13	10	86.48	7.23	8.36	−13.52	10
		400	80.38	8.22	10.23	−19.62	
		1000	75.29	2.68	3.55	−24.71	
R-MMC	6.89	10	101.09	11.40	11.27	1.09	10
		400	95.41	7.33	7.68	−4.59	
		1000	95.42	7.43	7.79	−4.58	
SCOPOLAMINE	4.79	10	114.29	17.54	15.35	14.29	10
		200	103.53	6.94	6.70	3.53	
		500	116.90	10.80	9.20	16.90	
		1000	95.50	4.35	4.56	−4.50	
SDB-005	15.58	2	97.58	13.21	13.54	−2.43	2
		200	83.76	12.33	14.72	−16.24	
SDB-006	14.09	2	90.27	10.73	11.89	−9.73	2
		200	117.67	11.46	9.74	17.67	
SERTRALINE	11.56	10	89.30	17.10	19.10	−10.70	10
		200	95.09	6.69	7.04	−4.91	
		500	92.96	11.71	12.60	−7.05	
		1000	83.18	6.98	8.40	−16.82	
SILDENAFIL	10.31	10	97.10	12.42	12.79	−2.90	10
		200	94.56	4.16	4.40	−5.44	
		500	116.58	14.42	12.37	16.58	
		1000	100.72	4.77	4.74	0.72	
STANOZOLOL	14.10	10	81.20	10.20	12.60	−18.80	10
		200	106.30	2.27	2.14	6.30	
		500	82.75	6.85	8.28	−17.25	
		1000	113.05	3.13	2.77	13.05	
TAPENTADOL	7.34	10	102.70	15.96	15.55	2.70	10
		400	113.93	9.75	8.56	13.93	
		1000	111.03	7.76	6.99	11.03	
TEMAZEPAM	11.68	10	81.18	13.09	16.13	−18.82	10
		200	95.26	10.67	11.20	−4.74	
		500	104.31	8.87	8.50	4.31	
		1000	93.68	2.71	2.89	−6.32	
TETRACAINE	9.02	10	88.71	9.01	10.16	−11.29	10
		400	90.25	8.27	9.17	−9.75	
		1000	90.99	3.46	3.80	−9.01	
THC	15.94	1	110.00	14.14	12.86	10.00	1
		200	81.64	2.73	3.35	−18.36	
THCCOOH	14.99	10	81.03	14.59	18.00	−18.97	10
		2000	80.85	1.74	2.15	−19.15	
THIOPROPAMINE	3.76	10	89.12	9.50	10.66	−10.88	10
		400	85.71	3.51	4.10	−14.29	
		1000	96.40	4.48	4.64	−3.60	
THJ	15.98	2	94.81	5.51	5.82	−5.19	2
		200	100.23	6.66	6.65	0.23	
THJ-018	15.55	2	106.61	8.13	7.63	6.61	2
		200	97.09	2.10	2.17	−2.91	
THJ-2201 (5-FLUORO THJ-018)	14.65	2	117.90	6.19	5.25	17.90	2
		200	111.52	3.44	3.08	11.52	
TILETAMINE	5.70	10	86.11	8.33	9.67	−13.89	10
		400	90.63	6.78	7.48	−9.37	
		1000	100.92	5.24	5.20	0.92	
TRAMADOL	6.94	10	94.98	16.61	17.49	−5.02	10
		200	101.02	7.83	7.75	1.02	
		500	113.97	12.30	10.79	13.97	
		1000	100.55	4.94	4.92	0.55	
TRAZODONE	8.36	10	116.14	15.97	13.75	16.14	10
		200	88.39	8.65	9.79	−11.61	
		500	118.90	7.40	6.30	18.90	
		1000	87.81	6.41	7.30	−12.19	
TRIAZOLAM	11.46	10	95.01	17.38	18.29	−4.99	10
		200	86.91	6.67	7.67	−13.09	
		500	96.91	9.02	9.31	−3.09	

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Table 2 (*continued*)

ANALYTE	RT	CONCENTRATION [ng/ml]	EVERAGE RECOVERY [%]	SD [%]	CV [%]	BIAS [%]	LOQ [ng/mL]
		1000	83.57	6.25	7.47	−16.43	
TRIMIPRAMINE	11.01	10	100.98	14.64	14.50	0.98	10
		200	112.75	11.74	10.41	12.75	
		500	109.20	8.35	7.65	9.20	
		1000	94.96	5.21	5.49	−5.04	
U-47700	9.12	10	104.03	9.73	9.36	4.03	10
		400	104.94	6.91	6.59	4.94	
		1000	96.12	6.22	6.47	−3.88	
UR-144	15.57	2	115.52	6.89	5.97	15.52	2
		200	109.04	3.55	3.26	9.04	
UR-144 metabolite	13.81	2	85.78	7.48	8.72	−14.22	2
		200	81.92	8.33	10.17	−18.08	
W-15	13.31	10	113.39	8.35	7.36	13.39	10
		400	92.11	5.05	5.49	−7.89	
		1000	100.86	5.83	5.78	0.86	
WIN 54.461	12.45	2	93.03	14.18	15.24	−6.97	2
		200	81.33	4.67	5.74	−18.67	
WIN 55.212–2	13.66	2	91.88	14.63	15.92	−8.12	2
		200	95.10	9.24	9.72	−4.90	
XLR-11	14.71	2	118.07	8.67	7.34	18.07	2
		200	113.57	5.06	4.46	13.57	
XLR12	14.80	2	84.04	6.33	7.53	−15.96	2
		200	92.80	9.97	10.74	−7.20	
YANGONIN	11.88	10	117.19	12.23	10.44	17.19	10
		400	101.10	11.72	11.59	1.10	
		1000	97.54	9.25	9.49	−2.46	
ZALEPLON	10.04	10	83.20	10.97	13.18	−16.80	10
		200	98.20	3.96	4.03	−1.80	
		500	113.89	10.78	9.47	13.89	
		1000	109.73	4.50	4.10	9.73	
ZOLPIDEM	7.93	10	105.59	7.91	7.49	5.58	10
		200	104.70	7.60	7.26	4.70	
		500	112.03	12.32	11.00	12.03	
		1000	92.37	4.44	4.80	−7.63	
ZOPICLONE	6.81	10	117.10	15.20	13.00	17.10	10
		200	108.64	9.42	8.67	8.64	
		500	114.50	8.80	7.70	14.50	
		1000	84.73	3.26	3.85	−15.27	
ZUCLOPENTHIXOL	12.19	10	88.95	9.07	10.19	−11.05	10
		200	80.19	5.77	7.20	−19.81	
		500	85.68	8.17	9.53	−14.32	
		1000	85.84	4.26	4.97	−14.16	
ALPHA-HYDROXYMIDAZOLAM	10.01	10	83.08	14.59	17.56	−16.92	10
		200	90.07	6.48	7.19	−9.93	
		500	111.40	17.60	15.80	11.40	
		1000	87.62	0.98	1.12	−12.38	

determined ranges of LOQ values were 1–200 ng/mL. The results obtained during the validation are summarized in Table 2. In addition, the results obtained for the LOQ value with the extracted analyte peaks are presented in Fig. S3 and Fig. S4 for 1 and 10 ng/mL respectively. The developed method was verified by proficiency tests carried out by LGC Standards. Samples containing the following substances were identified: benzoylecgonine, cocaine, desmethyldiazepam, diazepam, 5F-ADB, dihydrocodeine, and paracetamol. Quantitative studies were carried out for phenazepam. The obtained results met the criteria of SWGTOX guidelines.

3.4. The real-life samples

The developed analytical method was implemented for routine analyses at the Institute of Forensic Genetics in Bydgoszcz. In 2020, 3413 blood samples were analyzed for the presence of psychoactive substances, drugs, and their metabolites as ordered by trial authorities in forensic cases. This is a type of test that, by trial authorities in forensic cases, as described in Section 2.3. Only in the case of 701 of the analyzed samples. Only in the case of 701 of the analyzed samples none of the analyzed substances was found. In the remaining samples, the presence of the following analytes was detected (the number of samples in which the given analyte was found): 3-chloromethcathinone (19), 3-MMC/4-MMC (23), 3,4-MDMA (182), 4-chloromethcathinone (33), 4- lfuoropentedrone (1), 4-methylcathinone (16), 6-MAM (1), 7- aminoclonazepam (39), 7-aminonitrazepam (3), alpha-ethylaminopentiophenone (4), alpha-ethylaminohexanophenone (23), ALHPA-PHP (3), ALPHA-PVP (17), alprazolam (24), amitritpyline (2), amphetamine (1863), benzoylecgonine (88), cannabidiol (20), carbamazepine (14), cathine (2), clomipramine (3), clonazepam (36), cocaethylene (13), cocaine (31), codeine (13), deschloroetizolam (1), desmethyldiazepam (48), dextromethorphan (5), diazepam (77), diphenidine (3), doxepin (2), eddp (14), estazolam (4), eutylone (20), fentanyl (6), flubromazepam (1), fluoxetine (9), hydrocodone (3), JWH-080 (1), ketamine (29), lidocaine (205), lorazepam (6), meperidine (1), methadone (15), methamphetamine (45), methandienone (3), mianserin (5), midazolam (58), MMB220 (1), MMB-2201 (2), morphine (52), nitrazepam (2), norclomipramine (3), norketamine (27), nortriptyline (2), oxazepam (8), oxymorphone (1), paracetamol (141), paroxetine (6), pcpp/mcpp/ocpp (10), pregabalin (16), propafenone (3), propranolol (1), quetiapine (13), sertraline, (16) sildenafil (20), temazepam (10), THC (663), THCCOOH (709), tramadol (44), trazodone (17), trimipramine (1), zolpidem (13), zopiclone (2), zuclopethixol (4), alpha-hydroxymidazolam (65). The most common analytes turned out to be

AMPHETAMINE (55%), THCCOOH (21%), THC (19%), methamphetamine (13%), lidocaine (6%), 3,4-MDMA (5%) and paracetamol (4%).

4. Conclusions

The analytical method developed in this study and introduced into routine analyses enables the simultaneous analysis of 520 psychoactive substances, reducing the time and cost of analyzing a single blood sample for NPS. It also opens new possibilities for analysing this type of substances. The applied liquid–liquid extraction method as well as the sensitive and specific LC-MS/MS analysis enables a quick, sensitive and specific analysis of blood samples for psychoactive substances and their metabolites. By applying the developed method, we meet the challenges posed by today's toxicology. We are able to analyze many substances and their metabolites, as well as reveal the specific cause of poisoning or death that involves ingesting a toxic substance. The developed method also makes it possible to easily extend the assay to other substances, which is extremely important in the case of substances appearing on the black market.

Statements and Declaration:

Ethical standards:

The manuscript does not contain clinical studies or patient data.

Declaration of Competing Interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Jakub Czarny reports was provided by National Centre for Research and Development.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.microc.2022.107922.

References

[1] M.H. Baumann, R.G. Glennon, J.L. Wiley, Neuropharmacology of new psychoactive substances (NPS), The Science Behind the Headlines (32), (2017). Doi:10.1016/B978-0-12-415816-0.00018-3.

[2] European Monitoring Centre for Drugs and Drug Addiction (EMCDDA), European Drug Report 2018, Trends and Developments, 2018. 10.2810/800331.

[3] National Forensic Laboratory Information System. Emerging 2C-Phenethylamines, Piperazines, and Tryptamines in NFLIS, 2006-2011, (2012) 1-8. https://www.nflis.deadiversion.usdoj.gov/ DesktopModules/ReportDownloads/Reports/NFLIS_SR_Emerging_II.pdf.

[4] S.L. Hill, S.H.L. Thomas, Clinical toxicology of newer recreational drugs, Clin. Toxicol. 49 (8) (2011) 705–719, https://doi.org/10.3109/15563650.2011.615318.

[5] J.M. Prosser, L.S. Nelson, The toxicology of bath salts: a review of synthetic cathinones, J. Med. Toxicol. 8 (1) (2012) 33–42, https://doi.org/10.1007/s13181-011-0193-z.

[6] The European Monitoring Centre for Drugs and Drug Addiction (EMCDDA), New psychoactive substances in Europe. An update from the EU Early Warning System, 2015. 10.2810/372415.

[7] The European Monitoring Centre for Drugs and Drug Addiction (EMCDDA), European Drug Report. Trends and Developments, 2015. 10.2810/084165.

[8] H. Torrance, G. Cooper, The detection of mephedrone (4-methylmethcathinone) in 4 fatalities in Scotland, Forensic Sci. Int. 202 (1–3) (2010) e62–e63, https://doi.org/10.1016/j.forsciint.2010.07.014.

[9] M. Wikström, G. Thelander, I. Nyström, R. Kronstrand, Two fatal intoxications with the new designer drug methedrone (4-methoxymethcathinone), J. Anal. Toxicol. 34 (9) (2010) 594–598, https://doi.org/10.1093/jat/34.9.594.

[10] P.D. Maskell, G. De Paoli, C. Seneviratne, D.J. Pounder, Mephedrone (4-methylmethcathinone)-related deaths, J Anal Toxicol. 35 (3) (2011) 188–191, https://doi.org/10.1093/anatox/35.3.188.

[11] N. Carter, G.N. Rutty, C.M. Milroy, A.R.W. Forrest, Deaths associated with MBDB misuse, Int. J. Legal Med. 113 (3) (2000) 168–170, https://doi.org/10.1007/s004140050291.

[12] B.L. Murray, C.M. Murphy, M.C. Beuhler, Death following recreational use of designer drug "bath salts" containing 3,4-methylenedioxypyrovalerone (MDPV), J. Med. Toxicol. 8(1) (2012) 69-75. 10.1007/s13181-011-0196-9.

[13] P. Adamowicz, D. Zuba, B. Byrska, Fatal intoxication with 3-methyl-N-methylcathinone (3-MMC) and 5-(2-aminopropyl)benzofuran (5-APB), Forensic Sci. Int. 245 (2014) 126–132, https://doi.org/10.1016/j.forsciint.2014.10.016.

[14] P. Adamowicz, D. Zuba, Fatal intoxication with methoxetamine, J. Forensic Sci. 60 (s1) (2015) S264–S268, https://doi.org/10.1111/1556-4029.12594.

[15] M. Sykutera, M. Cychowska, E. Bloch-Boguslawska, A fatal case of pentedrone and α-pyrrolidinovalerophenone poisoning, J. Anal. Toxicol. 39(4) (2015) 324-329. 10.1093/jat/bkv011.

[16] H. Nagai, K. Saka, M. Nakajima, H. Maeda, R. Kuroda, A. Igarashi, T. Tsujimura-Ito, A. Nara, M. Komori, K.-I. Yoshida, Sudden death after sustained restraint following self-administration of the designer drug α-pyrrolidinovalerophenone, Int. J. Cardiol. 172 (1) (2014) 263–265, https://doi.org/10.1016/j.ijcard.2013.12.262.

[17] M. Coppola, R. Mondola, Synthetic cathinones: chemistry, pharmacology and toxicology of a new class of designer drugs of abuse marketed as "bath salts" or "plant food", Toxicol. Lett. 211 (2) (2012) 144–149, https://doi.org/10.1016/j.toxlet.2012.03.009.

[18] J.P. Kelly, Cathinone derivatives: a review of their chemistry, pharmacology and toxicology, Drug Test. Anal. 3 (7–8) (2011) 439–453, https://doi.org/10.1002/dta.313.

[19] K.A. Seely, J. Lapoint, J.H. Moran, L. Fattore, Spice drugs are more than harmless herbal blends: a review of the pharmacology and toxicology of synthetic cannabinoids, Prog. Neuropsychopharmacol Biol. Psychiatry 39 (2) (2012) 234–243, https://doi.org/10.1016/j.pnpbp.2012.04.017.

[20] S. Odoardi, M. Fisichella, F.S. Romolo, S. Strano-Rossi, High-throughput screening for new psychoactive substances (NPS) in whole blood by DLLME extraction and UHPLC-MS/MS analysis, J. Chromatogr. B Anal. Technol. Biomed. Life Sci. 1000 (2015) 57-68. 10.1016/j.jchromb.2015.07.007.

[21] Scientific Working Group for Forensic Toxicology (SWGTOX), Standard Practices for Method Validation in Forensic Toxicology. J. Anal. Toxicol. 37(7) (2013) 452-474. 10.1093/jat/bkt054.

Validation of a simple and quick method for determination of psychoactive substances, drugs and their metabolites from human blood by LC-MS/MS

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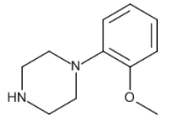
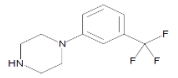
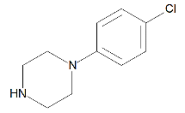
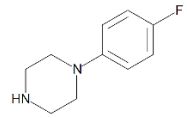
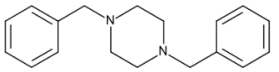
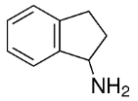
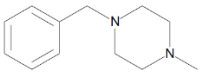
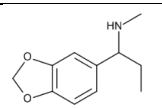
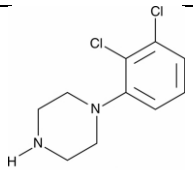
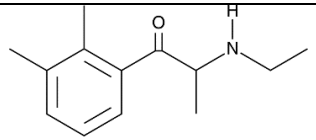
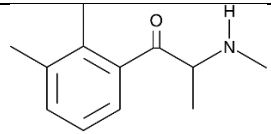
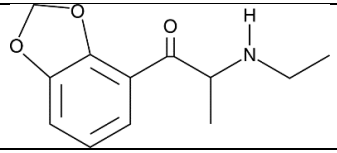
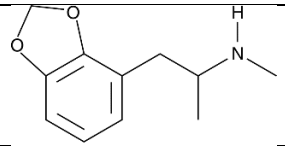
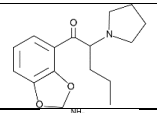
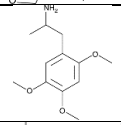
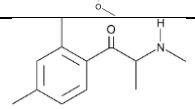
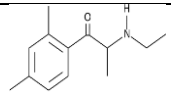
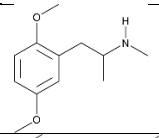
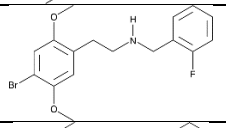
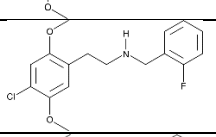
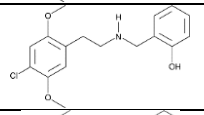
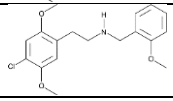
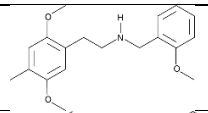
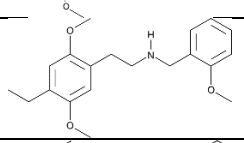
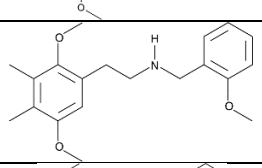
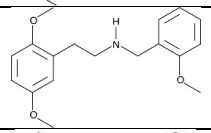
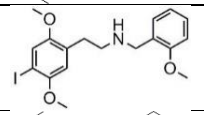
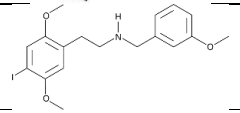
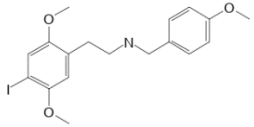
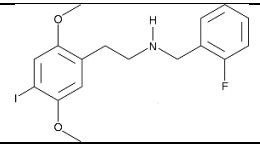
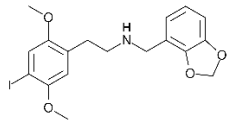
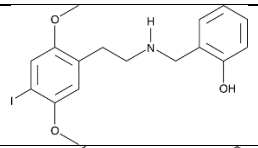
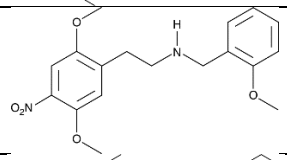
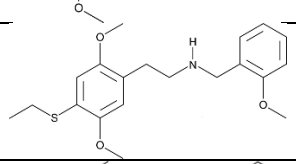
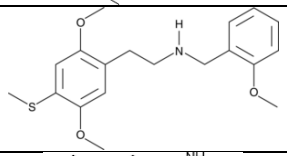
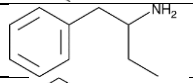
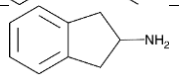
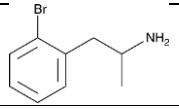
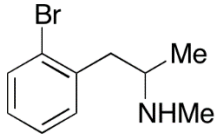
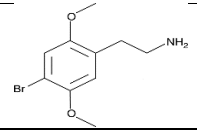
Table S1. Full chemical name, its abbreviation, full chemical structure, precursor ion, and CAS number.

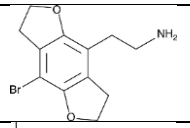
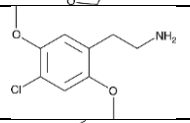
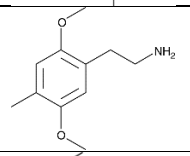
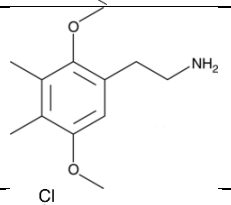
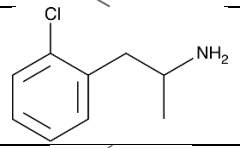
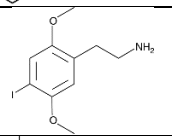
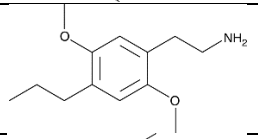
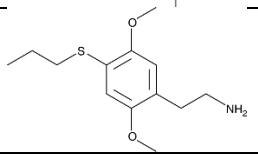
PRECURSOR ION (Q1)	ANALYTE	FORMAL NAME	SYNONYM	FULL CHEMICAL STRUCTUTRE	CAS NUMBER
193,263	1-(2-METHOXYPHENYL)PIPERAZINE	1-(2-METHOXYPHENYL)PIPERAZINE	1-(2-METHOXYPHENYL)PIPERAZINE		38869-49-7
231,278	1-(3-TRIFLUOROMETHYLPHENYL)PIPERAZINE (TFMPP)	1-(3-TRIFLUOROMETHYLPHENYL)PIPERAZINE	TFMPP		16015-69-3
197,469	1-(4-CHLOROPHENYL)PIPERAZINE (pCPP)	1-(4-CHLOROPHENYL)PIPERAZINE	pCPP		38212-33-8
181,26	1-(4-FLUOROPHENYL)PIPERAZINE (FPP)	1-(4-FLUOROPHENYL)PIPERAZINE	FPP		2252-63-3

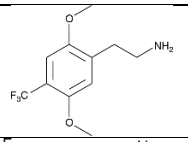
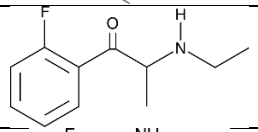
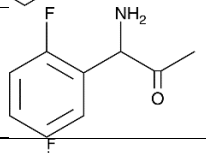
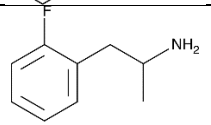
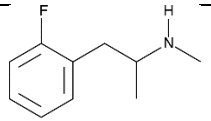
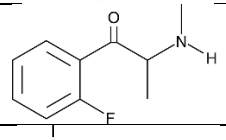
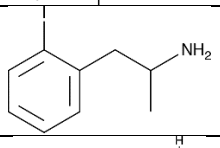
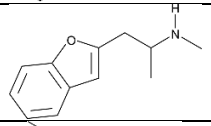
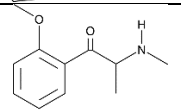
267,107	1,4-DIBENZYLPIPERAZINE (DBZP)	1,4-DIBENZYLPIPERAZINE	DBZP		2298-55-7
134,019	1-AMINOINDAN	2,3-dihydro-1H-inden-1-amine	1-AI		34698-41-4
191,061	1-METHYL-4-BENZYLPIPERAZINE (MBZP)	1-methyl-4-(phenylmethyl)-piperazine	MBZP		374898-00-7
194,261	1-METHYLAMINO-1-(3,4-METHYLENEDIOXYPHENYL)PROPANE	1-METHYLAMINO-1-(3,4-METHYLENEDIOXYPHENYL)PROPANE	M-ALPHA		127292-43-7
230,937	2,3-DICHLOROPHENYLPIPERAZINE (DCPP)	2,3-DICHLOROPHENYLPIPERAZINE	2,3-DCPP		119532-26-2
206,062	2,3-DIMETHYLETHCATHINONE (2,3-DMEC)	2,3-DIMETHYLETHCATHINONE; 1-(2,3-dimethylphenyl)-2-(ethylamino)propan-1-one	2,3-DMEC		2705531-06-0
192,202	2,3-DIMETHYLMETHCATHINONE (2,3-DMMC)	2,3-DIMETHYLMETHCATHINONE; 1-(2,3-dimethylphenyl)-2-(methylamino)propan-1-one,	2,3-DMMC		1797981-99-7
222,247	2,3-ETHYLONE ISOMER	1-(1,3-benzodioxol-4-yl)-2-(ethylamino)-1-propanone	2,3-Methylenedioxy-α ethylaminopropiophenone		2749504-06-9

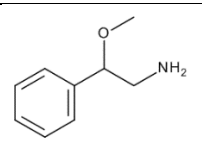
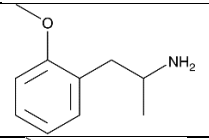
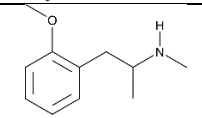
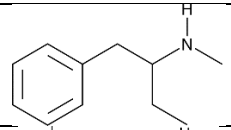
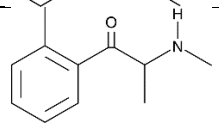
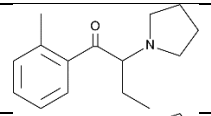
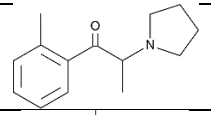
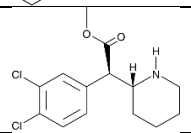
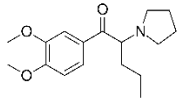
194,351	2,3-MDMA	2,3-Methylenedioxymethylamphetamine	2,3-MDMA		168968-01-2
276,236	2,3-MDPV	2,3-Methylenedioxy Pyrovalerone	2,3-MDPV		24622-62-6
226,297	2,4,5-TRIMETHOXYAMPHETAMINE	2,4,5-trimethoxy-α-methyl-benzeneethanamine	2,4,5-TRIMETHOXYAMPHETAMINE		15995-72-9
192,19	2,4-DIMETHYLMETHCATHINONE (2,4-DMMC)	1-(2,4-dimethylphenyl)-2-(methylamino)-1-propanone	2,4-DMMC		2412098-39-4
206,063	2,4-DMEC	1-(2,4-dimethylphenyl)-2-(ethylamino)propan-1-one	2,4-DMEC		2702352-15-4
210,264	2,5-DMMA	2,5-dimethoxy-N,α-dimethyl-benzeneethanamine	2,5-DMMA		54687-43-3
368,124	25B-NBF	4-bromo-N-[(2-fluorophenyl)methyl]-2,5-dimethoxy-benzeneethanamine	25B-NBF		1539266-17-5
324,164	25C-NBF	4-chloro-N-[(2-fluorophenyl)methyl]-2,5-dimethoxy-benzeneethanamine	25C-NBF		1539266-21-1
322,138	25C-NBOH	2-[[[2-(4-chloro-2,5-dimethoxyphenyl)ethyl]amino]methyl]-phenol	25C-NBOH		1539266-20-0
336,16	25C-NBOMe	2-(4-chloro-2,5-dimethoxyphenyl)-N-(2-methoxybenzyl)ethanamine	25C-NBOMe		1539266-19-7

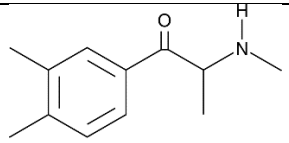
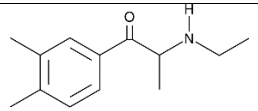
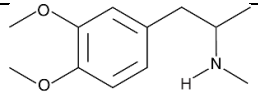
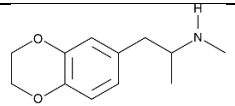
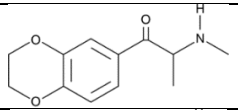
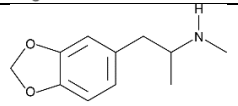
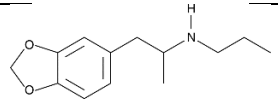
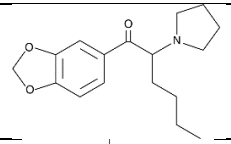
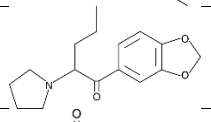
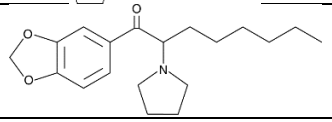
316,169	25D-NBOMe	2,5-dimethoxy-N-[(2-methoxyphenyl)methyl]-4-methyl-benzeneethanamine	25D-NBOMe		1539266-35-7
330,231	25E-NBOMe	4-ethyl-2,5-dimethoxy-N-[(2-methoxyphenyl)methyl]-benzeneethanamine	25E-NBOMe		1539266-39-1
330,142	25G-NBOMe	2,5-dimethoxy-N-[(2-methoxyphenyl)methyl]-3,4-dimethyl-benzeneethanamine	25G-NBOMe		1797132-54-7
302,346	25H-NBOMe	2-(2,5-dimethoxyphenyl)-N-(2-methoxybenzyl)ethanamine	25H-NBOMe		1566571-52-5
428,183	25-I-NB2OMe	2-(4-Iodo-2,5-dimethoxyphenyl)-N-[(2-methoxyphenyl)methyl] ethanamine	25-I-NB2OMe		1043868-97-8
428,176	25I-NB3OMe	2-(4-iodo-2,5-dimethoxyphenyl)-N-(3-methoxybenzyl)ethanamine	25I-NB3OMe		1566571-40-1
428,177	25I-NB4OMe	2-(4-iodo-2,5-dimethoxyphenyl)-N-(4-methoxybenzyl)ethan-1-amine, monohydrochloride	25I-NB4OMe		1566571-64-9
416,016	25I-NBF	N-(2-fluorobenzyl)-2-(4-iodo-2,5-dimethoxyphenyl)ethanamine	25I-NBF		1539266-13-1
442,154	25I-NBMD	N-(1,3-benzodioxol-4-ylmethyl)-2-(4-iodo-2,5-dimethoxyphenyl)ethanamine	25I-NBMD		1539266-14-2

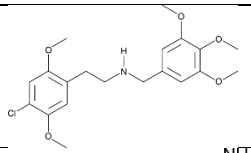
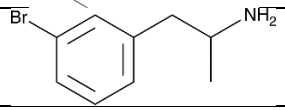
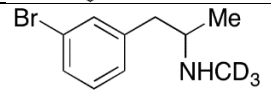
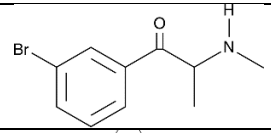
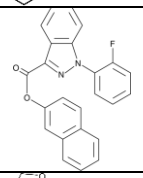
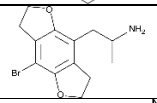
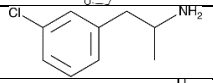
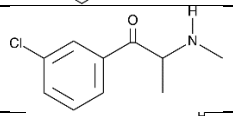
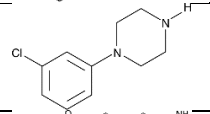
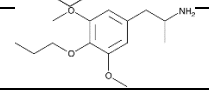
414,121	25I-NBOH	2-(((4-iodo-2,5-dimethoxyphenethyl)amino)methyl)phenol	25I-NBOH		1539266-12-0
347,2	25N-NBOMe	2,5-dimethoxy-N-[(2-methoxyphenyl)methyl]-4-nitro-benzeneethanamine	25N-NBOMe		1566571-65-0
362,264	25T2-NBOMe	4-(ethylthio)-2,5-dimethoxy-N-[(2-methoxyphenyl)methyl]-benzeneethanamine	25T2-NBOMe		1539266-51-7
348,035	25T-NBOMe	2,5-dimethoxy-N-[(2-methoxyphenyl)methyl]-4-(methylthio)-benzeneethanamine	25T-NBOMe		1539266-47-1
150,209	2-AMINO-1-PHENYLBUTANE	α-ethyl-benzeneethanamine	2-AMINO-1-PHENYLBUTANE		20735-15-3
134,257	2-AMINOINDANE	2-AMINOINDANE	2-AI		2338-18-3
214,186	2-BROMOAMPHETAMINE	2-bromo-α-methyl-benzeneethanamine	2-BA		861006-36-2
228,188	2-BROMOMETHAMPHETAMINE	1-(2-bromophenyl)-n-methylpropan-2-amine	2-BROMOMETHAMPHETAMINE		23695-11-6
259,957	2C-B	4-Bromo-2,5-dimethoxyphenethylamine	2C-B		56281-37-9

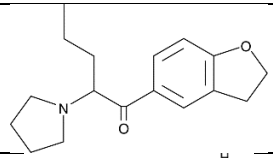
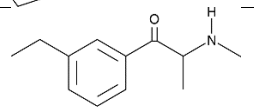
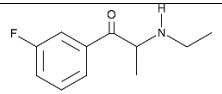
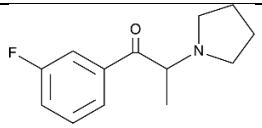
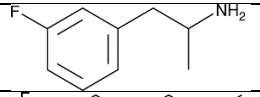
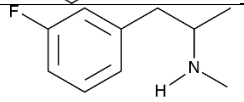
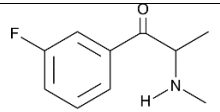
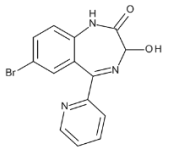
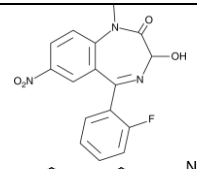
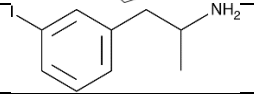
283,976	2C-B_FLY	8-bromo-2,3,6,7-tetrahydro-benzo[1,2-b:4,5-b']difuran-4-ethanamine	2C-B_FLY		178557-21-6
216,441	2C-C	2,5-Dimethoxy-4-chlorophenethylamine	2C-C		88441-15-0
195,583	2C-D	2,5-Dimethoxy-4-methylphenethylamine	2C-D		25505-65-1
210,052	2C-G	3,4-Dimethyl-2,5-dimethoxyphenethylamine	2C-G		327175-14-4
170,196	2-CHLOROAMPHETAMINE	2-chloro-α-methyl-benzeneethanamine	2-CA		35334-29-3
307,947	2C-I	2,5-Dimethoxy-4-iodophenethylamine	2C-I		64584-32-3
224,065	2C-P	2,5-Dimethoxy-4-propylphenethylamine	2C-P		1359704-27-0
256,022	2C-T-7	2,5-Dimethoxy-4-propylthiophenethylamine	2C-T-7		850140-15-7

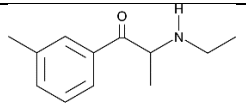
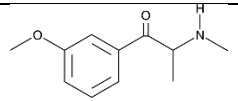
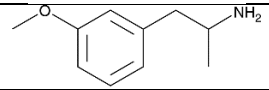
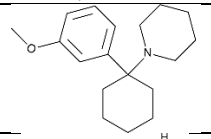
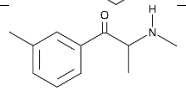
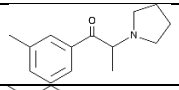
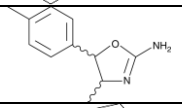
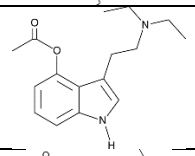
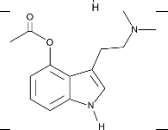
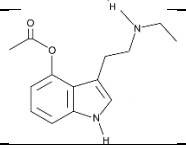
250,269	2C-TFM	2,5-dimethoxy-4-(trifluoromethyl)-benzeneethanamine	2C-TFM		159277-13-1
196,255	2-FEC	2-(ethylamino)-1-(2-fluorophenyl)-1-propanone	2-FEC		2446466-63-1
168,199	2-FIC	1-amino-1-(2-fluorophenyl)-2-propanone	2-FIC		1909305-71-0
154,13	2-FLUOROAMPHETAMINE	2-fluoro-α-methyl-benzeneethanamine	2-FA		1626-69-3
168,247	2-FLUOROMETHAMPHETAMINE (2-FMA)	2-fluoro-N-α-dimethyl-benzeneethanamine	2-FMA		1780004-19-4
182,187	2-FLUOROMETHCATHINONE (2-FMC)	1-(2-fluorophenyl)-2-(methylamino)propan-1-one	2-FMC		1346599-37-8
262,178	2-IODOAMPHETAMINE	2-iodo-α-methyl-benzeneethanamine	2-IA		22080-10-0
190,239	2-MAPB	N,α-dimethyl-2-benzofuranethanamine	2-MAPB		100389-74-0
194,219	2-MeOMC	1-(2-methoxyphenyl)-2-(methylamino)propan-1-one	2-MeOMC		No. Description

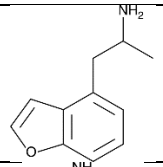
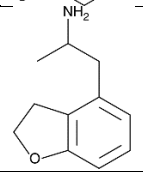
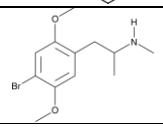
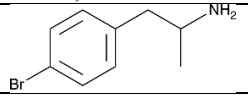
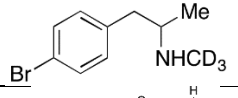
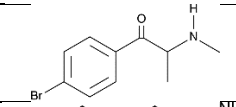
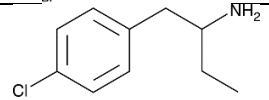
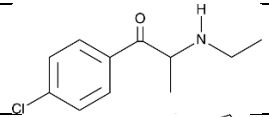
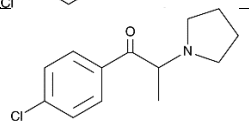
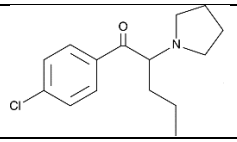
152,214	2-METHOXY-2-PHENYLETHYLAMINE	2-methoxy-2-phenylethanamine	2-methoxy-2-phenylethanamine		62064-68-0
166,068	2-METHOXYAMPHETAMINE (2-MA)	2-methoxy-α-methyl-benzeneethanamine	2-MA		72739-03-8
180,322	2-METHOXYMETHAMPHETAMINE (2-MeOMA)	2-methoxy-N,α-dimethyl-benzeneethanamine	2-MeOMA		5588-10-3
164,237	2-METHYLAMINO-1-PHENYLBUTANE	α-ethyl-N-methyl-benzeneethanamine	2-METHYLAMINO-1-PHENYLBUTANE		84952-63-6
178,06	2-METHYLMETHCATHINONE (2-MMC)	2-(methylamino)-1-(2-methylphenyl)-1-propanone	2-MMC		1246815-51-9
232,265	2-METHYL-PBP	2-(pyrrolidin-1-yl)-1-(o-tolyl)butan-1-one	2-METHYL-PBP		No. Description
218,291	2-METHYL-PPP	1-(2-methylphenyl)-2-(1-pyrrolidinyl)-1-propanone	2-METHYL-PPP		2749897-10-5
303,454	3,4-DICHLOROMETHYLPHENIDATE (3,4-CTMP)	(αR,2R)-*rel*-α-(3,4-dichlorophenyl)-2-piperidineacetic acid	3,4-CTMP		214149-42-5
292,246	3,4-DIMETHOXY-ALPHA-PVP	3',4'-Dimethoxy-α-pyrrolidinopentiophenone	3,4-DMPV		850351-99-4

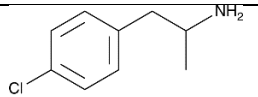
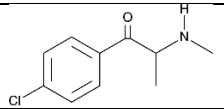
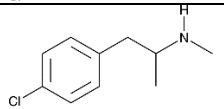
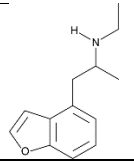
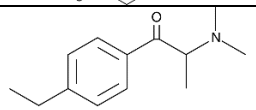
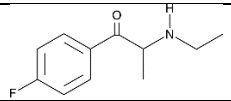
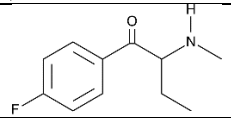
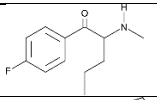
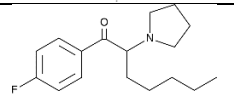
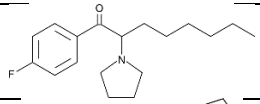
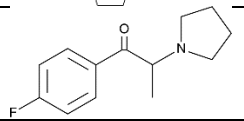
192,031	3,4-DIMETHYLMETHCATHINONE (3,4-DMMC)	1-(3,4-dimethylphenyl)-2-(methylamino)-1-propanone	3,4-DMMC		1081772-06-6
206,146	3,4-DMEC	1-(3,4-dimethylphenyl)-2-(ethylamino)propan-1-one	3,4-DMEC		2748561-69-3
210,063	3,4-DMMA	3,4-dimethoxy-N,α-dimethyl-benzeneethanamine	3,4-DMMA		70932-18-2
208,248	3,4-EDMA	1-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-N-methylpropan-2-amine	3,4-EDMA		2748304-41-6
222,191	3,4-EDMC	1-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-(methylamino)-1-propanone	3,4-EDMC		30253-44-2
194,025	3,4-MDMA (ECSTAZY)	N,α-dimethyl-1,3-benzodioxole-5-ethanamine	3,4-MDMA		64057-70-1
222,051	3,4-MDPA	α-methyl-N-propyl-1,3-benzodioxole-5-ethanamine	3,4-MDPA		3,4-MDPA
290,285	3,4-MDPHP	1-(1,3-benzodioxol-5-yl)-2-(1-pyrrolidinyl)-1hexanone	3,4-MDPHP		24622-61-5
276,144	3,4-METHYLENDIOXYPYROVALERONE	1-(1,3-benzodioxol-5-yl)-2-(1-pyrrolidinyl)-1-pentanone	3,4-MDPV		24622-62-6
318,23	3,4-METHYLENEDIOXY_PV9	1-(1,3-benzodioxol-5-yl)-2-(1-pyrrolidinyl)-1-octanone	3,4-METHYLENEDIOXY PV9		24646-40-0

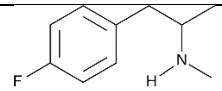
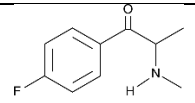
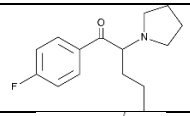
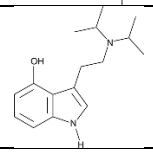
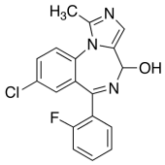
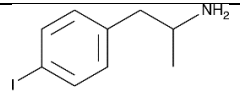
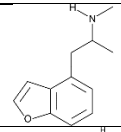
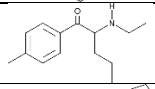
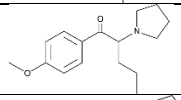
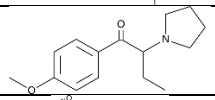
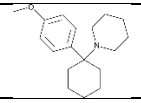
396,257	30C-NBOMe	2-(4-chloro-2,5-dimethoxyphenyl)-N-(3,4,5-trimethoxybenzyl)ethanamine	30C-NBOMe		2749391-65-7
214,192	3-BROMOAMPHETAMINE	3-bromo-α-methyl-benzeneethanamine	3-BA		1210708-61-4
228,18	3-BROMOMETHAMPHETAMINE	3-BROMOMETHAMPHETAMINE	3-BMA		28100-41-6
244,143	3-BROMOMETHCATHINONE (3-BMC)	1-(3-bromophenyl)-2-(methylamino)-1-propanone	3-BMC		676487-42-6
383,161	3-CAF	1-(2-fluorophenyl)-1H-indazole-3-carboxylic acid	3-CAF		2219324-25-9
298,069	3C-B-FLY	8-bromo-2,3,6,7-tetrahydro-α-methyl-benzo[1,2-b:4,5-b']difuran-4-ethanamine	3C-B-FLY		178557-19-2
170,206	3-CHLOROAMPHETAMINE	3-chloro-α-methyl-benzeneethanamine	3-CA		35378-15-5
198,231	3-CHLOROMETHCATHINONE (3-CMC)	1-(3-chlorophenyl)-2-(methylamino)-1-propanone	3-CMC		1607439-32-6
197,249	3-CHLOROPHENYLPIPERAZINE (mCPP)	1-(3-chlorophenyl)-piperazine	mCPP		13078-15-4
254,286	3C-P	3,5-dimethoxy-α-methyl-4-propoxy-benzeneethanamine	3C-P		2749897-26-3

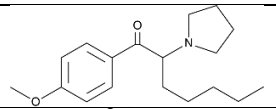
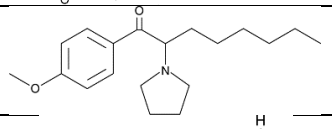
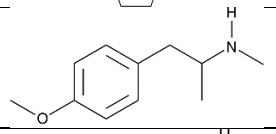
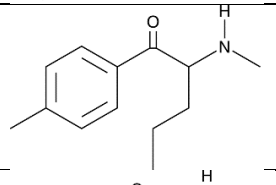
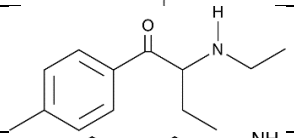
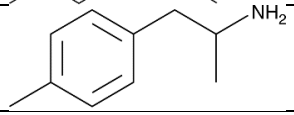
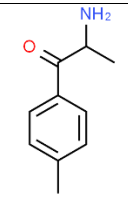
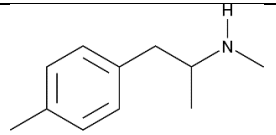
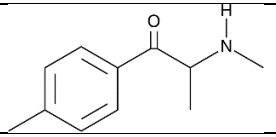
274,249	3-DESOXY-3,4-MDPV	1-(2,3-dihydro-5-benzofuranyl)-2-(1-pyrrolidinyl)-1-pentanone	3-DESOXY-3,4-MDPV		2117405-33-9
192,22	3-ETHYLMETHCATHINONE (3-EMC)	1-(3-ethylphenyl)-2-(methylamino)-1-propanone	3-EMC		2446466-60-8
196,262	3-FEC	2-(ethylamino)-1-(3-fluorophenyl)-1-propanone	3-FEC		2446466-64-2
222,28	3-FLUORO-ALFA-PPP	1-(3-fluorophenyl)-2-(1-pyrrolidinyl)-1-propanone	3-FLUORO-ALFA-PPP		1214940-15-4
154,134	3-FLUOROAMPHETAMINE	3-fluoro-α-methyl-benzeneethanamine	3-FA		1716-59-2
168,223	3-FLUOROMETHAMPHETAMINE (3-FMA)	1-(3-fluorophenyl)-N-methylpropan-2-amine	3-FMA		1324717-74-9
182,014	3-FLUOROMETHCATHINONE (3-FMC)	1-(3-fluorophenyl)-2-(methylamino)propan-1-one	3-FMC		1346600-40-5
331,895	3-HYDROXYBROMAZEPAM	7-bromo-3-hydroxy-5-pyridin-2-yl-1,3-dihydro-1,4-benzodiazepin-2-one	3-HYDROXYBROMAZEPAM		13132-73-5
330,031	3-HYDROXYFLUNITRAZEPAM	5-(2-fluorophenyl)-1,3-dihydro-3-hydroxy-1-methyl-7-nitro-2H-1,4-benzodiazepin-2-one	3-HYDROXYFLUNITRAZEPAM		67739-71-3
262,179	3-IODOAMPHETAMINE	3-iodo-α-methyl-benzeneethanamine	3-IA		20110-56-9

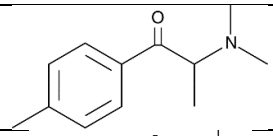
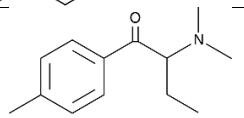
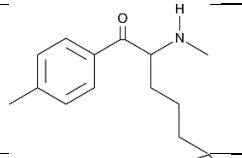
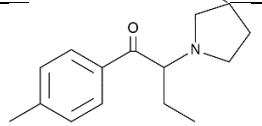
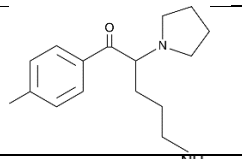
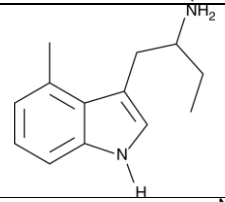
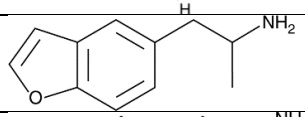
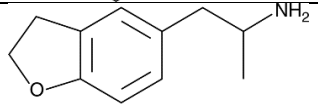
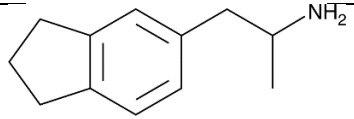
192,185	3-MEC	2-(ethylamino)-1-(3-methylphenyl)-1-propanone	3-MEC		2493976-59-1
194,225	3-MeOMC	1-(3-methoxyphenyl)-2-(methylamino)propan-1-one	3-MeOMC		1435933-70-2
166,07	3-METHOXYAMPHETAMINE (3-MA)	3-methoxy-α-methyl-benzeneethanamine	3-MA		35294-10-1
274,19	3-METHOXYPHENCYCLIDINE	1-[1-(3-methoxyphenyl)cyclohexyl]-piperidine	3-MeO PCP		72242-03-6
178,046	3-METHYLMETHCATHINONE (3-MMC)	2-(methylamino)-1-(3-methylphenyl)-1-propanone	3-MMC		1246816-62-5
218,209	3-METHYL-PPP	1-(3-methylphenyl)-2-(1-pyrrolidinyl)-1-propanone	3-METHYL-PPP		2749302-38-1
191,255	4,4'-DMAR	4,5-dihydro-4-methyl-5-(4-methylphenyl)-2-oxazolamine	4,4'-DMAR		1445569-01-6
275,216	4-AcO-DET	3-[2-(diethylamino)ethyl]-1H-indol-4-ol 4-acetate	4-AcO-DET		1135424-15-5
247,314	4-AcO-DMT	3-[2-(dimethylamino)ethyl]-1H-indol-4-ol-4-acetate	4-AcO-DMT		2748484-99-1
261,3	4-AcO-MET	3-[2-(ethylmethylamino)ethyl]-1H-indol-4-ol 4-acetate	4-AcO-MET		2748591-02-6

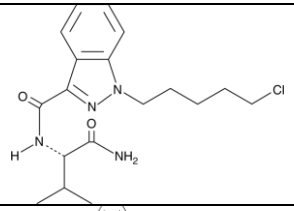
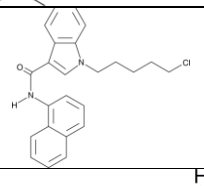
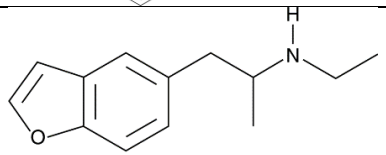
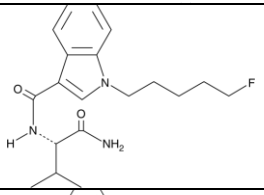
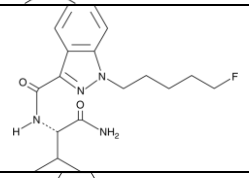
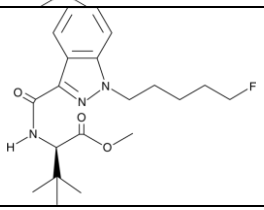
176,148	4-APB	α-methyl-4-benzofuranethanamine	4-APB		286834-82-0
178,238	4-APDB	2,3-dihydro-α-methyl-4-benzofuranethanamine	4-APDB		1203342-42-0
288,233	4-BROMO-2,5-DMMA	4-bromo-2,5-dimethoxy-N,α-dimethyl-benzeneethanamine	4-BROMO-2,5-DMMA		155638-80-5
214,182	4-BROMOAMPHETAMINE	4-bromo-α-methyl-benzeneethanamine	4-BA		58400-88-7
228,205	4-BROMOMETHAMPHETAMINE	1-(4-Bromophenyl)-n-methylpropan-2-amine	4-BMA		30651-67-3
243,495	4-BROMOMETHCATHINONE (BREFEDRONE)	1-(4-bromophenyl)-2-(methylamino)-1-propanone	4-BMC		135333-27-6
184,174	4-CAB	4-chloro-α-ethyl-benzeneethanamine	4-CAB		23292-08-2
212,21	4-CEC	1-(4-chlorophenyl)-2-(ethylamino)-1-propanone	4-CEC		22198-75-0
238,267	4-CHLORO-ALPHA-PPP	1-(4-chlorophenyl)-2-(1-pyrrolidinyl)-1-propanone	4-CHLORO-ALPHA-PPP		28117-79-5
266,3	4-CHLORO-ALPHA-PVP	1-(4-chlorophenyl)-2-(1-pyrrolidinyl)-1-pentanone	4-CHLORO-ALPHA-PVP		5881-77-6

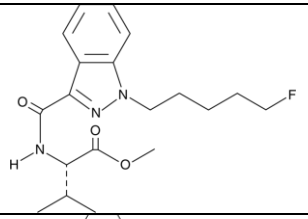
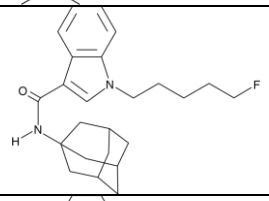
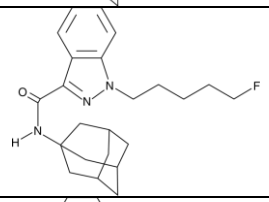
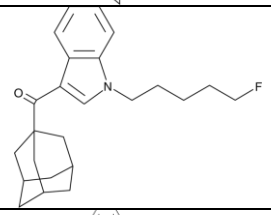
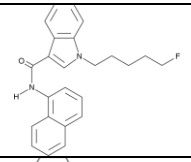
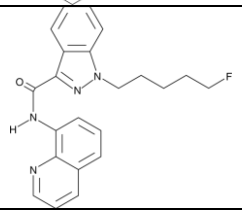
170,197	4-CHLOROAMPHETAMINE	4-chloro-α-methyl-benzeneethanamine	4-CA		3706-38-5
198	4-CHLOROMETHCATHINONE (4-CMC)	1-(4-chlorophenyl)-2-(methylamino)-1-propanone	4-CMC		2319878-22-1
184,235	4-CMA	4-chloro-N,α-dimethyl-benzeneethanamine	4-CMA		30572-91-9
204,264	4-EAPB	1-(benzofuran-4-yl)-N-ethylpropan-2-amine	4-EAPB		2514946-32-6
206,207	4-ETHYL-N,N-DMC	2-(dimethylamino)-1-(4-ethylphenyl)-1-propanone	4-ETHYL-N,N-DMC		2702382-98-5
196,26	4-FEC	2-(ethylamino)-1-(4-fluorophenyl)-1-propanone	4-FEC		2705473-25-0
196,234	4-FLUORO BUPHEDRONE	1-(4-fluorophenyl)-2-(methylamino)-1-butanone	4-FBP		2624137-27-3
210,264	4-FLUORO PENTEDRONE	1-(4-fluorophenyl)-2-(methylamino)pentan-1-one	4-FPD		2469350-88-5
278,165	4-FLUORO PV8	1-(4-fluorophenyl)-2-(pyrrolidin-1-yl)heptan-1-one	4-fluoro α-PHPP		2748485-01-8
292,257	4-FLUORO PV9	1-(4-fluorophenyl)-2-(1-pyrrolidinyl)-1-octanone	F-α-POP		2117405-40-8
222,267	4-FLUORO-ALPHA-PPP	1-(4-fluorophenyl)-2-(1-pyrrolidinyl)-1-propanone	4'-fluoro-α-PPP		2748590-18-1

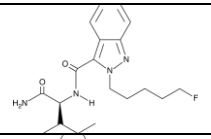
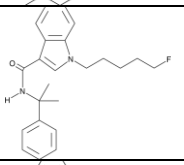
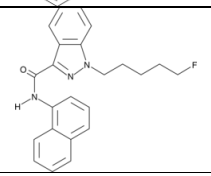
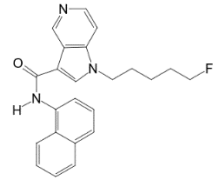
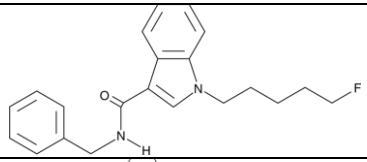
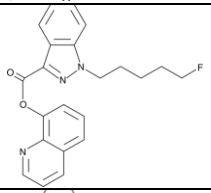
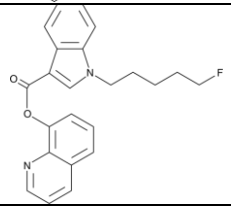
168,214	4-FLUOROMETHAMPHETAMINE (4-FMA)	4-fluoro-N-α-dimethyl-benzeneethanamine	4-FMA		52063-62-4
182,011	4-FLUOROMETHCATHINONE (4-FMC)	1-(4-fluorophenyl)-2-(methylamino)propan-1-one	4-FMC		7589-35-7
250,25	4F-PVP	1-(4-fluorophenyl)-2-(1-pyrrolidinyl)-1-pentanone	4-fluoro-α-PVP		850352-31-7
262,005	4-HYDROXY DiPT	3-[2-[*bis*(1-methylethyl)amino]ethyl]-1H-indol-4-ol,	4-OH DiPT		63065-90-7
341,932	4-HYDROXYMIDAZOLAM	8-chloro-6-(2-fluorophenyl)-1-methyl-4h-imidazo[1,5-a][1,4]benzodiazepin-4-ol	4-HYDROXYMIDAZOLAM		59468-85-8
262,177	4-IODOAMPHETAMINE	4-iodo-α-methyl-benzeneethanamine	4-IA		21894-58-6
190,254	4-MAPB	1-(benzofuran-4-yl)-N-methylpropan-2-amine	4-MAPB		No. Description
220,297	4-MEAP	2-(ethylamino)-1-(4-methylphenyl)-1-pentanone	4-MEAP		18297-05-7
262,212	4-MEO-ALPHA-PVP	1-(4-methoxyphenyl)-2-(1-pyrrolidinyl)-1-pentanone	4-MeO-α-PVP		5537-19-9
248,282	4-MeOPBP	1-methoxyphenyl)-2-(pyrrolidin-1-yl)butan-1-one	4-MeOPBP		2749897-35-4
274,176	4-METHOXY PHENCYCLIDINE	1-[1-(4-methoxyphenyl)cyclohexyl]-piperidine,	4-MeO PCP		2185-93-5

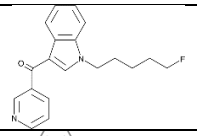
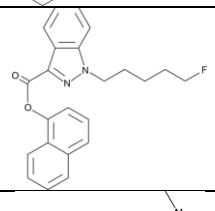
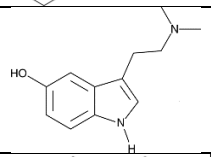
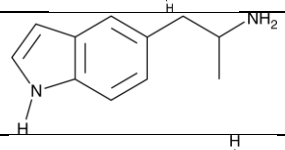
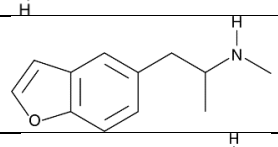
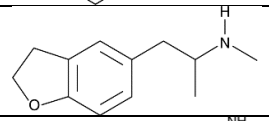
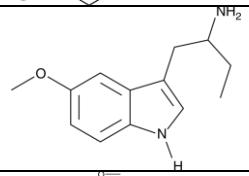
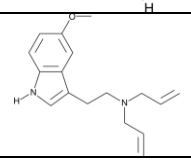
290,295	4-METHOXY PV8	1-(4-methoxyphenyl)-2-(pyrrolidin-1-yl)heptan-1-one	4-MeO PV8		2749302-60-9
304,286	4-METHOXY PV9	1-(4-methoxyphenyl)-2-(pyrrolidin-1-yl)octan-1-one	4-MeO PV9		2748590-60-3
180,289	4-METHOXYMETHAMPHETAMINE (PMMA)	4-methoxy-N,α-dimethyl-benzeneethanamine	PMMA		3398-68-3
206,274	4-METHYL PENTEDRONE	2-(methylamino)-1-(*p*-tolyl)pentan-1-one	4-MPD		1373918-61-6
206,11	4-METHYL-ALPHA-ETHYLAMINOBUTIOPHENONE	2-(ethylamino)-1-(4-methylphenyl)-1-butanone	4-METHYL-ALPHA-ETHYLAMINOBUTIOPHENONE		18268-19-4
150,227	4-METHYLAMPHETAMINE	α,4-dimethyl-benzeneethanamine	4-MA		41632-56-8
164,232	4-METHYLCATHINONE	2-Amino-1-(4-methylphenyl)-1-propanone	4-METHYLCATHINONE		31952-47-3
164,25	4-METHYLMETHAMPHETAMINE (4-MMA)	N,α,4-trimethyl-benzeneethanamine	4-MMA		161697-16-1
178,066	4-METHYLMETHCATHINONE (4-MMC)	2-(methylamino)-1-(4-methylphenyl)-1-propanone	4-MMC		1189726-22-4

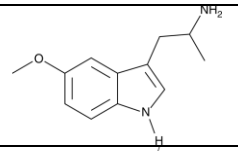
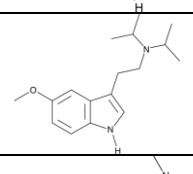
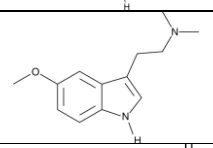
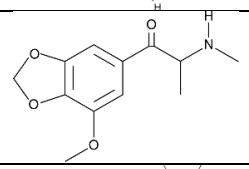
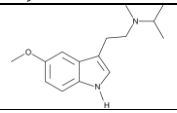
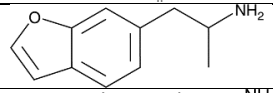
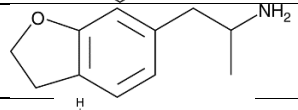
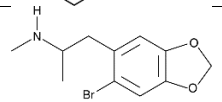
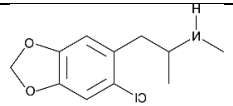
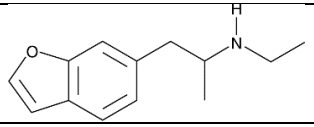
192,249	4-METHYL-N,N-DMC	2-(dimethylamino)-1-(4-methylphenyl)-1-propanone	4-METHYL-N,N-DMC		1448845-14-4
206,209	4-METHYL-N-METHYLBUPHEDRONE	2-(dimethylamino)-1-(4-methylphenyl)-1-butanone	4-METHYL-N-METHYLBUPHEDRONE		2748589-93-5
220,287	4-METHYL-N-METHYLHEXANOPHENONE	2-(methylamino)-1-(*p*-tolyl)hexan-1-one,	4'-Methylhexedrone		2168553-84-0
232,31	4-METHYL-PBP	1-(4-methylphenyl)-2-(1-pyrrolidinyl)-1-butanone	4-METHYL-PBP		1214-15-9
260,347	4-METHYL-PHP	2-(pyrrolidin-1-yl)-1-(*p*-tolyl)hexan-1-one	PV4		1391052-36-0
203,04	4-METHYL-α-ETHYLTRYPTAMINE	α-ethyl-4-methyl-1H-indole-3-ethanamine	4-methyl-α-ET		28289-30-7
176,082	5-APB	α-methyl-5-benzofuranethanamine	5-APB		286834-80-8
178,29	5-APDB	2,3-dihydro-α-methyl-5-benzofuranethanamine	5-APDB		152623-94-4
176,173	5-APDI	2,3-dihydro-α-methyl-1H-indene-5-ethanamine	5-APDI		152623-95-5

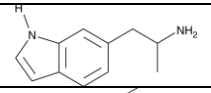
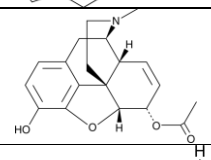
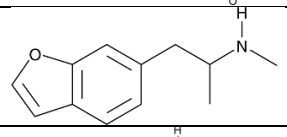
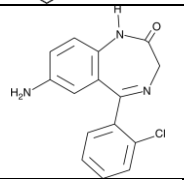
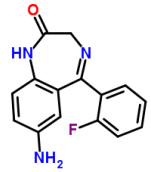
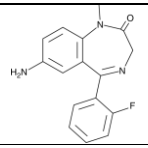
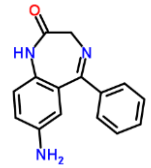
365,216	5-CHLORO AB-PINACA	N-[(1S)-1-(aminocarbonyl)-2-methylpropyl]-1-(5-chloropentyl)-1H-indazole-3-carboxamide	5-chloro ABP		1801552-02-2
391,226	5-CHLORO-NNEI	1-(5-chloropentyl)-N-1-naphthalenyl-1H-indole-3-carboxamide	5-CHLORO-NNEI		1800101-23-8
204,961	5-EAPB	N-ethyl-α-methyl-5-benzofuranethanamine	5-EAPB		1823776-22-2
348,07	5F-ABICA	N-[(1S)-1-(aminocarbonyl)-2-methylpropyl]-1-(5-fluoropentyl)-1H-indole-3-carboxamide	5F-ABICA		1801338-26-0
349,193	5F-AB-PINACA	N-[(1S)-1-(aminocarbonyl)-2-methylpropyl]-1-(5-fluoropentyl)-1H-indazole-3-carboxamide	5F-AB-PINACA		1800101-60-3
378,193	5F-ADB (5F-MDMB-PINACA)	N-[[1-(5-fluoropentyl)-1H-indazol-3-yl]carbonyl]-3-methyl-D-valine, methyl ester	5F-ADB		1715016-75-3

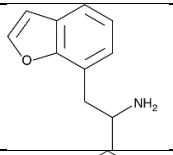
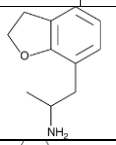
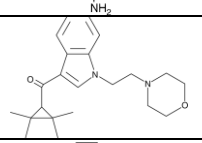
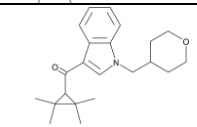
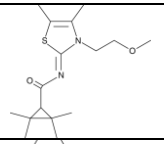
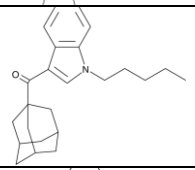
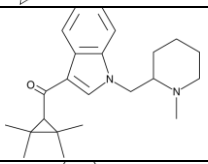
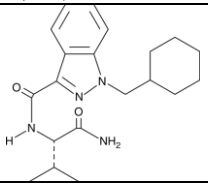
364,092	5F-AMB (5F-AMB-PINACA)	N-[[1-(5-fluoropentyl)-1H-indazol-3-yl]carbonyl]-L-valine, methyl ester	5F-AMB		1801552-03-3
383,14	5F-APICA (STS-135)	1-(5-fluoropentyl)-N-tricyclo[3.3.1.13,7]dec-1-yl-1H-indole-3-carboxamide	STS-135		1354631-26-7
384,207	5F-APINACA (AKB-48-5F)	N-((3s,5s,7s)-adamantan-1-yl)-1-(5-fluoropentyl)-1H-indazole-3-carboxamide	5F-APINACA		1400742-13-3
368,294	5-F-JWH-018 ADAMANTYL ANALOG	[1-(5-fluoropentyl)-1H-indol-3-yl]tricyclo[3.3.1.13,7]dec-1-yl-methanone	AM2201 adamantyl analog		1364933-62-9
375,043	5-FLUORO MN-24 (5-FLUORO NNEI)	1-(5-fluoropentyl)-N-(naphthalen-1-yl)-1H-indole-3-carboxamide	5-FLUORO MN-24		1445580-60-8
377,255	5-FLUORO THJ	1-(5-fluoropentyl)-N-8-quinolinyl-1H-indazole-3-carboxamide	5-FLUORO THJ		2180934-72-7

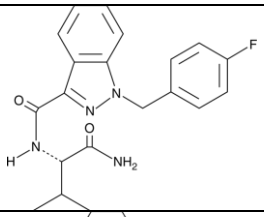
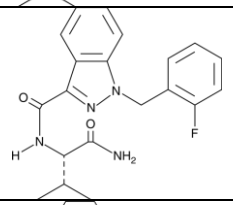
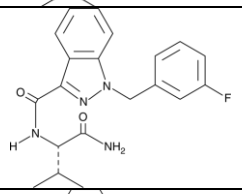
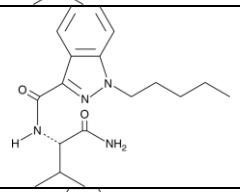
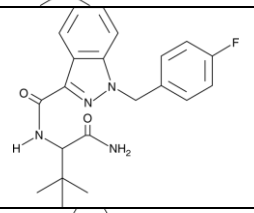
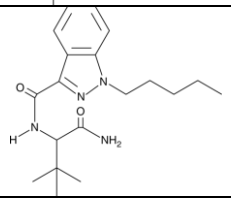
363,254	5-FLUORO-2-ADB-PINACA_ISOMER_2	N-(1-amino-3S-methyl-1-oxopentan-2S-yl)-2-(5-fluoropentyl)-2H-indazole-3-carboxamide	5-FLUORO-2-ADB-PINACA_ISOMER_2		2365471-68-5
367,233	5-FLUORO-CUMYL-PICA	1-(5-fluoropentyl)-N-(1-methyl-1-phenylethyl)-1H-indole-3-carboxamide	SGT-67		1400742-18-8
376,497	5-FLUORO-MN-18	1-(5-fluoropentyl)-N-1-naphthalenyl-1H-indazole-3-carboxamide	5-FLUORO-MN-18		1445581-91-8
376,066	5-FLUORO-MN-21 (5-FLUORO-PCN)	1-(5-Fluoropentyl)-N-(naphthalen-1-yl)-1H-pyrrolo(3,2-C)pyridine-3-carboxamide	5-FLURO-PCN		325373-36-9
339,222	5-FLUORO-SDB-006	1-(5-fluoropentyl)-N-(phenylmethyl)-1H-indole-3-carboxamide	5-FLUORO-SDB-006		1776086-02-2
378,028	5F-NPB-22	1-(5-fluoropentyl)-1H-Indazole-3-carboxylic acid, 8-quinolinyl ester	5F-NPB-22		1445579-79-2
377,092	5F-PB-22	1-(5-fluoropentyl)-8-quinolinyl ester-1H-indole-3-carboxylic acid	5F-PB-22		1400742-41-7

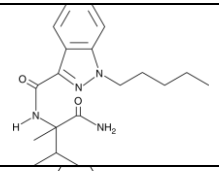
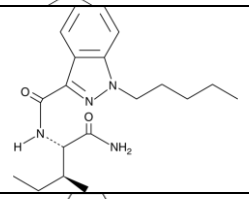
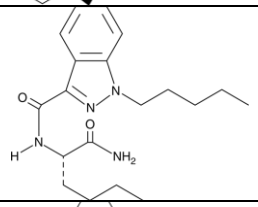
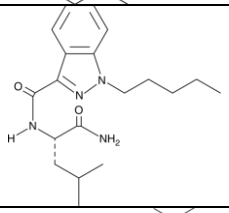
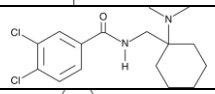
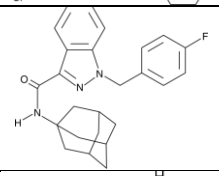
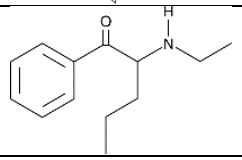
311,223	5-F-PENTYL-3-PYRIDINOYLINDOLE	[1-(5-fluoropentyl)-1H-indol-3-yl]-3-pyridinyl-methanone	5-F-PENTYL-3-PYRIDINOYLINDOLE		NOCAS_1018128
377,212	5F-SDB-005	1-(5-fluoropentyl)-1H-indazole-3-carboxylic acid, 1-naphthalenyl ester	5F-SDB-005		2185863-14-1
205,058	5-HYDROXY DMT	3-[2-(dimethylamino)ethyl]-1H-indol-5-ol	5-OH DMT		55206-22-9
175,275	5-IT	α-methyl-1H-indole-5-ethanamine	5-IT		3784-30-3
190,252	5-MAPB	N,α-dimethyl-5-benzofuranethanamine	5-MAPB		1823925-53-6
192,202	5-MAPDB	2,3-dihydro-N,α-dimethyl-5-benzofuranethanamine	5-MAPDB		2748590-04-5
219,295	5-MeO-ALPHA-ET	α-ethyl-5-methoxy-1H-indole-3-ethanamine	5-MeO-α-ET		4765-10-0
271,063	5-MeO-DALT	5-methoxy-N,N-di-2-propen-1-yl-1H-indole-3-ethanamine	5-MeO-DALT		928822-98-4

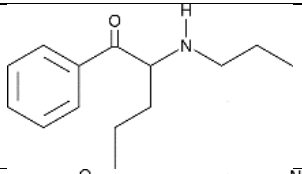
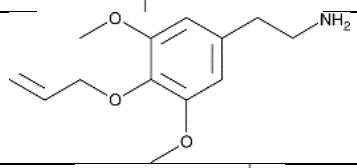
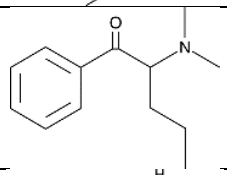
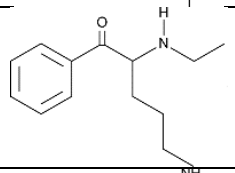
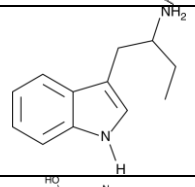
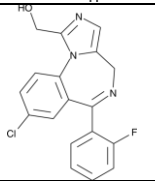
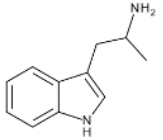
205,05	5-METHOXY AMT	5-methoxy-α-methyl-1H-indole-3-ethanamine	5-MeO AMT		1137-04-8
275,078	5-METHOXY DiPT	5-methoxy-N,N-*bis*(1-methylethyl)-1H-indole-3-ethanamine	5-MeO DiPT		4021-34-5
219,968	5-METHOXY DMT	5-methoxy-N,N-dimethyl-1H-indole-3-ethanamine	5-MeO DMT		1019-45-0
238,277	5-METHOXY METHYLONE	1-(7-methoxy-1,3-benzodioxol-5-yl)-2-(methylamino)-1-propanone	5-METHOXY METHYLONE		2702151-27-5
247,988	5-METHOXY MiPT	5-methoxy-N-methyl-N-(1-methylethyl)-1H-Indole-3-ethanamine	5-MeO MiPT		96096-55-8
176,049	6-APB	α-methyl-6-benzofuranethanamine	6-APB		286834-84-2
178,157	6-APDB	2,3-dihydro-α-methyl-6-benzofuranethanamine	6-APDB		1281872-58-9
272,17	6-BROMO-MDMA	1-(6-bromobenzo[d][1,3]dioxol-5-yl)-N-methylpropan-2-amine	6-BROMO-MDMA		No. Description
228,238	6-CHLORO-MDMA	1-(6-chlorobenzo[d][1,3]dioxol-5-yl)-N-methylpropan-2-amine	6-CHLORO-MDMA		319920-71-3
204,15	6-EAPB	N-ethyl-α-methyl-6-benzofuranethanamine	6-EAPB		1823318-37-1

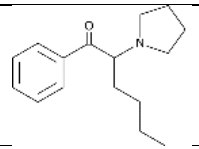
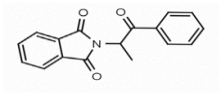
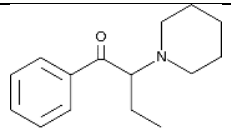
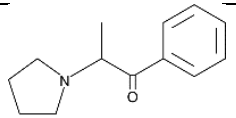
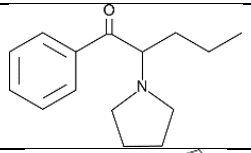
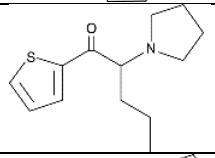
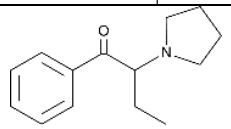
175,258	6-IT	α-methyl-1H-indole-6-ethanamine	6-IT		21005-63-0
328,01	6-MAM	(5α,6α)-7,8-didehydro-4,5-epoxy-17-methyl-morphinan-3,6-diol 6-acetate	6-MAM		2784-73-8
190,239	6-MAPB	N,α-dimethyl-6-benzofuranethanamine	6-MAPB		2731011-08-6
286,241	7-AMINOCLONAZEPAM	7-amino-5-(2-chlorophenyl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one	7-AMINOCLONAZEPAM		4959-17-5
270,396	7-AMINODESMETHYLFLUNITRAZEPAM	7-Amino-5-(o-fluorophenyl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one	7-AMINODESMETHYLFLUNITRAZEPAM		894-76-8
283,767	7-AMINOFLUNITRAZEPAM	7-amino-5-(2-fluorophenyl)-1,3-dihydro-1-methyl-2H-1,4-benzodiazepin-2-one	7-AMINOFLUNITRAZEPAM		34084-50-9
252,005	7-AMINONITRAZEPAM	7-amino-5-phenyl-1,3-dihydro-1,4-benzodiazepin-2-one	7-AMINONITRAZEPAM		4928-02-3

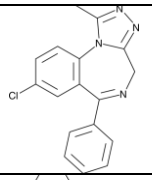
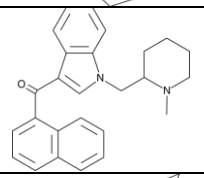
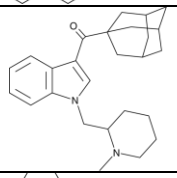
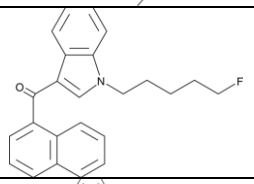
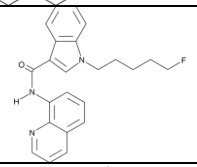
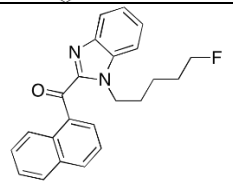
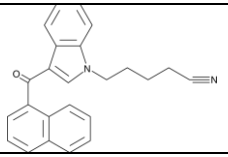
176,239	7-APB	α-methyl-7-benzofuranethanamine	7-APB		286834-86-4
178,233	7-APDB	2,3-dihydro-α-methyl-7-benzofuranethanamine	7-APDB		No. Description
355,053	A-796260	[1-[2-(4-morpholinyl)ethyl]-1H-indol-3-yl](2,2,3,3-tetramethylcyclopropyl)-methanone	A-796260		895155-26-7
340,308	A-834735	[1-[(tetrahydro-2H-pyran-4-yl)methyl]-1H-indol-3-yl](2,2,3,3-tetramethylcyclopropyl)-methanone	A-834735		895155-57-4
311,15	A-836339	[N(Z)]-N-[3-(2-methoxyethyl)-4,5-dimethyl-2(3H)-thiazolylidene]-2,2,3,3-tetramethyl-cyclopropanecarboxamide	A-836339		959746-77-1
350,211	AB-001	(1s,3s)-adamantan-1-yl(1-pentyl-1H-indol-3-yl)methanone	AB-001		1345973-49-0
352,92	AB005	[1-[(1-methyl-2-piperidinyl)methyl]-1H-indol-3-yl](2,2,3,3-tetramethylcyclopropyl)-methanone	AB005		895155-25-6
357,16	AB-CHMINACA	N-[(1S)-1-(aminocarbonyl)-2-methylpropyl]-1-(cyclohexylmethyl)-1H-indazole-3-carboxamide	AB-CHMINACA		1185887-21-1

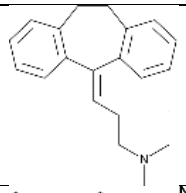
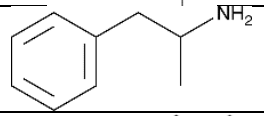
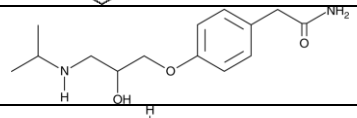
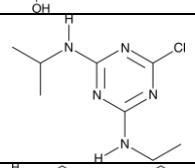
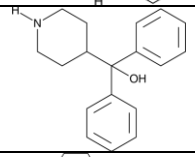
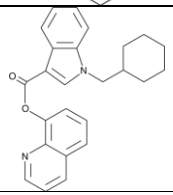
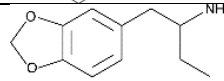
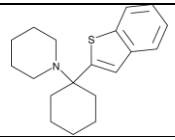
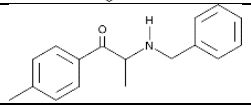
369,13	AB-FUBINACA	N-[(1S)-1-(aminocarbonyl)-2-methylpropyl]-1-[(4-fluorophenyl)methyl]-1H-indazole-3-carboxamide	AB-FUBINACA		1185282-01-2
369,269	AB-FUBINACA 2-FLUOROBENZYL ISOMER	N-[(1S)-1-(aminocarbonyl)-2-methylpropyl]-1-[(2-fluorophenyl)methyl]-1H-indazole-3-carboxamide	AB-FUBINACA 2-FLUOROBENZYL ISOMER		1185282-16-9
369,241	AB-FUBINACA 3-FLUOROBENZYL ISOMER	N-[(1S)-1-(aminocarbonyl)-2-methylpropyl]-1-[(3-fluorophenyl)methyl]-1H-indazole-3-carboxamide	AB-FUBINACA 3-FLUOROBENZYL ISOMER		1185282-19-2
331,065	AB-PINACA	(S)-N-(1-amino-3-methyl-1-oxobutan-2-yl)-1-pentyl-1H-indazole-3-carboxamide	AB-PINACA		1445752-09-9
382,972	ADB-FUBINACA	N-[1-(aminocarbonyl)-2,2-dimethylpropyl]-1-[(4-fluorophenyl)methyl]-1H-indazole-3-carboxamide	ADB-FUBINACA		1445583-51-6
345,052	ADB-PINACA	N-[1-(aminocarbonyl)-2,2-dimethylpropyl]-1-pentyl-1H-indazole-3-carboxamide	ADB-PINACA		1633766-73-0

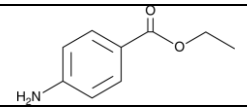
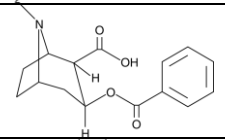
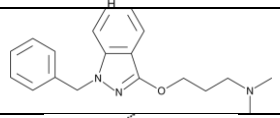
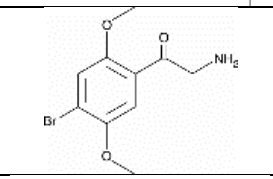
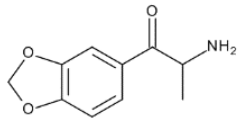
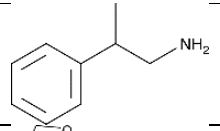
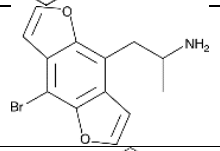
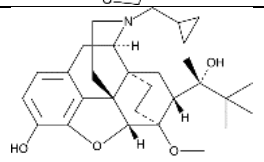
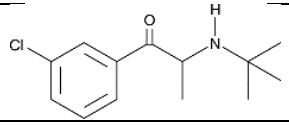
345,335	ADB-PINACA ISOMER_1	N-(1-amino-2,3-dimethyl-1-oxobutan-2-yl)-1-pentyl-1H-indazole-3-carboxamide	ADB-PINACA ISOMER_1		No. Description
345,304	ADB-PINACA ISOMER_2	N-((2S,3S)-1-amino-3-methyl-1-oxopentan-2-yl)-1-pentyl-1H-indazole-3-carboxamide	ADB-PINACA ISOMER_2		No. Description
345,292	ADB-PINACA ISOMER_3	(S)-N-(1-amino-1-oxohexan-2-yl)-1-pentyl-1H-indazole-3-carboxamide	ADB-PINACA ISOMER_3		No. Description
345,305	ADB-PINACA ISOMER_4	(S)-N-(1-amino-4-methyl-1-oxopentan-2-yl)-1-pentyl-1H-indazole-3-carboxamide	ADB-PINACA ISOMER_4		No. Description
329,174	AH-7921	3,4-dichloro-N-[[1-(dimethylamino)cyclohexyl]methyl]-benzamide	AH-7921		55154-30-8
404,265	AKB48_N-(4-FLUOROBENZYL)_ANALOG	1-[(4-fluorophenyl)methyl]-N-tricyclo[3.3.1.1^{3,7}]dec-1-yl-1H-indazole-3-carboxamide	AFB-48		2180933-90-6
206,323	ALPHA-ETHYLAMINOPENTIOPHENONE	2-(ethylamino)-1-phenyl-1-pentanone	ALFA-ETHYLAMINOPENTIOPHENONE		18268-16-1

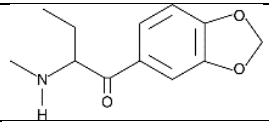
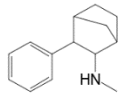
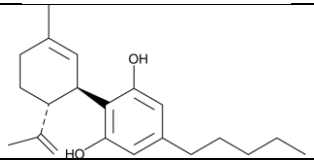
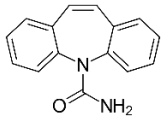
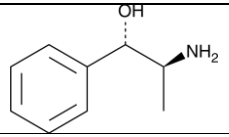
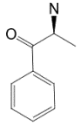
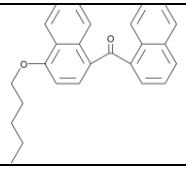
220,315	ALPHA-PROPYLAMINOPENTIOPHENONE	1-phenyl-2-(propylamino)-1-pentanone	ALFA-PROPYLAMINOPENTIOPHENONE		18268-15-0
238,321	ALLYLESCALINE	3,5-dimethoxy-4-(2-propen-1-yloxy)-benzeneethanamine	ALLYLESCALINE		39201-76-8
206,291	ALPHA-DIMETHYLAMINOPENTIOPHENONE	2-(dimethylamino)-1-phenyl-1-pentanone	ALPHA-DIMETHYLAMINOPENTIOPHENONE		2168229-67-0
220,312	ALPHA-ETHYLAMINOHEXANOPHENONE	2-(ethylamino)-1-phenyl-1-hexanone	ALPHA-ETHYLAMINOHEXANOPHENONE		18410-62-3
188,767	ALPHA-ETHYLTRYPTAMINE	α-ethyl-1H-indole-3-ethanamine	α-ET		2235-90-7
341,989	ALPHA-HYDROXYMIDAZOLAM	8-chloro-6-(2-fluorophenyl)-4H-imidazo[1,5-a][1,4]benzodiazepine-1-methanol	ALPHA-HYDROXYMIDAZOLAM		59468-90-5
175,029	ALPHA-METHYLTRYPTAMINE	alpha-Methyl-1H-indole-3-ethanamine	ALPHA-METHYLTRYPTAMINE		299-26-3

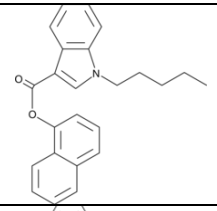
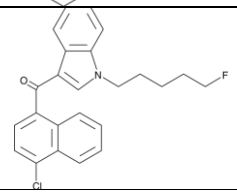
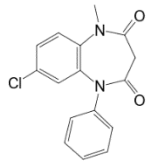
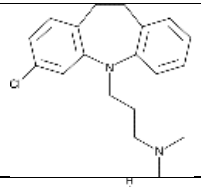
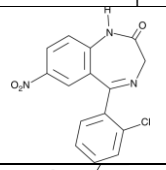
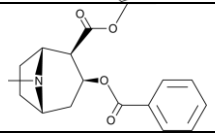
246,318	ALPHA-PHP	1-phenyl-2-(1-pyrrolidinyl)-1-hexanone	α-PHP		13415-59-3
280,193	ALPHA-PHTALIMIDOPROPIOPHENONE	2-(1-oxo-1-phenylpropan-2-yl)isoindole-1,3-dione	ALPHA-PHTALIMIDOPROPIOPHENONE		19437-20-8
232,294	ALPHA-PIPBP	1-phenyl-2-(1-piperidinyl)-1-butanone	α-PipBP		92728-82-0
204,261	ALPHA-PPP	1-phenyl-2-(1-pyrrolidinyl)-1-propanone	α-PPP		92040-10-3
232,243	ALPHA-PVP	1-phenyl-2-(1-pyrrolidinyl)-1-pentanone	α-PVP		5485-65-4
238,017	ALPHA-PVT	2-(1-pyrrolidinyl)-1-(2-thienyl)-1-pentanone	α-PVT		2748622-52-6
224,19	ALPHA-PYRROLIDINOBUTHIOPHENONE	1-phenyl-2-(1-pyrrolidinyl)-1-butanone	α-PBP		13415-54-8

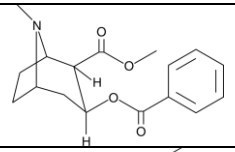
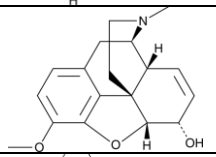
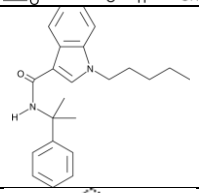
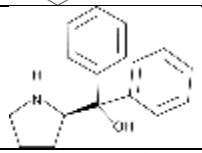
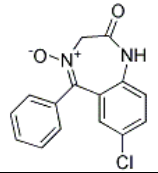
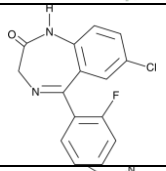
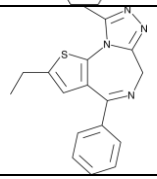
309,934	ALPRAZOLAM	8-chloro-1-methyl-6-phenyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine	ALPRAZOLAM		28981-97-7
383,315	AM1220	[1-[(1-methyl-2-piperidinyl)methyl]-1H-indol-3-yl]-1-naphthalenyl-methanone	AM1220		137642-54-7
391,166	AM-1248	[1-[(1-methyl-2-piperidinyl)methyl]-1H-indol-3-yl]tricyclo[3.3.1.13,7]dec-1-yl-methanone	AM-1248		335160-66-2
360,031	AM-2201	[1-(5-fluoropentyl)-1H-indol-3-yl]-1-naphthalenyl-methanone	AM-2201		335161-24-5
376,237	AM2201 8-QUINOLINYL CARBOXAMIDE	1-(5-fluoropentyl)-N-8-quinolinyl-1H-indole-3-carboxamide	AM2201 8-QUINOLINYL CARBOXAMIDE		2365471-42-5
361,184	AM2201 BENZIMIDAZOLE ANALOG	[1-(5-fluoropentyl)benzimidazol-2-yl]-naphthalen-1-ylmethanone	FUBIMINA		1984789-90-3
353,245	AM2232	3-(1-naphthalenylcarbonyl)-1H-Indole-1-pentanenitrile	AM2232		335161-19-8

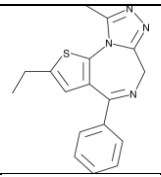
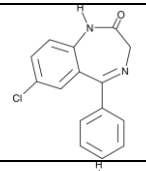
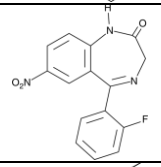
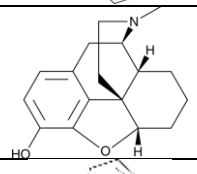
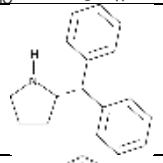
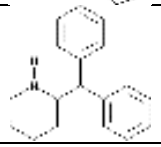
278,073	AMITRIPTYLINE	3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)-N,N-dimethyl-1-propanamine	AMITRIPTYLINE		549-18-8
136,03	AMPHETAMINE	α-methyl-benzeneethanamine	AMPHETAMINE		2706-50-5
267,122	ATENOLOL	4-[2-hydroxy-3-[(1-methylethyl)amino]propoxy]-benzeneacetamide	ATENOLOL		29122-68-7
216,245	ATRAZINE	6-chloro-N2-ethyl-N4-(1-methylethyl)-1,3,5-triazine-2,4-diamine	ATRAZINE		1912-24-9
268,279	AZACYCLONOL	α,α-diphenyl-4-piperidinemethanol	AZACYCLONOL		115-46-8
385,123	BB-22	1-(cyclohexylmethyl)-1H-indole-3-carboxylic acid, 8-quinolinyl ester	BB-22		1400742-42-8
194,03	BDB	α-ethyl-1,3-benzodioxole-5-ethanamine	BDB		42542-07-4
300,293	BENOCYCLIDINE	1-(1-benzo[b]thien-2-ylcyclohexyl)-piperidine	BCP		112726-66-6
254,273	BENZEDRONE	1-(4-methylphenyl)-2-[(phenylmethyl)amino]-1-propanone	4-MBC		1797979-43-1

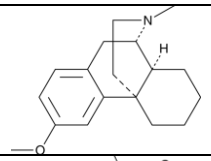
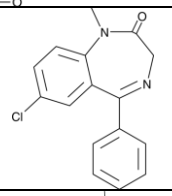
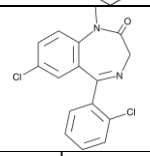
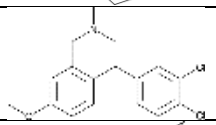
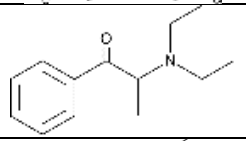
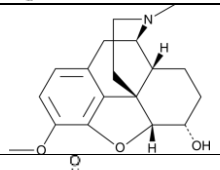
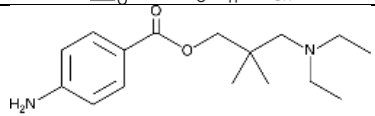
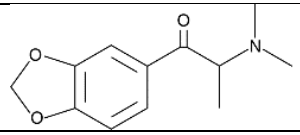
166,03	BENZOCAINE	4-amino-benzoic acid, ethyl ester	BENZOCAINE		94-09-7
290,034	BENZOYLECGONINE	(1R,2R,3S,5S)-3-(benzoyloxy)-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylic acid	BENZOYLECGONINE		519-09-5
310,213	BENZYDAMINE	N,N-dimethyl-3-[[1-(phenylmethyl)-1H-indazol-3-yl]oxy]-1-propanamine	BENZYDAMINE		642-72-8
274,896	bk-2C-B	2-amino-1-(4-bromo-2,5-dimethoxyphenyl)-ethanone	bk-2C-B		2303508-66-7
194,195	bk-MDA	3,4-Methylenedioxycathinone	bk-MDA		80535-73-5
136,133	BMPEA	β-methyl-benzeneethanamine	BMPEA		20388-87-8
293,977	BROMO-DRAGON-FLY	8-bromo-α-methyl-benzo[1,2-b:4,5-b']difuran-4-ethanamine	BROMO-DRAGON-FLY		219986-78-4
468,189	BUPRENORPHINE	αS,5α,7α)-17-(cyclopropylmethyl)-α-(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro-3-hydroxy-6-methoxy-α-methyl-6,14-ethenomorphinan-7-methanol	BUPRENORPHINE		53152-21-9
239,672	BUPROPION	1-(3-chlorophenyl)-2-[(1,1-dimethylethyl)amino]-1-propanone	BUPROPION		31677-93-7

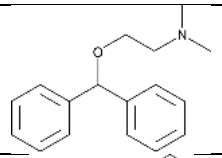
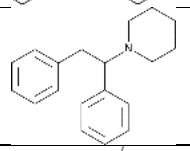
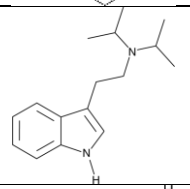
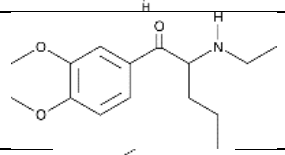
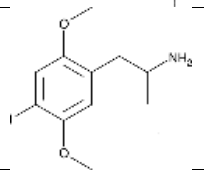
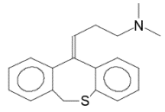
222,185	BUTYLONE (bk-MBDB)	1-(1,3-benzodioxol-5-yl)-2-(methylamino)-1-butanone	bk-MBDB		17763-12-1
202,289	CAMFETAMINE	N-Methyl-3-phenylnorbornan-2-amine	CAMFETAMINE		92499-19-9
315,323	CANNABIDIOL	2-[1R-3-methyl-6R-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl-1,3-benzenediol	CBD		13956-29-1
237,209	CARBAMAZEPINE	5H-Dibenzo[b,f]azepine-5-carboxamide	CARBAMAZEPINE		298-46-4
152,256	CATHINE	α-[(1S)-1-aminoethyl]-benzenemethanol	(+)-Norpseudoephedrine		492-39-7
150,03	CATHINONE	(2*S*)-2-amino-1-phenylpropan-1-one	CATHINONE		71031-15-7
369,1	CB-13	1-naphthalenyl[4-(pentylox)-1-naphthalenyl]-methanone	CRA-13		432047-72-8

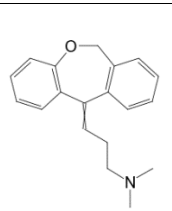
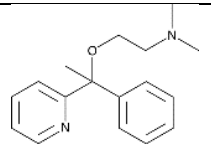
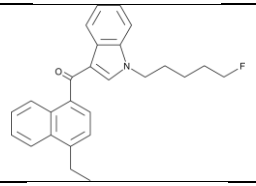
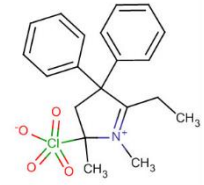
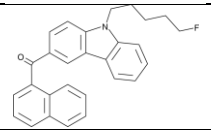
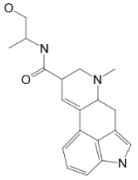
358,214	CBL-018	naphthalen-1-yl 1-pentyl-1H-indole-3-carboxylate	CBL-018		2365471-54-9
394,203	CI2201	(4-chloro-1-naphthalenyl)[1-(5-fluoropentyl)-1H-indol-3-yl]-methanone	CI2201		1391486-12-6
301,995	CLOBAZAM	-Chloro-1-methyl-5-phenyl-1H-1,5-benzodiazepine-2,4(3H,5H)-dione	CLOBAZAM		22316-47-8
315,043	CLOMIPRAMINE	3-chloro-10,11-dihydro-N,N-dimethyl-5H-dibenz[b,f]azepine-5-propanamine	CLOMIPRAMINE		17321-77-6
316,097	CLONAZEPAM	5-(2-chlorophenyl)-1,3-dihydro-7-nitro-2H-1,4-benzodiazepin-2-one	CLO		1622-61-3
318,094	COCAETHYLENE	(1R,2R,3S,5S)-3-(benzoyloxy)-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylic acid	COCAETHYLENE		529-38-4

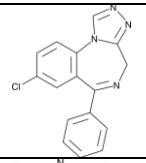
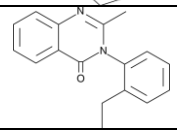
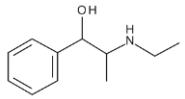
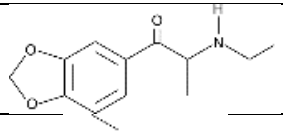
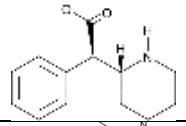
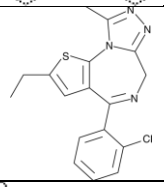
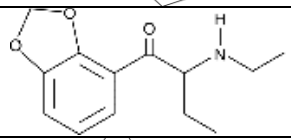
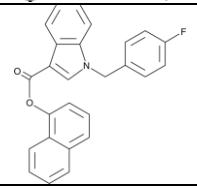
304,198	COCAINE	(1R,2R,3S,5S)-3-(benzoyloxy)-8-(methyl)-8-azabicyclo[3.2.1]octane-2-carboxylic acid	COCAINE		50-36-2
300,058	CODEINE	(5α,6α)-7,8-didehydro-4,5-epoxy-3-methoxy-17-methyl-morphinan-6-ol	CODEINE		76-57-3
349,217	CUMYL-PICA	N-(1-methyl-1-phenylethyl)-1-pentyl-1H-indole-3-carboxamide	CUMYL-PICA		1400742-32-6
254,299	D2PM	α,α-diphenyl-2R-pyrrolidinemethanol	D2PM		172152-19-1
286,956	DEMOXEPAM	7-Chloro-5-phenyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one 4-Oxide	DEMOXEPAM		963-39-3
289,917	DESALKYLFLURAZEPAM	7-chloro-5-(2-fluorophenyl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one	DESALKYLFLURAZEPAM		2886-65-9
310,255	DESCHLOROETIZOLAM	2-ethyl-9-methyl-4-phenyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepine	DESCHLOROETIZOLAM		40054-73-7

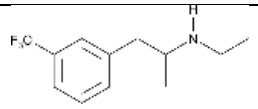
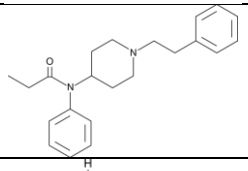
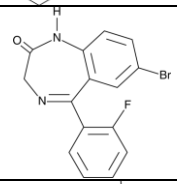
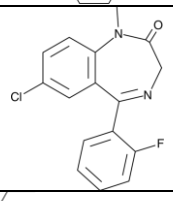
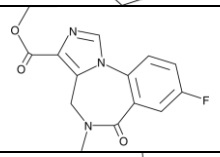
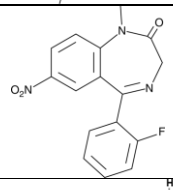
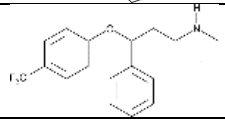
218,287	DESCHLORO-N-ETHYL-KETAMINE	2-(ethylamino)-2-phenyl-cyclohexanone,	O-PCE		4551-92-2
267,085	DESIPRAMINE	5-[3-(Methylamino)propyl]-5H-dibenz[b,f]azepine	DESIPRAMINE		50-47-5
271,978	DESMETHYLDIAZEPAM (NORDIAZEPAM)	7-chloro-1,3-dihydro-5-phenyl-2H-1,4-benzodiazepin-2-one	NORDIAZEPAM		1088-11-5
299,977	DESMETHYLFLUNITRAZEPAM	5-(2-fluorophenyl)-1,3-dihydro-7-nitro-2H-1,4-benzodiazepin-2-one	DESMETHYLFLUNITRAZEPAM		2558-30-7
272,254	DESOMORPHINE	4,5α-epoxy-17-methyl-morphinan-3-ol	DESOMORPHINE		427-00-9
238,301	DESOXY-D2PM	2-(diphenylmethyl)-pyrrolidine	DESOXY-D2PM		188398-87-0
252,331	DESOXYPIPRADROL (2-DPMP)	2-(diphenylmethyl)-piperidine	2-DPMP		5807-81-8

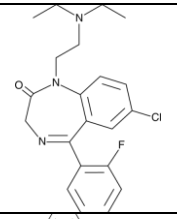
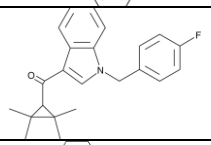
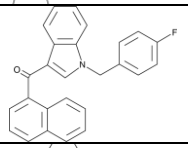
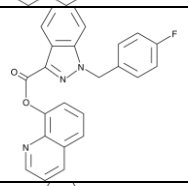
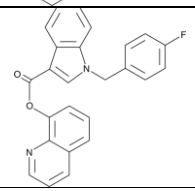
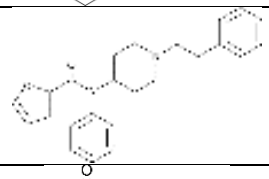
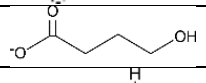
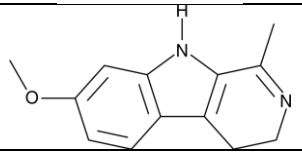
272,289	DEXTROMETHORPHAN	(9α,13α,14α)-3-methoxy-17-methyl-morphinan	DXM		125-71-3
285,397	DIAZEPAM	7-chloro-1,3-dihydro-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one	DIAZEPAM		439-14-5
320,306	DICLAZEPAM	7-chloro-5-(2-chlorophenyl)-1,3-dihydro-1-methyl-2H-1,4-benzodiazepin-2-one	DICLAZEPAM		2894-68-0
322,115	DICLOFENSINE	4-(3,4-dichlorophenyl)-1,2,3,4-tetrahydro-7-methoxy-2-methyl-isoquinoline	Ro 8-4650		34041-84-4
206,061	DIETHYLCATHINONE (AMFEPRAMONE)	2-(diethylamino)-1-phenyl-1-propanone	DIETHYLCATHINONE (AMFEPRAMONE)		134-80-5
302,062	DIHYDROCODEINE	4,5α-epoxy-3-methoxy-17-methyl-morphinan-6α-ol	DIHYDROCODEINE		125-28-0
279,175	DIMETHOCAINE	3-(diethylamino)-2,2-dimethyl-1-(4-aminobenzoate)-1-propanol	DIMETHOCAINE		553-63-9
222,209	DIMETHYLONE (bk-MDDMA)	1-(1,3-benzodioxol-5-yl)-2-(dimethylamino)-1-propanone	bk-MDDMA		109367-07-9

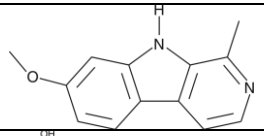
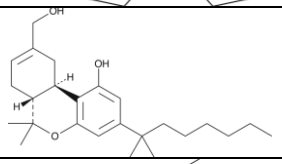
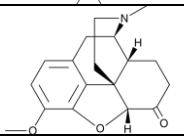
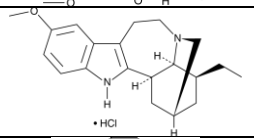
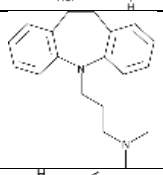
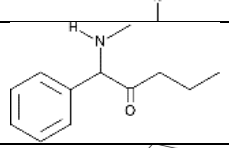
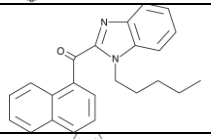
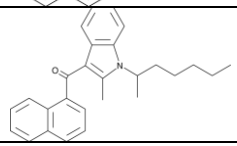
256,071	DIPHENHYDRAMINE	2-(diphenylmethoxy)-N,N-dimethyl-ethanamine	DPH		147-24-0
266,099	DIPHENIDINE	1-(1,2-diphenylethyl)-piperidine	DEP		28383-15-5
244,891	DiPT	N,N-*bis*(1-methylethyl)-1H-indole-3-ethanamine	DiPT		14780-24-6
266,292	DL-4662	1-(3,4-dimethoxyphenyl)-2-(ethylamino)pentan-1-one	DL-4662		1674389-55-9
322,068	DOI	4-iodo-2,5-dimethoxy-a-methyl-benzeneethanamine	DOI		42203-78-1
296,089	DOTHIEPIN	(3Z)-3-(6*H*-benzo[c][1]benzothiepin-11-ylidene)-*N*,*N*-dimethylpropan-1-amine	DOTHIEPIN		113-53-1

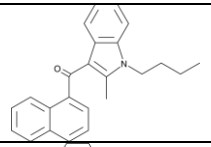
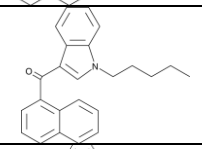
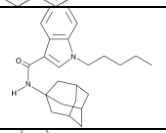
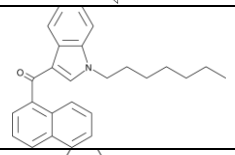
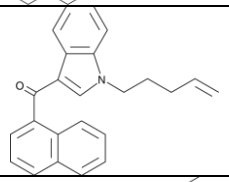
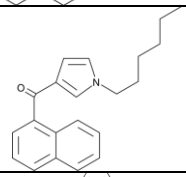
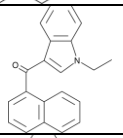
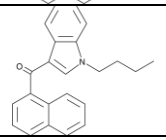
279,918	DOXEPIN	3-(dibenz[b,e]oxepin-11(6H)-ylidene)-N,N-dimethyl-1-propanamine	DOXEPIN		1229-29-4
271,067	DOXYLAMINE	N,N-dimethyl-2-[1-phenyl-1-(2-pyridinyl)ethoxy]monoethanamine	NSC 74772		469-21-6
388,297	EAM-2201	(4-ethyl-1-naphthalenyl)[1-(5-fluoropentyl)-1H-indol-3-yl]-methanone	EAM-2201		1364933-60-7
278,507	EDDP	5-ethyl-3,4-dihydro-1,2-dimethyl-4,4-diphenyl-2H-pyrrolium	EDDP		31161-17-8
410,225	EG-2201	[9-(5-fluoropentyl)-9H-carbazol-3-yl]-1-naphthalenyl-methanone	EG-2201		2365471-72-1
326,4	ERGOMETRINE	(6*aR*,9*R*)-*N*-[(2*S*)-1-hydroxypropan-2-yl]-7-methyl-6,6*a*,8,9-tetrahydro-4*H*-indolo[4,3-fg]quinoline-9-carboxamide	ERGOMETRINE		60-79-7

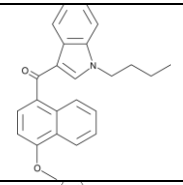
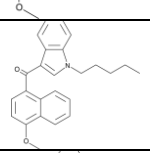
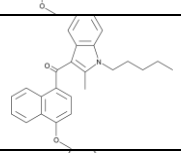
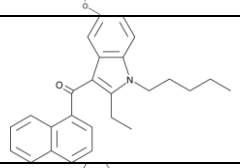
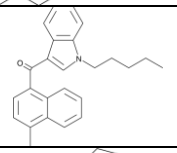
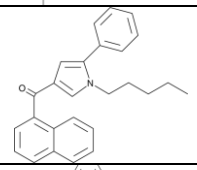
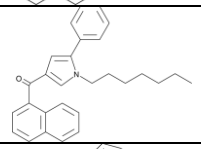
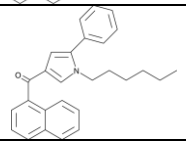
295,921	ESTAZOLAM	8-chloro-6-phenyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine	ESTAZOLAM		29975-16-4
264,918	ETAQUALONE	3-(2-ethylphenyl)-2-methyl-4(3H)-quinazolinone	ETAQUALONE		7432-25-9
180,064	ETHCATHINONE METABOLITE	2-(Ethylamino)-1-phenylpropan-1-ol	ETHCATHINONE METABOLITE		63401-08-1
222,228	ETHYLONE (bk-MDEA)	1-(1,3-benzodioxol-5-yl)-2-(ethylamino)-1-propanone	MDEC		1454266-19-3
248,328	ETHYLPHENIDATE	αR,2R)-*rel*-α-phenyl-2-piperidineacetic acid, ethyl ester	ETHYLPHENIDATE		214149-46-9
343,91	ETIZOLAM	4-(2-chlorophenyl)-2-ethyl-9-methyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepine	ETIZOLAM		40054-69-1
236,294	EUTYLONE (bk-EBDB)	1-(benzo[d][1,3]dioxol-4-yl)-2-(ethylamino)butan-1-one	bk-EBDB		17764-18-0
396,194	FDU-PB-22	1-[(4-fluorophenyl)methyl]-1H-indole-3-carboxylic acid, 1-naphthalenyl ester	FDU-PB-22		1883284-94-3

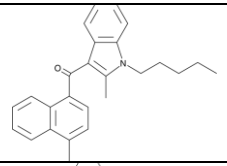
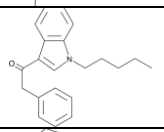
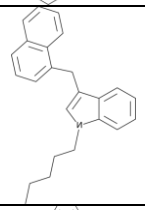
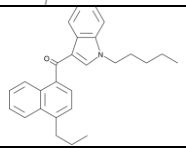
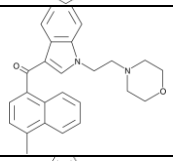
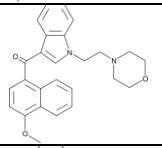
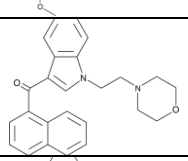
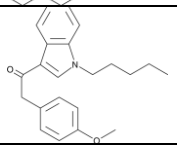
232,018	FENFLURAMINE	N-ethyl-α-methyl-3-(trifluoromethyl)-benzeneethanamine	FENFLURAMINE		404-82-0
337,171	FENTANYL	N-phenyl-N-[1-(2-phenylethyl)-4-piperidinyl]-propanamide	FENTANYL		437-38-7
334,716	FLUBROMAZEPAM	7-bromo-5-(2-fluorophenyl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one	FLUBROMAZEPAM		2647-50-9
303,922	FLUDIAZEPAM	7-chloro-5-(2-fluorophenyl)-1,3-dihydro-1-methyl-2H-1,4-benzodiazepin-2-one	FLUDIAZEPAM		3900-31-0
303,986	FLUMAZENIL	8-fluoro-5,6-dihydro-5-methyl-6-oxo-4H-imidazo[1,5-a][1,4]benzodiazepine-3-carboxylic acid, ethyl ester	FLUMAZENIL		78755-81-4
313,814	FLUNITRAZEPAM	5-(2-fluorophenyl)-1,3-dihydro-1-methyl-7-nitro-2H-1,4-benzodiazepin-2-one	FLUNITRAZEPAM		1622-62-4
310,021	FLUOXETINE	N-methyl-γ-[4-(trifluoromethyl)phenoxy]-benzenepropanamine	FLUOXETINE		56296-78-7

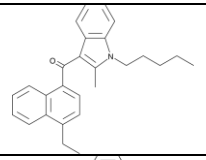
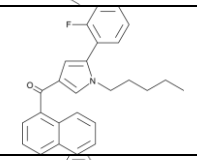
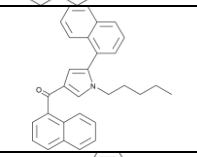
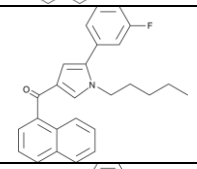
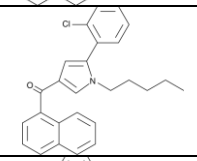
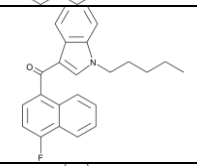
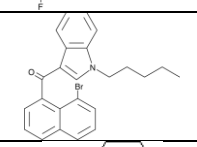
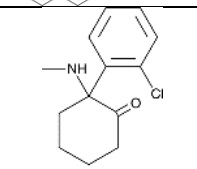
388,023	FLURAZEPAM	7-chloro-1-[2-(diethylamino)ethyl]-5-(2-fluorophenyl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one	FLURAZEPAM		17617-23-1
350,227	FUB-144	[1-[(4-fluorophenyl)methyl]-1H-indol-3-yl](2,2,3,3-tetramethylcyclopropyl)-methanone	FUB-144		2185863-15-2
380,203	FUB-JWH-018	(1-(4-fluorobenzyl)-1H-indol-3-yl)(naphthalen-1-yl)methanone	FUB-JWH-018		2365471-45-8
398,186	FUB-NPB-22	quinolin-8-yl 1-(4-fluorobenzyl)-1H-indazole-3-carboxylate	5-FLUORO NIN		2244864-90-0
396,975	FUB-PB-22	1-[(4-fluorophenyl)methyl]-1H-indole-3-carboxylic acid, 8-quinolinyl ester	FUB-PB-22		1800098-36-5
375,29	FURANYLFENTANYL (Fu-F)	N-phenyl-N-[1-(2-phenylethyl)-4-piperidinyl]-2-furancarboxamide	Fu-F		101365-56-4
102,935	GHB	4-hydroxy-butanoic acid	GHB		502-85-2
215,051	HARMALINE	4,9-dihydro-7-methoxy-1-methyl-3H-pyrido[3,4-b]indole	HARMALINE		304-21-2

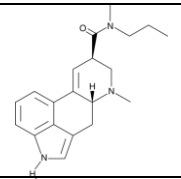
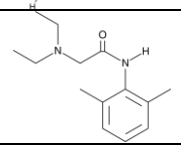
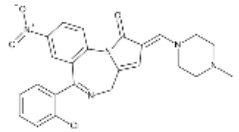
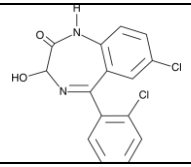
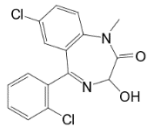
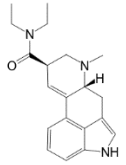
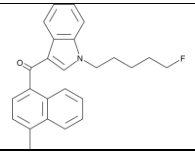
212,795	HARMINE	7-methoxy-1-methyl-9H-pyrido[3,4-b]indole	HARMINE		442-51-3
387,195	HU-210	3-(1,1'-dimethylheptyl)-6aR,7,10,10aR-tetrahydro-1-hydroxy-6,6-dimethyl-6H-dibenzo[b,d]pyran-9-methanol	HU-210		112830-95-2
300,05	HYDROCODONE	4,5α-epoxy-3-methoxy-17-methyl-morphinan-6-one	HYDROCODONE		125-29-1
312,288	IBOGAINE	12-methoxy-ibogamine	NSC 29847		5934-55-4
281,078	IMIPRAMINE	10,11-dihydro-N,N-dimethyl-5H-dibenz[b,f]azepine-5-propanamine	IMIPRAMINE		113-52-0
192,055	ISOPENTEDRONE	1-(methylamino)-1-phenyl-2-pentanone	ISOPENTEDRONE		1429402-13-0
343,221	JWH 018 BENZIMIDAZOLE ANALOG	naphthalen-1-yl(1-pentyl-1H-benzo[d]imidazol-2-yl)methanone	BIM-018		2316839-70-8
384,202	JWH-011	[2-methyl-1-(1-methylhexyl)-1H-indol-3-yl]-1-naphthalenyl-methanone	JWH-011		155471-13-9

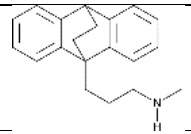
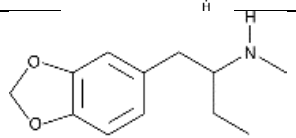
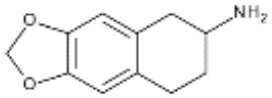
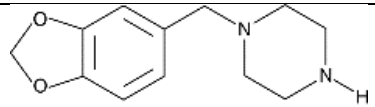
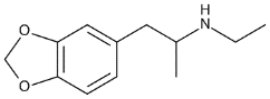
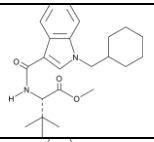
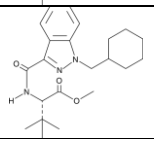
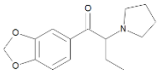
342,097	JWH-016	1-butyl-2-methyl-1H-indol-3-yl)-1-naphthalenyl-methanone	JWH-016		155471-09-3
342,063	JWH-018	1-naphthalenyl(1-pentyl-1H-indol-3-yl)-methanone	AM678		209414-07-3
365,291	JWH-018 ADAMANTYL CARBOXAMIDE	1-pentyl-N-tricyclo[3.3.1.1^{3,7}]dec-1-yl-1H-indole-3-carboxamide	APICA		1345973-50-3
370,197	JWH-020	(1-heptyl-1H-indol-3-yl)-1-naphthalenyl-methanone	JWH-020		209414-09-5
340,223	JWH-022	1-naphthalenyl[1-(4-penten-1-yl)-1H-indol-3-yl]-methanone	JWH-022		209414-16-4
306,155	JWH-031	(1-hexyl-1H-pyrrol-3-yl)-1-naphthalenyl-methanone	JWH-031		162934-74-9
300,22	JWH-071	(1-ethyl-1H-indol-3-yl)-1-naphthalenyl-methanone	JWH-071		209414-05-1
328,077	JWH-073	(1-butyl-1H-indol-3-yl)-1-naphthalenyl-methanone	JWH-073		208987-48-8

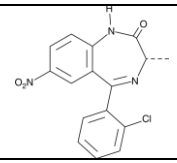
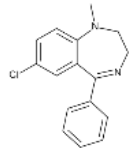
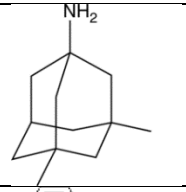
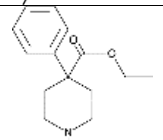
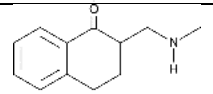
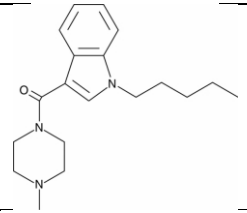
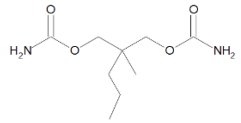
358,107	JWH-080	(1-butyl-1H-indol-3-yl)(4-methoxy-1-naphthalenyl)-methanone	JWH-080		210179-44-5
372,132	JWH-081	(4-methoxy-1-naphthalenyl)(1-pentyl-1H-indol-3-yl)-methanone	JWH-081		210179-46-7
386,111	JWH-098	(4-methoxy-1-naphthalenyl)(2-methyl-1-pentyl-1H-indol-3-yl)-methanone	JWH-098		316189-74-9
370,219	JWH-116	(2-ethyl-1-pentyl-1H-indol-3-yl)-1-naphthalenyl-methanone	JWH-116		619294-64-3
356,234	JWH-122	(4-methyl-1-naphthalenyl)(1-pentyl-1H-indol-3-yl)-methanone	JWH-122		619294-47-2
367,929	JWH-145	1-naphthalenyl(1-pentyl-5-phenyl-1H-pyrrol-3-yl)-methanone	JWH-145		914458-19-8
396,312	JWH-146	(1-heptyl-5-phenyl-1H-pyrrol-3-yl)-1-naphthalenyl-methanone	JWH-146		914458-21-2
382,164	JWH-147	(1-hexyl-5-phenyl-1H-pyrrol-3-yl)-1-naphthalenyl-methanone	JWH-147		914458-20-1

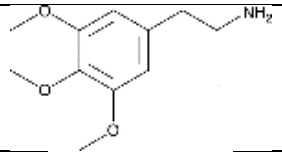
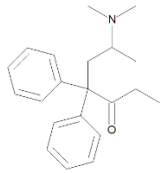
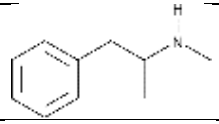
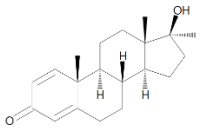
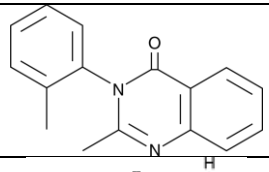
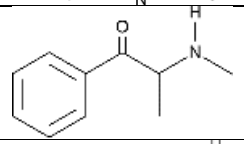
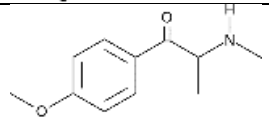
370,172	JWH-149	(4-methyl-1-naphthalenyl)(2-methyl-1-pentyl-1H-indol-3-yl)-methanone	JWH-149		548461-82-1
306,156	JWH-167	1-(1-pentyl-1H-indol-3-yl)-2-phenyl-ethanone	JWH-167		864445-37-4
328,281	JWH-175	3-(1-naphthalenylmethyl)-1-pentyl-1H-indole	JWH-175		619294-35-8
384,268	JWH-182	(1-pentyl-1H-indol-3-yl)(4-propyl-1-naphthalenyl)-methanone	JWH-182		824960-02-3
399,123	JWH-193	(4-methyl-1-naphthalenyl)[1-[2-(4-morpholinyl)ethyl]-1H-indol-3-yl]-methanone	JWH-193		133438-58-1
415,117	JWH-198	(4-methoxy-1-naphthalenyl)[1-[2-(4-morpholinyl)ethyl]-1H-indol-3-yl]-methanone	JWH-198		166599-76-4
385,076	JWH-200	[1-[2-(4-morpholinyl)ethyl]-1H-indol-3-yl]-1-naphthalenyl-methanone	JWH-200		103610-04-4
336,263	JWH-201	2-(4-methoxyphenyl)-1-(1-pentyl-1H-indol-3-yl)-ethanone	JWH-201		864445-47-6

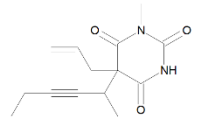
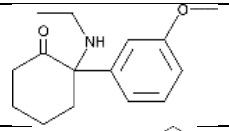
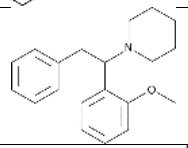
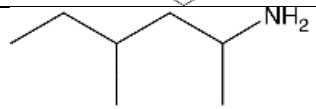
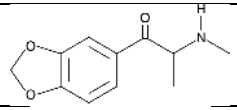
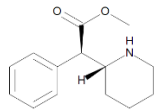
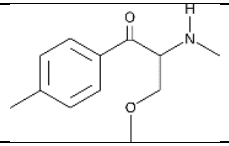
384,326	JWH-213	(4-ethyl-1-naphthalenyl)(2-methyl-1-pentyl-1H-indol-3-yl)-methanone	JWH-213		824959-83-3
386,153	JWH-307	[5-(2-fluorophenyl)-1-pentyl-1H-pyrrol-3-yl]-1-naphthalenyl-methanone	JWH-307		914458-26-7
418,325	JWH-309	1-naphthalenyl[5-(1-naphthalenyl)-1-pentyl-1H-pyrrol-3-yl]-methanone	JWH-309		914458-42-7
386,132	JWH-368	[5-(3-fluorophenyl)-1-pentyl-1H-pyrrol-3-yl]-1-naphthalenyl-methanone	JWH-368		914458-31-4
402,279	JWH-369	[5-(2-chlorophenyl)-1-pentyl-1H-pyrrol-3-yl]-1-naphthalenyl-methanone	JWH-369		914458-27-8
360,213	JWH-412	(4-fluoro-1-naphthalenyl)(1-pentyl-1H-indol-3-yl)-methanone	JWH-412		1364933-59-4
422,179	JWH-424	(8-bromonaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone	JWH-424		1366068-04-3
238,083	KETAMINE	2-(2-chlorophenyl)-2-(methylamino)-cyclohexanone	CI-581		1867-66-9

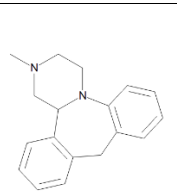
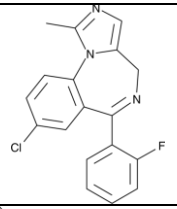
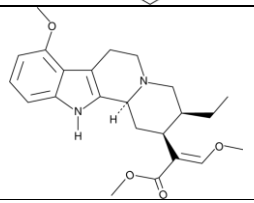
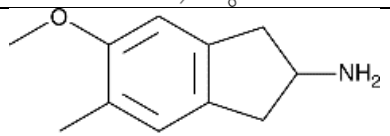
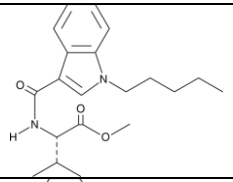
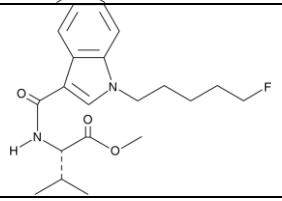
324,164	LAMPA	8β)-9,10-didehydro-N,6-dimethyl-N-propyl-ergoline-8-carboxamide	LAMPA		40158-98-3
235,081	LIDOCAINE	2-(diethylamino)-N-(2,6-dimethylphenyl)-acetamide	NSC 40030		137-58-6
464,983	LOPRAZOLAM	(2Z)-6-(2-Chlorophenyl)-2,4-dihydro-2-[(4-methyl-1-piperazinyl)methylene]-8-nitro-1H-imidazo[1,2-a][1,4]benzodiazepin-1-one	LOPRAZOLAM		61197-73-7
321,924	LORAZEPAM	7-chloro-5-(2-chlorophenyl)-1,3-dihydro-3-hydroxy-2H-1,4-benzodiazepin-2-one	NSC 279758		846-49-1
335,939	LORMETAZEPAM	7-Chloro-5-(2-chlorophenyl)-3-hydroxy-1-methyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one	LORMETAZEPAM		848-75-9
324,277	LSD	Lysergic Acid Diethylamide	LSD		50-37-3
374,126	MAM-2201	[1-(5-fluoropentyl)-1H-indol-3-yl](4-methyl-1-naphthalenyl)-methanone	MAM-2201		1354631-24-5

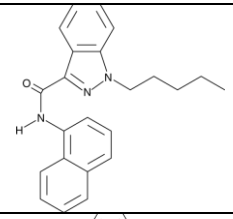
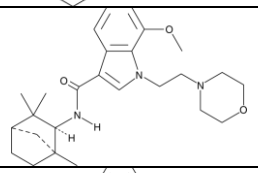
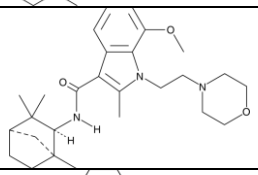
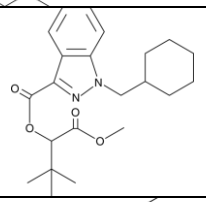
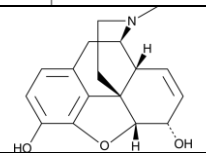
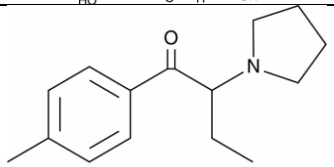
278,114	MAPROTILINE	N-methyl-9,10-ethanoanthracene-9(10H)-propanamine	Ba 34276		10347-81-6
208,04	MBDB	α-ethyl-N-methyl-1,3-benzodioxole-5-ethanamine	MBDB		128767-12-4
192,204	MDAT	6,7-Methylenedioxy-2-aminotetralin	MDAT		101625-35-8
221,272	MDBP	1-(1,3-benzodioxol-5-ylmethyl)-piperazine	MDBP		38063-96-6
208,054	MDEA	N-Ethyl-alpha-methyl-1,3-benzodioxole-5-ethanamine	MDEA		82801-81-8
385,124	MDMB-CHMICA (MMB-CHMINACA)	N-[[1-(cyclohexylmethyl)-1H-indol-3-yl]carbonyl]-3-methyl-L-valine	MMB-CHMINACA		1971007-95-0
386,303	MDMB-CHMINACA	N-[[1-(cyclohexylmethyl)-1H-indazol-3-yl]carbonyl]-3-methyl-L-valine	MDMB-CHMINACA		1185888-32-7
262,024	MDPBP	1-(1,3-benzodioxol-5-yl)-2-(1-pyrrolidinyl)-1-butanone	MDPBP		784985-33-7

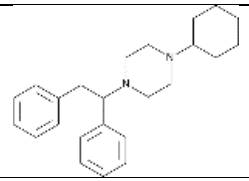
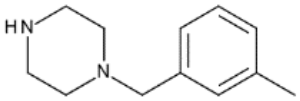
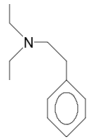
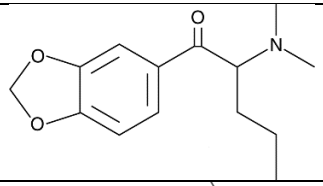
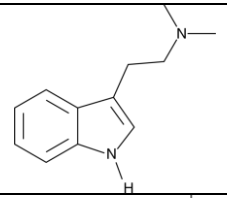
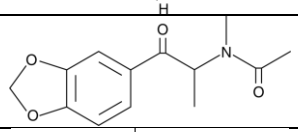
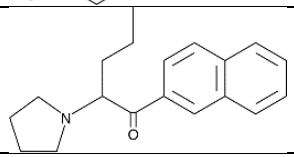
329,969	MECLONAZEPAM	(3S)-5-(2-chlorophenyl)-1,3-dihydro-3-methyl-7-nitro-2H-1,4-benzodiazepin-2-one	Ro11-3128		58662-84-3
271,019	MEDAZEPAM	7-Chloro-1-methyl-1,3-dihydro-2H-1,4-benzodiazepine	MEDAZEPAM		2898-12-6
180,261	MEMANITINE	1-Amino-3,5-dimethyladamantane	MEMANTINE		41100-52-1
248,14	MEPERIDINE	1-methyl-4-phenyl-4-piperidinecarboxylic acid, ethyl ester	NIH 10522		50-13-5
190,139	MEPHTETRAMINE (MTTA)	3,4-dihydro-2-[(methylamino)methyl]-1(2H)-naphthalenone	MTTA		2749302-69-8
314,241	MEPIRAPIM	(4-methyl-1-piperazinyl)(1-pentyl-1H-indol-3-yl)-methanone	MEPIRAPIM		2365542-30-7
219,029	MEPROBAMATE	Carbamic acid 2-methyl-2-propyltrimethylene ester	MEPROBAMATE		57-53-4

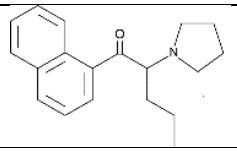
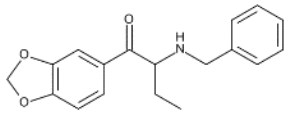
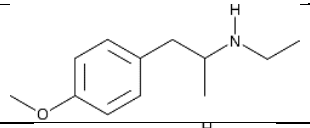
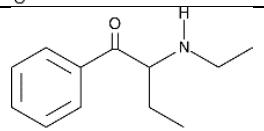
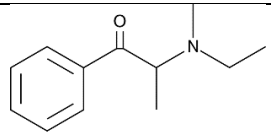
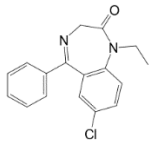
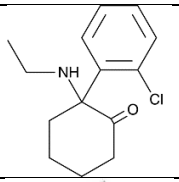
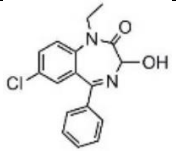
212,183	MESCALINE	3,4,5-trimethoxy-benzeneethanamine	TMPEA		832-92-8
310,094	METHADONE	6-(dimethylamino)-4,4-diphenyl-3-heptanone	MEPHENON		1095-90-5
150,063	METHAMPHETAMINE	N,α-dimethyl-benzeneethanamine	MA		826-10-8
301,06	METHANDIENONE	(17β)-17-Hydroxy-17-methylandrosta-1,4-dien-3-one	METHANDIENONE		72-63-9
251,007	METHAQUALONE	2-methyl-3-(2-methylphenyl)-4(3H)-quinazolinone	NSC 111388		72-44-6
164,056	METHCATHINONE	2-(methylamino)-1-phenyl-1-propanone	DL-EPHEDRONE		49656-78-2
193,998	METHEDRONE (bk-PMMA)	1-(4-methoxyphenyl)-2-(methylamino)-1-propanone	PMMC		879665-92-6

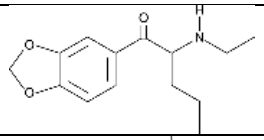
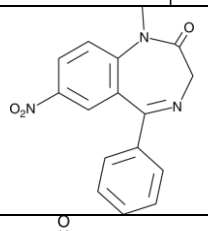
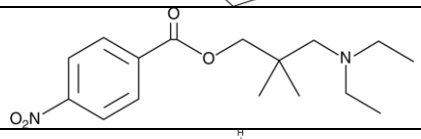
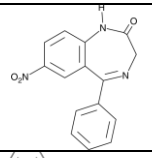
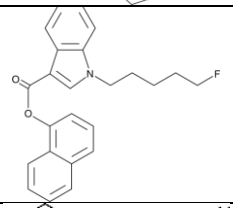
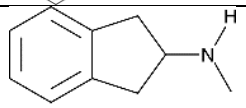
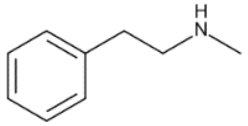
263,072	METHOHEXITAL	5-Allyl-1-methyl-5-(1-methyl-pent-2-ynyl)-pyrimidine-2,4,6-trione	METHOHEXITAL		151-83-7
248,059	METHOXETAMINE	2-(ethylamino)-2-(3-methoxyphenyl)-cyclohexanone	MXE		1239908-48-5
297,324	METHOXPHENIDINE	1-(1-(2-methoxyphenyl)-2-phenylethyl)piperidine	MXP		2055777-48-3
116,066	METHYLHEXANAMINE	4-methyl-2-hexanamine	DMMA		13803-74-2
208,272	METHYLONE (bk-MDMA)	1-(1,3-benzodioxol-5-yl)-2-(methylamino)-1-propanone	bk-MDMA		186028-80-8
234,3	METHYLPHENIDATE	2-Piperidineacetic acid	METHYLPHENIDATE		113-45-1
208,3	MEXEDRONE	3-methoxy-2-(methylamino)-1-(*p*-tolyl)propan-1-one	MEXEDRONE		9002622

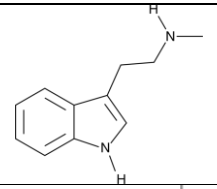
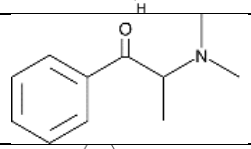
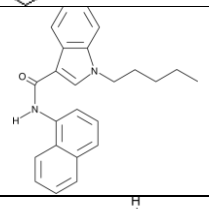
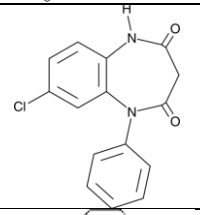
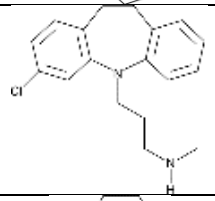
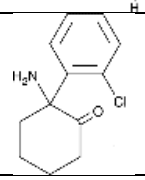
265,493	MIANSERIN	Dibenzo[c,f]pyrazino[1,2-a]azepine, 1,2,3,4,10,14b-hexahydro-2-methyl-	MIANSERIN		24219-97-4
326,065	MIDAZOLAM	8-chloro-6-(2-fluorophenyl)-1-methyl-4H-imidazo[1,5-a][1,4]benzodiazepine	MIDAZOLAM		59467-70-8
399,094	MITRAGYNINE	(αE,2S,3S,12bS)-3-ethyl-1,2,3,4,6,7,12,12b-octahydro-8-methoxy-α-(methoxymethylene)-indolo[2,3-a]quinolizine-2-acetic acid, methyl ester	MITRAGYNINE		4098-40-2
178,131	MMAI	2,3-dihydro-5-methoxy-6-methyl-1H-inden-2-amine	MMAI		132980-17-7
345,251	MMB018	N-[(1-pentyl-1H-indol-3-yl)carbonyl]-L-valine, methyl ester	AMB-PICA		1971007-97-2
363,251	MMB2201	N-[[1-(5-fluoropentyl)-1H-indol-3-yl]carbonyl]-L-valine, methyl ester	5-FLUORO AMB-PICA		1971007-87-0

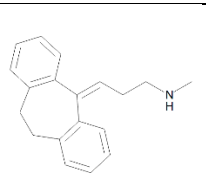
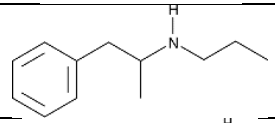
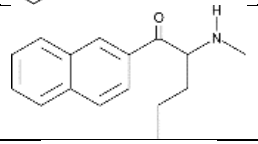
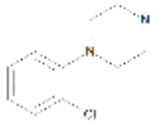
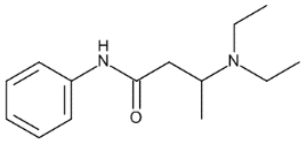
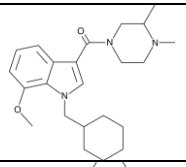
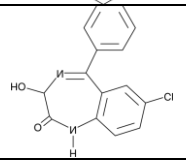
358,061	MN-18	N-1-naphthalenyl-1-pentyl-1H-indazole-3-carboxamide	MN-18		1391484-80-2
440,336	MN-25	7-methoxy-1-[2-(4-morpholinyl)ethyl]-N-[(1S,2S,4R)-1,3,3-trimethylbicyclo[2.2.1]hept-2-yl]-1H-indole-3-carboxamide	UR-12		501926-82-5
454,347	MN-25-2-METHYL DERIVATIVE	7-methoxy-2-methyl-1-[2-(4-morpholinyl)ethyl]-N-[(1S,2S,4R)-1,3,3-trimethylbicyclo[2.2.1]hept-2-yl]-1H-indole-3-carboxamide	MN-25-2-METHYL DERIVATIVE		501927-29-3
387,261	MO-CHMINACA	1-methoxy-3,3-dimethyl-1-oxobutan-2-yl 1-(cyclohexylmethyl)-1H-indazole-3-carboxylate	MO-AMB		2365471-04-9
286,043	MORPHINE	7,8-didehydro-4,5α-epoxy-17-methyl-morphinan-3,6α-diol	MORPHINE		57-27-2
232,059	MPBP	4'-Methyl-alpha-pyrrolidinobutiophenone	MPBP		1214-15-9

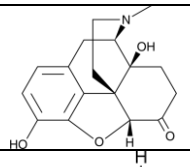
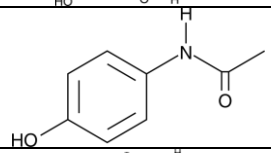
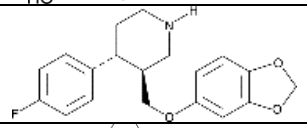
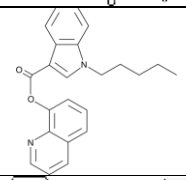
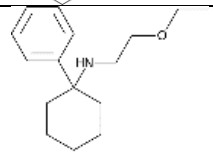
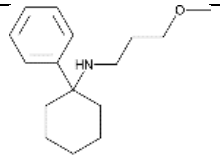
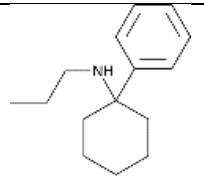
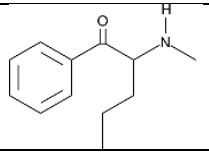
349,38	MT-45	1-cyclohexyl-4-(1,2-diphenylethyl)-piperazine	I-C6		57314-55-3
191,273	N-(3-METHYLBENZYL)PIPERAZINE	N-(3-Methylbenzyl)piperazine	N-(3-METHYLBENZYL)PIPERAZINE		5321-48-2
178,273	N,N-DIETHYLPHENETHYLAMINE	*N*,*N*-diethyl-2-phenylethanamine	N,N-DIETHYLPHENETHYLAMINE		5300-21-0
250,302	N,N-DIMETHYLPENTYLONE (bk-DMBDP)	1-(1,3-benzodioxol-5-yl)-2-(dimethylamino)-1-pentanone	bk-DMBDP		17763-13-2
189,572	N,N-DMT	N,N-dimethyl-1H-indole-3-ethanamine	NSC 63795		61-50-7
250,245	N-ACETYL-3,4-MDMC	N-[2-(1,3-benzodioxol-5-yl)-1-methyl-2-oxoethyl]-N-methyl-acetamide	N-ACETYL-3,4-MDMC		1227293-15-3
282,065	NAPHYRONE	1-(2-naphthalenyl)-2-(1-pyrrolidinyl)-1-pentanone	NRG-1		850352-11-3

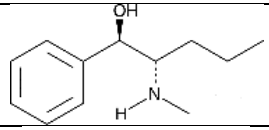
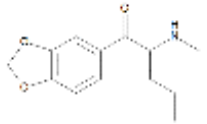
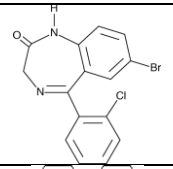
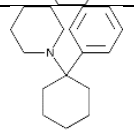
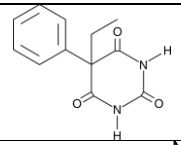
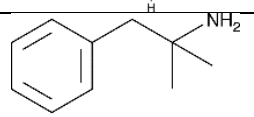
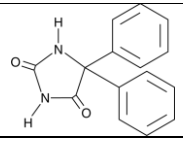
282,125	NAPHYRONE-1-NAPHTYL ISOMER	1-(naphthalen-1-yl)-2-(pyrrolidin-1-yl)pentan-1-one	α-Naphyrone		1349245-31-3
298,241	N-BENZYLNORBUTYLONE	N-Benzyl-(3,4-methylenedioxyphenyl)-2-aminobutan-1-one	N-BENZYLNORBUTYLONE		1823865-05-9
194,253	N-ETHYL-4-METHOXYAMPHETAMNE	N-ethyl-4-methoxy-a-methyl-benzeneethanamine	PMEA		93963-24-7
192,296	N-ETHYLBUPHEDRONE	2-(ethylamino)-1-phenylbutan-1-one	NEB		2731709-73-0
192,099	N-ETHYL-N-METHYLCATHINONE	2-(ethyl(methyl)amino)-1-phenylpropan-1-one	N-ETHYL-N-METHYLCATHINONE		1157739-24-6
299,364	N-ETHYLNORDAZEPAM	7-chloro-1-ethyl-5-phenyl-3*H*-1,4-benzodiazepin-2-one	N-ETHYLNORDAZEPAM		5571-65-3
252,18	N-ETHYLNORKETAMINE	2-(2-chlorophenyl)-2-(ethylamino)-cyclohexanone	N-ETHYLNORKETAMINE		2525095-53-6
315,994	N-ETHYLOXAZEPAM	N-Ethyl-9-chloro-4-hydroxy-6-phenyl-2,5-diazabicyclo[5.4.0]undeca-5,8,10,12-tetraen-3-one	N-ETHYLOXAZEPAM		62659-64-7

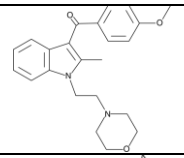
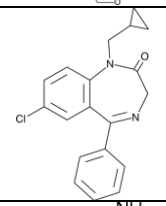
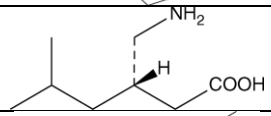
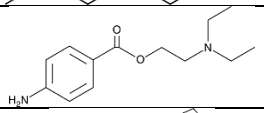
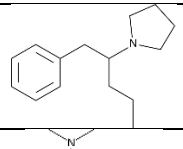
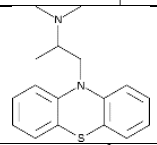
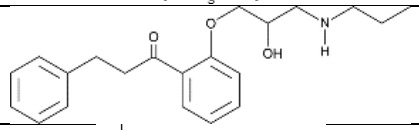
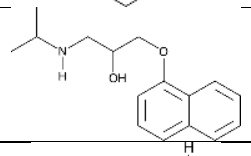
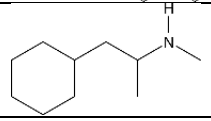
250,269	N-ETHYLPENTYLONE	1-(1,3-benzodioxol-5-yl)-2-(ethylamino)-1-pentanone	EPHYLONE		17763-02-9
296,187	NIMETAZEPAM	1,3-dihydro-1-methyl-7-nitro-5-phenyl-2H-1,4-benzodiazepin-2-one	Ro 5-3453		2011-67-8
309,822	NITRACAINE	3-(diethylamino)-2,2-dimethylpropyl 4-nitrobenzoate	NITRACAINE		1648893-21-3
281,974	NITRAZEPAM	1,3-dihydro-7-nitro-5-phenyl-2H-1,4-benzodiazepin-2-one	NSC 58775		146-22-5
376,276	NM2201	1-(5-fluoropentyl)-1H-indole-3-carboxylic acid, 1-naphthalenyl ester	CBL-2201		2042201-16-9
148,043	N-METHYL-2AI	2,3-dihydro-N-methyl-1H-inden-2-amine	NM-2AI		10408-85-2
136,182	N-METHYL-PEA	N-Methyl-2-phenylethylamine	N-METHYL-PEA		589-08-2

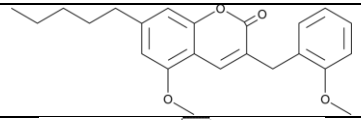
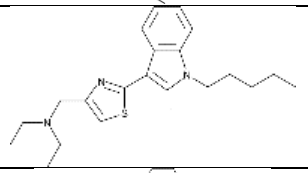
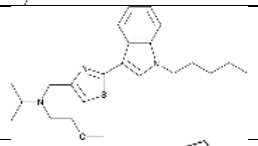
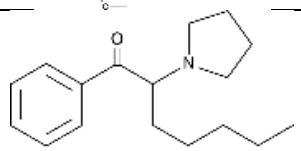
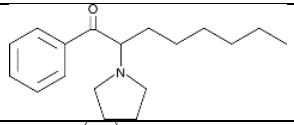
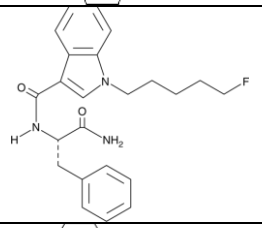
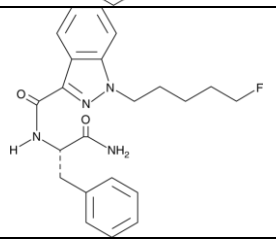
175,508	N-METHYLTRYPTAMINE	N-methyl-1H-indole-3-ethanamine	NMT		61-49-4
178,233	N,N-DMC	2-(dimethylamino)-1-phenyl-1-propanone	N,N-DMC		10105-90-5
357,005	NNEI	N-1-naphthalenyl-1-pentyl-1H-indole-3-carboxamide	MN-24		1338925-11-3
286,954	NORCLOBAZAM	8-chloro-1-phenyl-1H-1,5-benzodiazepine-2,4(3H,5H)-dione	N-DESMETHYLCLOBAZAM		22316-55-8
301,026	NORCLOMIPRAMINE	3-chloro-10,11-dihydro-N-methyl-5H-dibenz[b,f]azepine-5-propanamine	N-DESMETHYLCLOMIPRAMINE		29854-14-6
224,176	NORKETAMINE	2-amino-2-(2-chlorophenyl)-cyclohexanone	N-DESMETHYLKETAMINE		79499-59-5

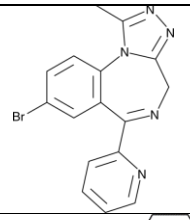
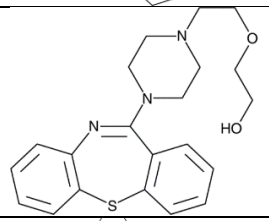
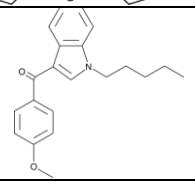
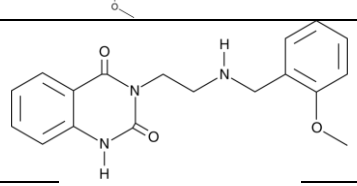
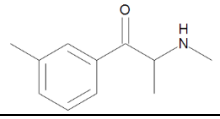
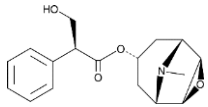
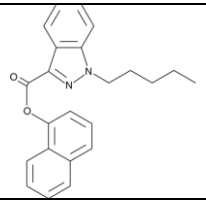
264,066	NORTRIPTYLINE	3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)-N-methyl-1-propanamine	NORTRIPTYLINE		894-71-3
178,103	N-PROPYLAMPHETAMINE	α-methyl-N-propyl-benzeneethanamine	NPA		59877-57-5
242,25	NRG-3	2-(methylamino)-1-(naphthalen-2-yl)pentan-1-one	NRG-3		2701928-05-2
197,229	o-CPP	ortho-Chlorophenylpiperazine	o-CPP		41202-32-8
235,279	OCTACAINE	Butanamide, 3-(diethylamino)-N-phenyl-	OCTACAINE		93940-32-0
384,309	ORG-28611	[1-(cyclohexylmethyl)-7-methoxy-1H-indol-3-yl](3,4-dimethyl-1-piperazinyl)-methanone	ORG-28611		784138-08-5
288,031	OXAZEPAM	7-chloro-1,3-dihydro-3-hydroxy-5-phenyl-2H-1,4-benzodiazepin-2-one	NSC 169448		604-75-1

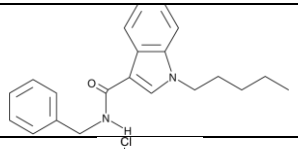
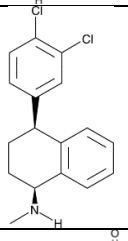
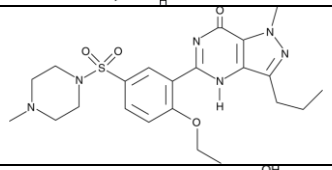
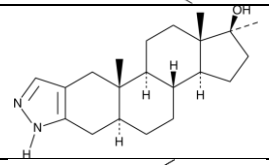
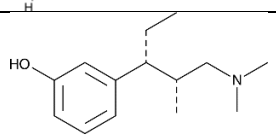
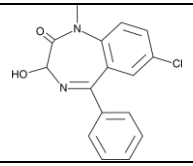
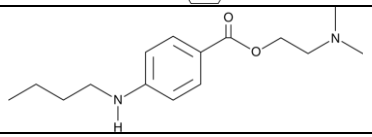
302,251	OXYMORPHONE	(5α)-4,5-epoxy-3,14-dihydroxy-17-methyl-morphinan-6-one	NSC 19045		76-41-5
152,016	PARACETAMOL	N-(4-hydroxyphenyl)-acetamide	ACETAMINOPHEN		103-90-2
330,014	PAROXETINE	3S,4R)-3-[(1,3-benzodioxol-5-yloxy)methyl]-4-(4-fluorophenyl)-piperidine	BRL29060A		78246-49-8
359,081	PB-22	1-pentyl-1H-indole-3-carboxylic acid, 8-quinolinyl ester	QUPIC		1400742-17-7
248,346	PCEEA	N-(2-ethoxyethyl)-1-phenylcyclohexanamine	PCEEA		1798021-89-2
248,342	PCMPA	N-(3-methoxypropyl)-1-phenyl-cyclohexanamine	PCMPA		1934-63-0
218,345	PCPr	1-phenyl-N-propyl-cyclohexanamine	PCPr		1934-55-0
192,062	PENTEDRONE	2-(methylamino)-1-phenyl-1-pentanone	PENTEDRONE		879669-95-1

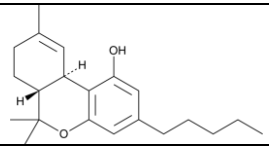
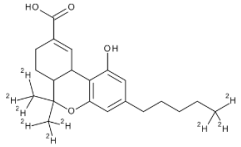
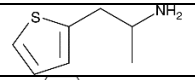
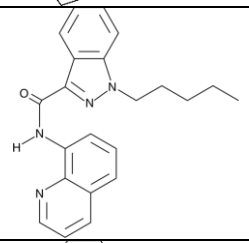
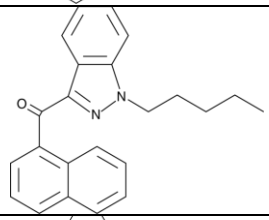
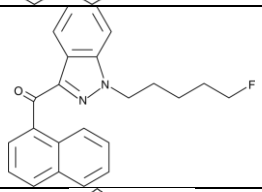
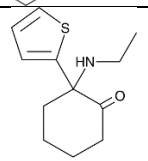
194,308	PENTEDRONE METABOLITE	α-[(1R)-1-(methylamino)butyl]-benzenemethanol	PENTEDRONE METABOLITE		1422513-91-4
235,658	PENTYLONE (bk-MBDP)	2-(methylamino)-3',4'-(methylenedioxy)-Valerophenone	PENTYLONE (bk-MBDP)		17763-01-8
350,845	PHENAZEPAM	7-bromo-5-(2-chlorophenyl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one	BD 98		51753-57-2
244,103	PHENCYCLIDINE (PCP)	1-(1-phenylcyclohexyl)-piperidine	PCP		956-90-1
231,014	PHENOBARBITAL	5-ethyl-5-phenyl-2,4,6(1H,3H,5H)-pyrimidinetrione	NSC 9848		50-06-6
150,067	PHENTERMINE	α,α-dimethyl-benzeneethanamine	PHENTERMINE		1197-21-3
253,004	PHENYTOIN	5,5-diphenyl-2,4-imidazolidinedione	PHENYTOIN		57-41-0

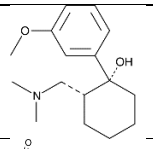
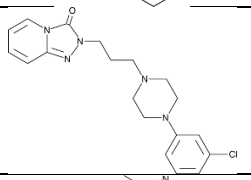
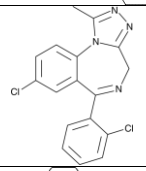
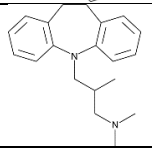
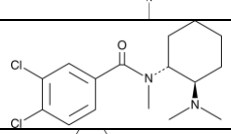
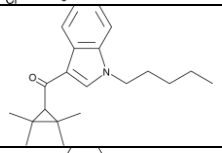
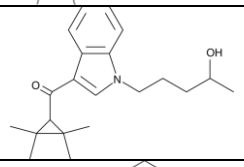
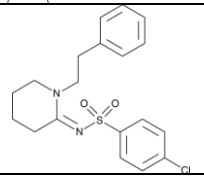
379,06	PRAVADOLINE	(4-methoxyphenyl)[2-methyl]-1-[2-(4-morpholinyl)ethyl]-1H-indol-3-yl]-methanone	WIN 48,098		92623-83-1
325,365	PRAZEPAM	7-chloro-1-(cyclopropylmethyl)-1,3-dihydro-5-phenyl-2H-1,4-benzodiazepin-2-one	NSC 277179		2955-38-6
160,078	PREGABALIN	3S-(aminomethyl)-5-methyl-hexanoic acid	CI 1008		148553-50-8
237,063	PROCAINE	4-amino-benzoic acid, 2-(diethylamino)ethyl ester	PROCAINE		51-05-8
218,162	PROLINTANE	1-[1-(phenylmethyl)butyl]-pyrrolidine	NSC169914		1211-28-5
285,029	PROMETHAZINE	N,N,α-trimethyl-10H-phenothiazine-10-ethanamine	PROMETHAZINE		58-33-3
342,045	PROPAFENONE	1-[2-[2-hydroxy-3-(propylamino)propoxy]phenyl]-3-phenyl-1-propanone	PROPAFENONE		34183-22-7
260,069	PROPRANOLOL	1-[(1-methylethyl)amino]-3-(1-naphthalenyloxy)-2-propano	NSC 91523		318-98-9
155,882	PROPYLHEXEDRINE	N,α-dimethyl-cyclohexaneethanamine	NSC 27110		1007-33-6

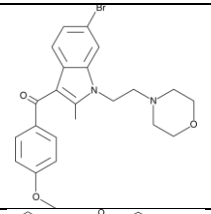
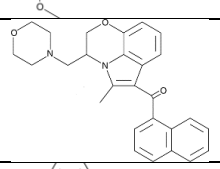
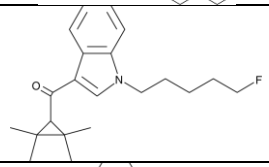
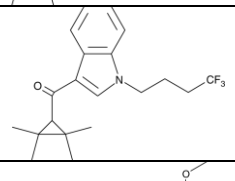
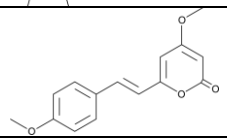
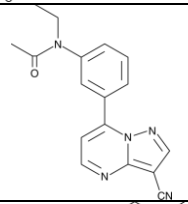
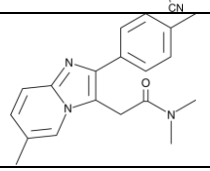
367,248	PSB-SB-1202	5-methoxy-3-[(2-methoxyphenyl)methyl]-7-pentyl-2H-1-benzopyran-2-one	PSB-SB-1202		1399049-60-5
356,299	PTI-1	N,N-diethyl-2-(1-pentyl-1H-indol-3-yl-4-thiazolemethanamine	PTI-1		1400742-46-2
400,341	PTI-2	N-(2-methoxyethyl)-N-(1-methylethyl)-2-(1-pentyl-1H-indol-3-yl)-4-thiazolemethanamine	PTI-2		No. Description
260,116	PV-8	1-phenyl-2-(1-pyrrolidinyl)-1-heptanone	α-PHPP		13415-55-9
274,307	PV9	1-phenyl-2-(1-pyrrolidinyl)-1-octanone	α-POP		2749897-19-4
396,09	PX-1	(S)-N-(1-amino-1-oxo-3-phenylpropan-2-yl)-1-(5-fluoropentyl)-1H-indole-3-carboxamide	5-FLUORO APP-PICA		2221100-71-4
397,253	PX-2	N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-1-(5-fluoropentyl)-1H-indazole-3-carboxamide	5-FLUORO APP-PINACA		2365471-47-0

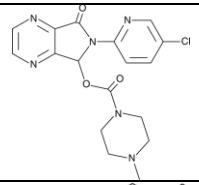
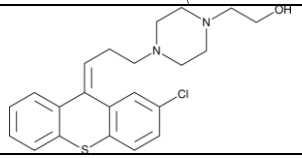
353,943	PYRAZOLAM	8-bromo-1-methyl-6-(2-pyridinyl)-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine	PYRAZOLAM		39243-02-2
384,09	QUETIAPINE	2-[2-(4-dibenzo[b,f][1,4]thiazepin-11-yl-1-piperazinyl)ethoxy]-ethanol	ICI 204636		111974-72-2
322,05	RCS-4	(4-methoxyphenyl)(1-pentyl-1H-indol-3-yl)methanone	E-4		1345966-78-0
326,3	RH-34	3-[2-[[(2-methoxyphenyl)methyl]amino]ethyl]-2,4(1H,3H)-quinazolinedione	RH-34		1028307-48-3
236,144	R-MMC	2-(Methylamino)-1-(3-methylphenyl)-1-propanone hydrochloride (1:1), 3-Methylmethcathinone	R-MMC		1246816-62-5
303,805	SCOPOLAMINE	(1α,2β,4β,5α,7β)-9-methyl-3-oxa-9-azatricyclo[3.3.1.02,4]non-7-yl ester αS-(hydroxymethyl)-benzeneacetic acid,	HYOSCINE		114-49-8
359,177	SDB-005	1-pentyl-1H-indazole-3-carboxylic acid, 1-naphthalenyl ester	SDB-005		2180934-13-6

321,153	SDB-006	1-pentyl-N-(phenylmethyl)-1H-indole-3-carboxamide	SDB-006		695213-59-3
306,988	SERTRALINE	1S,4S)-4-(3,4-dichlorophenyl)-1,2,3,4-tetrahydro-N-methyl-1-naphthalenamine	SERTRALINE		79559-97-0
475,047	SILDENAFIL	5-[2-ethoxy-5-[(4-methyl-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one	SILDENAFIL		139755-83-2
329,138	STANOZOLOL	(5α,17β)-17-methyl-2'H-androst-2-eno[3,2-c]pyrazol-17-ol	WIN 14,833		10418-03-8
222,343	TAPENTADOL	3-[(1R,2R)-3-(dimethylamino)-1-ethyl-2-methylpropyl]-phenol	TAPENTADOL		175591-09-0
301,993	TEMAZEPAM	7-chloro-1,3-dihydro-3-hydroxy-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one	NSC 246303		846-50-4
265,226	TETRACAINE	4-(butylamino)-benzoic acid, 2-(dimethylamino)ethyl ester	TETRACAINE		94-24-6

315,093	THC	6aR,7,8,10aR-tetrahydro-6,6,9-trimethyl-3-pentyl-6H-dibenzo[b,d]pyran-1-ol	DRONABINOL		1972-08-3
345,2	THCCOOH	(-)-11-Nor-9-carboxy-delta9-THC	THCCOOH		56354-06-4
142,098	THIOPROPAMINE	α-methyl-2-thiopheneethanamine	THIOPROPAMINE		53632-92-1
359,247	THJ	1-pentyl-N-(quinolin-8-yl)-1H-indazole-3-carboxamide	THJ		2180931-94-4
343,076	THJ-018	1-naphthalenyl(1-pentyl-1H-indazol-3-yl)-methanone	JWH 018 indazole analog		1364933-55-0
361,067	THJ-2201 (5-FLUORO THJ-018)	[1-(5-fluoropentyl)-1H-indazol-3-yl]-1-naphthalenyl-methanone	THJ-2201		1801552-01-1
224,246	TILETAMINE	2-(ethylamino)-2-(2-thienyl)-cyclohexanone	CI-634		14176-50-2

264,304	TRAMADOL	*el*-2R-[(dimethylamino)methyl]-1R-(3-methoxyphenyl)-cyclohexanol	CG 315		36282-47-0
372,082	TRAZODONE	2-[3-[4-(3-chlorophenyl)-1-piperazinyl]propyl]-1,2,4-triazolo[4,3-a]pyridin-3(2H)-one	TRAZODONE		25332-39-2
343,99	TRIAZOLAM	8-chloro-6-(2-chlorophenyl)-1-methyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine	U-33030		28911-01-5
294,788	TRIMIPRAMINE	10,11-dihydro-N,N,β-trimethyl-5H-dibenz[b,f]azepine-5-propanamine, (2Z)-2-butenedioate	TRIMIPRAMINE		521-78-8
329,037	U-47700	*trans*-3,4-dichloro-N-[2-(dimethylamino)cyclohexyl]-N-methyl-benzamide	U-47700		82657-23-6
312,107	UR-144	(1-pentyl-1H-indol-3-yl)(2,2,3,3-tetramethylcyclopropyl)-methanone	KM-X1		1199943-44-6
328,092	UR-144 metabolite	(1-(4-hydroxypentyl)-1H-indol-3-yl)(2,2,3,3-tetramethylcyclopropyl)methanone	XLR11 N-(4-hydroxypentyl) metabolite		1537884-04-5
377,154	W-15	4-chloro-N-[1-(2-phenylethyl)-2-piperidinylidene]-benzenesulfonamide	W-15		93100-99-3

457,176	WIN 54,461	[6-bromo-2-methyl-1-[2-(4-morpholinyl)ethyl]-1H-indol-3-yl](4-methoxyphenyl)-methanone	WIN 54,461		166599-63-9
427,117	WIN 55,212-2	[2,3-dihydro-5-methyl-3-(4-morpholinylmethyl)pyrrolo[1,2,3-de]-1,4-benzoxazin-6-yl]-1-naphthalenyl-methanone, methanesulfonate	WIN 55,212-2		131543-23-2
330,293	XLR-11	(1-(5-fluoropentyl)-1H-indol-3-yl)(2,2,3,3-tetramethylcyclopropyl)methanone	5-FLUORO UR-144		1364933-54-9
352,216	XLR12	(2,2,3,3-tetramethylcyclopropyl)[1-(4,4,4-trifluorobutyl)-1H-indol-3-yl]-methanone	XLR12		895155-78-9
259,148	YANGONIN	4-methoxy-6-[(1E)-2-(4-methoxyphenyl)ethenyl]-2H-pyran-2-one	YANGONIN		500-62-9
305,911	ZALEPLON	N-[3-(3-cyanopyrazolo[1,5-a]pyrimidin-7-yl)phenyl]-N-ethyl-acetamide	CL 284,846		151319-34-5
308,323	ZOLPIDEM	N,N,6-trimethyl-2-(4-methylphenyl)-imidazo[1,2-a]pyridine-3-acetamide	SL 80-0750		82626-48-0

389,014	ZOPICLONE	4-methyl-1-piperazinecarboxylic acid, 6-(5-chloro-2-pyridinyl)-6,7-dihydro-7-oxo-5H-pyrrolo[3,4-b]pyrazin-5-yl ester	RP 27267		43200-80-2
401,024	ZUCLOPENTHIXOL	4-[(3Z)-3-(2-chloro-9H-thioxanthen-9-ylidene)propyl]-1-piperazineethanol	ZUCLOPENTHIXOL		53772-83-1

[D4] Jolanta Powierska-Czarny, Jakub Czarny, Radosław Zbytniewski, Michał Raczkowski, Natalia Galant, **Jadwiga Musiał**., *Sposób wykrywania związków psychoaktywnych w próbkach biologicznych oraz zastosowanie tego sposobu do wykrywania substancji psychoaktywnych,* Zgłoszenie patentowe - Numer P.441164 UP

URZĄD PATENTOWY
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Kancelaria Ogólna

Warszawa, 2022-05-13

Nasz znak: POTWIERDZENIE/239275/P.441164
Wasz znak: 32078/PAT/22

POTWIERDZENIE

Urząd Patentowy RP stwierdza, że dnia 2022-05-13 przyjęto w formie elektronicznej wniosek o udzielenie patentu na wynalazek:

Sposób wykrywania związków psychoaktywnych w próbkach biologicznych oraz zastosowanie tego sposobu do wykrywania substancji psychoaktywnych

Zgłoszenie oznaczono numerem: **P.441164**
[WIPO ST 10/C PL441164]

Zgłaszający: **Instytut Genetyki Sadowej Jolanta Powierska - Czarny, Bydgoszcz, Polska**

Dokument wystawiony automatycznie przez system teleinformatyczny UPRP.

Pouczenie:

1. Strony oraz ich przedstawiciele i pełnomocnicy mają obowiązek zawiadomić Urząd o każdej zmianie swojego adresu. W razie zaniedbania tego obowiązku doręczenie pisma pod dotychczasowym adresem ma skutek prawny (art. 41 kpa).
2. O zgłoszeniu wynalazku Urząd Patentowy dokonuje ogłoszenia niezwłocznie po upływie 18 miesięcy od daty pierwszeństwa do uzyskania patentu. Zgłaszający może w okresie 12 miesięcy od daty pierwszeństwa złożyć wniosek o dokonanie ogłoszenia w terminie wcześniejszym (art. 43 ustawy z dnia 30 czerwca 2000r. Prawo własności przemysłowej (Dz. U. z 2021 r. poz. 324).
3. W korespondencji należy powoływać się na nr P.441164.

Klauzula informacyjna:
Zgodnie z art. 13 ust. 1 i 2 Rozporządzenia Parlamentu Europejskiego i Rady (UE) 2016/679 z dnia 27 kwietnia 2016 r. w sprawie ochrony osób fizycznych w związku z przetwarzaniem danych osobowych i w sprawie swobodnego przepływu takich danych oraz uchylenia dyrektywy 95/46/WE (dalej RODO) Urząd Patentowy Rzeczypospolitej Polskiej informuje, że:

1. Administratorem Pani/Pana danych osobowych jest Urząd Patentowy Rzeczypospolitej Polskiej z siedzibą w Warszawie, adres: al. Niepodległości 188/192, 00-950 Warszawa, skrytka pocztowa 203;
2. Inspektor Ochrony Danych, dane kontaktowe: adres: al. Niepodległości 188/192, 00-950 Warszawa, tel. bezpośredni (022) 579 00 25, fax (022) 579 00 01, e-mail: iod@uprp.pl;

3. Pani/Pana dane osobowe przetwarzane będą w celu realizowania zadań Urzędu Patentowego RP określonych przepisami ustawy z dnia 30 czerwca 2000 r. Prawo własności przemysłowej;
4. Podstawą prawną przetwarzania Pani/Pana danych osobowych jest ustawa z dnia 30 czerwca 2000 r. Prawo własności przemysłowej, rozporządzenia wykonawcze do ww. ustawy, umowy międzynarodowe oraz art. 6 ust. 1 lit. c RODO;
5. Pani/Pana dane osobowe mogą być przekazywane do podmiotów publicznych na zasadach obowiązujących w przepisach prawa oraz organizacjom międzynarodowym i organom unijnym, zgodnie z obowiązującymi przepisami prawa i umowami międzynarodowymi, po upływie terminów zastrzeżonych dla nieujawniania informacji o zgłoszeniu;
6. Pani/Pana dane osobowe będą przechowywane przez okres zgodny z zasadami archiwizacji dokumentów w Urzędzie Patentowym RP;
7. Posiada Pani/Pan prawo żądania dostępu do treści swoich danych osobowych, prawo ich sprostowania oraz prawo do ograniczenia ich przetwarzania;
8. Przysługuje Pani/Panu prawo wniesienia skargi do organu nadzorczego właściwego w zakresie ochrony danych osobowych gdy uzna Pani/Pan, że przetwarzanie Pani/Pana danych osobowych narusza przepisy RODO;
9. Podanie przez Panią/Pana danych osobowych jest wymogiem ustawowym niezbędnym do dalszego procedowania przez Urząd Patentowy RP.

UWAGA NA OSZUSTÓW!

Przed dokonaniem jakiejkolwiek opłaty do Urzędu Patentowego RP, sprawdź czy numer rachunku zgadza się z numerem konta Urzędu:

NBP O/O Warszawa: 93 1010 1010 0025 8322 3100 0000

Urząd Patentowy RP posiada tylko jeden numer rachunku i pobiera opłaty wyłącznie w złotych!

W przypadku jakichkolwiek wątpliwości prosimy o kontakt z Centrum Informacji w Urzędzie Patentowym RP pod nr tel.: 22 579 05 55. Aktualne ostrzeżenia o próbach wyłudzeń publikowane są na stronach Urzędu Patentowego RP (uprp.gov.pl) oraz w komunikatach FinCERT.pl - Bankowego Centrum Cyberbezpieczeństwa Związku Banków Polskich (zbp.pl).

W celu weryfikacji autentyczności korespondencji zeskanuj podany kod QR lub przejdź na stronę weryfikacji korespondencji Urzędu Patentowego RP dostępnej pod adresem **https://pue.uprp.gov.pl/public/stamp/verify** i przepisz kod stempla.

Kod stempla: fe4-9d5d-26b

[D5] Jakub Czarny, **Jadwiga Musiał**, Jolanta Powierska-Czarny, Michał Raczkowski, Natalia Galant, Bogusław Buszewski, Renata Gadzała-Kopciuch, *Determination of 465 psychoactive substances, drugs and their metabolites in urine by LC-MS/MS,* Analytical Methods, 2024, https://doi.org/10.1039/D4AY00777H, IF=2,7

Próbki moczu charakteryzują się wyższymi stężeniami analitów lub ich metabolitów niż próbki krwi. W ziązku z powyższym w próbkach moczu jest szansa na wykrycie analitów w późniejszym czasie niż w przypadku krwi. Połączenie badań obejmujących próbki krwi, moczu oraz włosów od jednego pacjenta/przestępcy czy też ofiary, umożliwiają retrospektywne podejście oraz wykrycie zarówno tych charakterystycznych jak i dotąd nie znanych metabolitów. Takie podejście do próbek pochodzących od jednej osoby daje szerokie możliwości również w kwestii wyciągnięcia konsekwencji prawnych oraz zdrowotnych. Jest to bardzo istotny fakt, szczególnie mając na uwadze ciągle wzrastającą liczbę zdarzeń drogowych, zatruć oraz przestępstw kryminalnych popełnianych pod wpływem substancji psychoaktywnych dostępnych w sprzedaży ulicznej. W publkacji [**D5**] skupiono się na przystosowaniu opracowanej metody analitycznej dla próbek krwi opisanych powyżej do analizy próbek moczu.

Celem prac było opracowanie metody ekstrakcji analitów z próbek moczu bazując na opracowanej dla próbek krwi procedurze analitycznej. Pozwoliłoby to na szybkie przystosowanie opracowanej metody do kolejnej matrycy, co umożliwiłoby analizę kompleksową próbek biologicznych pochodzących od jednej osoby. Nadal istotnym dla badań było spełnienie warunków jakimi miała charakteryzować się opracowana procedura analityczna: prosta, dająca możliwość łatwego rozszerzenia o kolejne anality, a przy tym selektywna z niską granicą oznaczalności. Biorąc pod uwagę wyniki otrzymane dla próbek krwi w tym przypadku również zdecydowano się na zastosowanie LLE oraz metody z użyciem krzywej wzorcowej uwzględniającej matrycę i rozcieńczenia próbki w końcowym etapie procedury.

Jednakże w celu optymalizacji procedury konieczne było zweryfikowanie wpływu β-glukuronidazy na wydajność ekstrakcji. Zwykle w przypadku próbek tej matrycy enzym ten jest wprowadzany do procedury. Zależało nam na tym, aby sprawdzić czy jest to niezbędny etap naszej procedury. Dzięki przeprowadzonym badaniom udowodniono, że etap z zastosowaniem β-glukuronidazy można pominąć, a ekstrakcja bez jej użycia jest wydajna, a przy tym znacznie szybsza i tańsza. Biorąc pod uwagę szeroki zakres analitów, a przez to znaczące różnice w stężeniach analitów tej matrycy, szczególnie jeśli chodzi o zawartość benzodiazepin względem pozostałych grup analitów zdecydowano na zastosowanie dwóch

rozcieńczeń: 10-krotnego i 100-krotnego, co umożliwiło objęcie zakresu stężeń występujących w próbkach zarówno dla benzodizepin, jak i innych grup substancji psychoaktywnych.

Opracowaną metodę analityczną, tak jak w przypadku wcześniej opisanych matryc, poddano procesowi walidacji zgodnie z wytycznymi SWGTOX [78]. Linowość sprawdzono poprzez analizę 6 powtórzeń krzywej wzorcowej przygotowanej w matrycy w zakresie stężeń od 0,05 do 50 ng/ml dla poszczególnych analitów. Ponadto, w każdej serii analizowano próbkę ślepą (matrycę) i matrycę z wzorcem wewnętrznym. Współczynniki korelacji obliczone dla każdego analitu wynosiły ≥0,99. Aby wyznaczyć precyzję i BIAS analizowano sześciokrotnie pięć poziomów stężeń analitów po uwzględnieniu rozcieńczenia próbki (10, 100, 1000, 2000 i 5000 ng/ml. Dla powyższych parametrów przyjęto zgodnie z wytycznymi granicę ±20%. Pomiary te wykorzystano także do wyznaczenia średniego odzysku analitów. Za LOQ przyjęto, tak jak w przypadku innych matryc, najniższy punkt krzywej wzorcowej, wyznaczony jako stosunek S/N ≥10. W celu weryfikacji powtarzalności metody przystąpiono do analizy próbek z badań biegłości.

Opracowana podczas przeprowadzonych badań metoda analityczna została wprowadzona do rutynowych analiz w Instytucie Genetyki Sądowej w Bydgoszczy.

Analytical Methods

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Determination of 465 psychoactive substances, drugs and their metabolites in urine by LC-MS/MS

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Abstract

Due to the emergence of new psychoactive substances on the drug market, there is a growing demand for analytical methods allowing identification and determination of as many newly available drugs as possible in the shortest possible time. Immunochemical methods are not sufficient to meet constantly growing requirements. Therefore, the aim of the study was to develop an analytical method enabling quick analysis of urine samples for psychoactive substances, drugs and their metabolites. Liquid-liquid extraction (LLE) and liquid chromatography coupled with mass spectrometry (LC-MS/MS) were used for this purpose. Extraction was performed using acetonitrile with ammonium formate and formic acid. Chromatographic separation was achieved with a Kinetex C18 column (Phenomenex, 3.0 x 100 mm; 2.6 µm). The mass spectrometer worked in the MRM pair monitoring mode (two pairs for each analyte). The developed method was validated for 477 substances belonging to various chemical groups. Out of such a large number of analytes, only 12 did not meet the validation criteria recommended by SWGTOX (CV: ± 20% and BIAS ± 20%). Thus the validated method makes it possible to determine 465 psychoactive substances in just 30 minutes. The designated limit of detection (LOD) is 0.5 ng/mL and the limits of quantification (LOQ) are in the range 10–100 ng/mL. The method was successfully applied to toxicological analyses of urine samples, which was an opportunity to develop it further to meet the needs of toxicology.

Keywords: New psychoactive substances (NPS), drugs, metabolites, urine analysis, liquid-liquid extraction (LLE), liquid chromatography tandem mass spectrometry (LC-MS/MS).

Introduction

In recent years, interest in psychoactive substances has increased significantly, particularly in their uncontrolled analogues called new psychoactive substances (NPS). Due to modifications in the structure of classic drugs, NPS fall through the net of administrative control, providing an attractive, often cheaper alternative to amphetamines, THC or opiates. Internet commerce can provide this type of substances to a very large group of customers, posing a significant threat to their health and life. Products of this type are advertised and sold in the form of, inter alia, "bath salts", "plant food" or "scientific research chemicals"[1]. Vendors do not indicate the actual active ingredients or the purity of the NPS offered[2-4]. Consequently, this increases the risk of an overdose and unforeseen side effects. Modifications in the structures of psychoactive substances are associated with the lack of available methods of analysis that would enable the detection of used substances and thus avoid legal consequences and colossal health consequences for many people. The increase in the number of NPS appearing in trade poses an excellent challenge for analysts. It is necessary to develop analytical methods that enable detecting and quantifying the most significant possible number of analytes in the shortest possible time. The negative impact of this type of substance on the body can be associated with enormous health consequences and even life-threatening, so it is crucial to detect the taken substance, introduce a treatment appropriate for a given substance, and then reduce the presence of this substance in trade. Screening analysis allows for the preliminary exclusion of NPS consumption. Still, it should be remembered that the concentrations of the legal highs used are so low that these methods may give a false negative result. In addition, they do not allow for unequivocal identification of the substance used.

Urine samples are frequently used in toxicological analyses as they have many advantages, including non-invasive sampling, high concentrations of drugs and metabolites that are tested for, and relatively long time windows for detection of substances used[5]. However, urine as matrix also poses several difficulties. Immunochemical tests are often used as a quick and cheap screening method[6]. These types of tests work on the principle of interaction between antibodies and substances used[7]. However, with these tests there is a high risk of obtaining false positive and false negative results due to the sensitivity limitations of these methods to given substances or groups of substances[2]. This means that immunochemical tests can be considered only as preliminary results for a given sample. Each positive should be confirmed by a different analytical method[8], e.g. gas spectrometry coupled with mass spectrometry (GC-MS). The problem arising in the case of analyses using GC-MS is usually the need to derivatize the sample

in order to enable the determination of analytes, which results, inter alia, in sample losses[2,3,6]. The solution to the problem of sample preparation for GC-MS analysis is liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS), which allows the analysis of multiple analytes with high sensitivity without the need for additional stages of sample preparation[4,6,9-11]. However, in this case, there is also a difficulty related to the form in which analytes occur, as in urine tests there are analytes in free form as well as associated with glucuronide[12]. Concentration of each form may differ because it depends both on the metabolism of a given organism and the time of sampling[2,12]. To counteract this problem glucuronide hydrolysis is performed to determine a specific analyte, irrespective of the form in which it appears in the sample[13,14]. Often, when preparing urine samples, solid phase extraction (SPE) is used[2,3,15,16]. However, this procedure also has its disadvantages: it is time-consuming and there can be large differences in the values of recoveries of individual analytes if multiple analytes are determined at the same time[2,16]. Among the recent studies, the use of dilution method to prepare urine samples for analysis with LC-MS/MS[1,17,18] seems promising. The aim of our work was to develop an analytical method that would allow us to detect and quantify as many analytes as possible in a relatively short time. In addition, we wanted to be able to quickly develop the developed method with the new NPS, which will be available for sale over time. In our research, we used dilution and LC-MS/MS analysis to develop a method for determining 477 psychoactive substances including classical drugs and new psychoactive substances in urine samples. In order to remove the matrix effect during the determinations, a calibration curve prepared for the matrix was used.

Experimental

Material and methods

Chemicals and reagents

Certified analytical standards were purchased from Cayman Chemical, CHIRON, Lipomed Services to Health, and LGC Standards. Acetonitrile for LC-MS, methanol for LC-MS and formic acid for LC-MS were purchased from S. WITKO CHS, and ammonium formate for LC-MS was purchased from Sigma Aldrich. The following equipment was used: Eppendorf tubes (2ml), vials (2ml), MS2 Minishaker IKA 200-2500 rpm, laboratory centrifuge: Sigma 4-16S, syringe filters: VWR 0,2 μm.

Standard solution, working solution

Acetonitrile with buffer was prepared by adding 20 µL ammonium formate, and 20 µL formic acid to a 100 mL volumetric flask and making up to the mark with acetonitrile.

Standard solutions in methanol at eight concentrations (0.5 ng/mL, 1 ng/mL, 5 ng/mL, 10 ng/mL, 50 ng/mL, 100 ng/mL, 200 ng/mL and 500 ng/mL) was prepared from 1 mg/mL standards with the dilution method.

The calibration curve in the matrix was made by measuring of 250 µL of urine without analytes was added to three Eppendorf tubes of 2 mL volume and adding 250 µL of ACN with ammonium formate and formic acid. The contents of the tubes were mixed (Vortex). The test tubes were placed in a minishaker (1400 rpm, 21^{o}C) for 10 minutes during the next step. Afterward, the samples were put in a freezer for 10 minutes and then placed in a centrifuge (2000 rcf) for 5 minutes. The supernatant was filtered through a syringe filter, and during the last step, the tubes were placed into a centrifuge (10000 rcf) for 1 minute. The urine extract (100 µL), 50 µL mix of the analytical standard at a concentration 10x as high as the reference in the calibration curve (to obtain the appropriate concentration in the sample after final dilution), 10 µL of atrazine solution – internal standard (1000 ng/mL), and 340 µL of mobile phase A:B (90:10,v/v) was put in a vial (2 mL). The calibration curve was analyzed in each series of tests.

Equipment

The liquid chromatography system consisted of an ExionLC AC Pump 2x, ExionLC Degaser, Exion AC Autosampler, and ExionLC Column Oven from AB SCIEX. The system was coupled to a mass spectrometer AB SCIEX 5500 QTRAP with electrospray ionization in positive and negative mode. For data acquisition, data handling and instrument control Analyst 1.6.3 and MultiQuant 3.0.3 software was used. Separation was carried out on a Kinetex C18 column (Phenomenex, 3.0 x 100 mm; 2.6 µm). A 20 µL sample was injected into the system at a flow rate of 0.5 mL/min. Mobile phases A: water with ammonium formate (2 mM) and formic acid (0.1 %v/v) and B MeOH with ammonium formate (2 mM) and formic acid (0.1%, v/v), were used with the gradient program below: 5% of B at 0 min, 5% of B at 1min, 95% of B maintained from 15 to 21 min, 5% of B maintained from 27 to 30 min. The mobile phase was delivered at a flow rate of 0.5 mL/min. Analytes were quantified in double ion monitoring (MRM) mode. All results were based on the peak area ratio between the drug and the analytical standard. The MS conditions were set as follows: CUR: 30, CAD: medium, TEM: 400, GS1: 40, GS2: 70, dwell time ≥ 5 ms.

Sample preparation

Urine samples and fortified samples:

First, 250 µL of urine and 20 µL of atrazine (2500 ng/mL) was added into 2 mL Eppendorf tubes; next 250 µL of ACN with buffer was added and mixed in a vortexer. During the next step, the test tubes were placed into a minishaker (1400 rpm, 21^{O}C) for 10 minutes. Afterwards the samples were placed in a freezer for 10 minutes for a better purification of the sample and then were put in a centrifuge (2000 rcf) for 5 minutes. The supernatant was filtered through a syringe filter and in the last step the tubes were placed in a centrifuge (10000 rcf) for 1 minute. The 10 µL of urine extract and 490 µL of mobile phase A:B (90:10, v/v) was put in a vial (2mL). Fortified samples are prepared analogously to the real samples. In the first, apart from the atrazine and urine, we add 50 µl of the mix of analytical standards (500 ng /mL). However, in the next step, we add 200 µL of ACN with a buffer instead of 250 µL as in the case of urine samples. We perform the remaining steps analogously to the real samples. The fortified samples were analyzed in each series of tests.

Method Validation

The spectrometric analysis parameters were optimized, and two MRM pairs were selected for each analyte according to the mass spectrometry standards.

This method was validated according to the SWGTOX validation guidelines for whole blood and urine[19]. The parameters such as selectivity, specificity, linearity, precision, BIAS, recovery, reproducibility, LOD and LOQ were validated.

Selectivity and specificity were assessed by spiking fortified samples with in small mix to test for any interference. Urine without analytes was used to identify matrix interferences. Samples were extracted and analyzed following the developed method in order to ascertain whether exogenous analytes may interfere with the analytes tested for the developed method.

Linearity was assessed by analyzing six separate calibration curves in the matrix by spiking blank urine with concentrations ranging from 0.05 to 50 ng/mL for each analyte. Calibration curves were generated by plotting the peak area ratio (PAR) versus the spiked analyte concentration. Blank matrix and blank matrix containing only IS was analyzed with each batch but not included in the calibration curves. The correlation coefficient (R2) was calculated and deemed acceptable for R2 values >0.99.)

Precision and BIAS was calculated by running six replicates of calibration standards for five concentrations (10, 100, 1000, 2000 and 5000 ng/mL). For precision and BIAS accuracy limit of ±20% was used. The six repetitions were also used to determine the mean recovery.

The limit of detection (LOD) value was determined as the lowest calibration standard which was expressed as S/N ratio ≥3, while the LOQ was determined to be the lowest calibration standard which was expressed as S/N ratio ≥10. The reproducibility of the analytical method has been verified by proficiency tests.

In order to verify the matrix effect, a standard curve in the matrix was used. The obtained points of the standard curve take into account the influence of the matrix on the analysis of real samples.

Results and discussion

Choice of the experimental conditions in HPLC and MS

In order to select the working parameters of the mass spectrometer, the analytical standards of the tested substances were individually optimized with the Analyst 1.6.3 software. During this step, values appropriate for each analyte were selected, such as the ionization mode, Q1, Q3, declustering potential (DP), entrance potential (EP), collision energy (CE), and collision cellExit potential (CXP). Among the psychoactive substances that were optimized, the negative ionization mode turned out to be better only for two of them (GHB and Phenobarbital). All other analytes are analyzed in positive ionization mode. The MRM pairs and DP, EP, CE, CXP values for each analyte have been collected in Table 1. MRM transitions were monitored only in specific detection windows that were defined as ± 0.5 min from the expected retention time. The developed method 465 analytes (two transitions for each analyte). After selecting the MS parameters, optimization of the chromatographic method was undertaken in order to obtain the best possible separation of all analytes. Optimum separation conditions were obtained with the following conditions of the gradient: 5% of B at 0 min, 5% of B at 1min, 95% of B maintained from 15 to 21 min, 5% of B maintained from 27 to 30 min. The mobile phase was delivered at a flow rate of 0.5 mL/min. Mobile phases A: water with ammonium formate (2 mM) and formic acid (0.1 %v/v) and B MeOH with ammonium formate (2 mM) and formic acid (0.1 %v/v), were used. Acetonitrile was also checked instead of methanol; however, it did not create more favorable conditions, and increased the harmfulness of the waste generated during the analyzes as well as their cost. Various contents of ammonium formate (from 2 to 5mM) were also tested. In this case, increasing the ammonium formate content did not improve the separation of the analytes on the chromatographic column. The chromatographic conditions selected in this way

were checked on three different columns: Kinetex C18 column (Phenomenex, 3.0 x 100 mm; 2.6 μm), Kinetex Biphenyl (Phenomenex, 3.0 x 100 mm; 2.6 μm) and Kinetex Phenyl-Hexyl (Phenomenex, 3.0 x 100 mm; 2.6 μm). The best separation was obtained for the first column, so it was selected for further analysis. This gradient method allowed separation of all compounds except 3-MMC and 4-MMC in a 30-min run time. The retention times of all compounds were from 1.41 to 16.76 min and are presented in Table 2.

Development of the extraction procedure

Work on the extraction process started with solid phase extraction (SPE) tests. However, the wide range of analytes belonging to different groups made it impossible to obtain satisfactory results. Individual columns dedicated to a given group of analytes generated numerous losses among other analytes. If several types of SPE columns were used, a single sample needed to be analyzed several times, which generates large losses, both in terms of time and reagent, and requires a much larger amount of sample for testing. Considering the obtained results, an attempt was made to develop an extraction method that would enable rapid isolation of all compounds contained in the developed procedure. Liquid-liquid extraction with cold ammonium formate in acetonitrile was selected for this purpose. To verify the extraction process, atrazine solution was added to each of the samples at the same level. The next step was to check the effect of freezing the sample at two stages of the sample preparation process. The sample was first placed in the freezer for 10 minutes after the addition of ACN with buffer and vortexing. The sample was placed in the freezer again after being removed from the centrifuge. The tests performed showed that while the first freezing of the sample is beneficial in the preparation of the sample, its re-freezing has no effect, so this step was removed from the procedure. The urine sample preparation procedure described above turned out to be the most advantageous in terms of recoveries obtained for individual analytes. The developed procedure allowed the isolation of all tested analytes from urine samples during one process. The results concerning the mean recovery of a given analyte are presented in Table 2.

Validation

The developed method of isolating and determining psychoactive compounds, drugs and their metabolites from urine samples was validated according to the SWGTOX guidelines. 465 out of 477 validated compounds met the validation criteria and were included in routine analysis of urine samples. The type of calibration curve in matrix was selected using the software used to process the results. The linear range of the curves was selected as the most appropriate, and the calibration curves in matrix were linear in the range of 0.5–50 ng/mL. The correlation

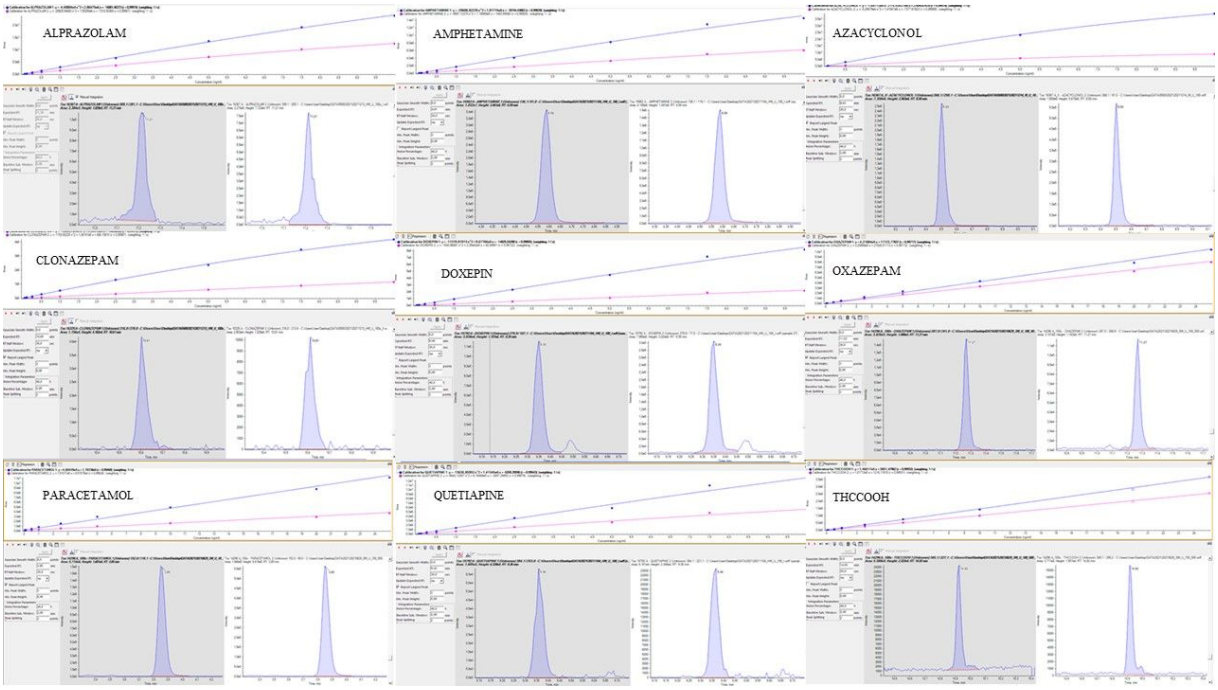
coefficient (R2) was calculated and deemed acceptable for R2 values >0.99. The use of this type of standard curve made it possible to eliminate the influence of the matrix effect in real samples. Extraction recoveries ranged from 18.43% (JWH-146) to 119.94% (1-(2-methoxyphenyl)piperazine). The method was found to be selective for the tested compounds. The only exception are 3-MMC and 4-MMC which do not separate on analysis. No interfering peaks were observed in the drug-free urine samples. The precision and accuracy values and recoveries for validated compounds are presented in Table 2. Due to the requirements and improvement of routine laboratory work, the lowest point of the curve was adopted as the LOD values. However, in the case of LOQ, the lowest concentration was assumed, which positively passed the validation of individual analytes. The LOD was estimated for 465 compounds and the value was 0.5 ng/mL. The LOQs values were from to 10 ng/mL to 100 ng/mL. The LOD and LOQ values for each analyte are also included in Table 2. For precision and bias, the accuracy limit of ±20% was used. Values of precision ranged from 0.87 % to 19.14% and bias from -19.92% to 19.94%. Twelve of the validated compounds did not meet the above criteria. The developed method was verified by proficiency tests carried out according to LGC Standards. The obtained results met the criteria of proficiency tests.

Use in real samples in Institute of Forensic Genetics in Bydgoszcz

The developed analytical method was incorporated into the routine analysis of urine samples in our laboratory. In 2021, 70 urine samples from drivers were analyzed. In only 18% of them, the presence of none of the 477 analyzed substances was found. 49 analytes were detected in the remaining samples. They were: 3,4-MDMA, 3-CMC, 3-hydroxybromazepam, 3-MMC, 4-MMC, 4-CMC, 4-methylamphetamine, 4-methylcathinone, 6-MAM, 7-aminoclonazepam, alpha-ethylaminohexanophenone, alprazolam, amphetamine, azacyclonol, benzoylecgonine, carbamazepine, cathine, clonazepam, cocaethylene, cocaine, codeine, DCPP, dextromethorphan, diazepam, dihydrocodeine, doxepin, EDDP, eutylone (BK-EBDB), fentanyl, fluoxetine, GHB, hydrocodone, lidocaine, methadone, methamphetamine, methcathinone, mianserin, morphine, nordiazepam (desmethyldiazepam), oxazepam, paracetamol, pregabalin, propranolol, quetiapine, sertraline, sildenafil, temazepam, THCCOOH, tramadol, trazodone. Figure 1 shows the calibration curves in matrix, and chromatograms of substances detected in real samples. One substance was found in 14 samples, Two substances were found in 12 samples, three substances were found in 8 samples, four substances were found in 4 samples, five substances were found in 1 sample, six substances were found in 7 samples, seven substances were found in 2 samples, eight substances were

found in 3 samples and fourteen substances were found in 1 sample. The most frequently detected substances were paracetamol (22 samples), amphetamine (20 samples), GHB (11 samples), THCCOOH (8 samples), and morphine (7 samples). The conducted research on a group of drivers allowed us to verify the method in terms of its suitability for routine analyzes.

Figure 1. The calibration curves in matrix and chromatograms of substances detected in real samples.



Conclusions

The developed analytical method enables quick, relatively cheap analysis of urine samples for psychoactive substances, drugs and their metabolites. The use of liquid-liquid extraction made it possible to isolate a large number of analytes (465) during a single sample preparation process, which significantly reduces the time of sample preparation as well as the consumption of reagents and the volume of harmful waste. The developed method is characterized by a much larger number of analyzed substances than the works mentioned above[6,8,11,17,18] in which the number of analytes is 62, 80, 7, 8, and 10, respectively. Moreover, the procedure of our method has been simplified o remove the stage of enzymatic hydrolysis, which was used in one of the studies[18]. Moreover, the developed procedure obtained lower LOD and LOQ values than in the previous works. An additional advantage is the possibility of further development of the method and its expansion with new analytes. The LC-MS/MS method used for the determination was successfully introduced into routine analyses. With it, a large number of substances can be analyzed quickly, which facilitates fast diagnosis and treatment of patients with suspected poisoning, or collecting evidence from e.g. road accident participants or suspects showing signs

of psychoactive substance abuse. The developed and fully validated method not only enables on-the-spot analyses but also creates great opportunities for further development of this method and the creation of new variants, e.g. tailored for specific needs of toxicologists. The method we developed has some shortcomings, including a small number of metabolites compared to the number of primary analytes. However, the enormous development opportunities of this method allow us to analyze primary substances in other matrices, such as blood, and add further metabolites to the list of analytes, which will improve the method developed by us in terms of a more comprehensive analysis of urine samples.

Statements and Declaration:

Conflict of interest:

The authors declare the following financial interest/personal relationships which may be considered as potential competing interests: Jakub Czarny reports was provided by National Centre for Research and Development.

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References:

1. J.M. Prosser, L.S. Nelson, The Toxicology of Bath Salts: A Review of Synthetic Cathinones. J. Med. Toxicol. 8 (2012) 33–42. doi: 10.1007/s13181-011-0193-z
2. M. Baron, M. Elie, L. Elie, An analysis of legal highs-do they contain what it says on the tin? Drug Test. Anal. 3 (2011) 576–581. doi: 10.1002/dta.274
3. S. Davies, D.M. Wood, G. Smith, J. Button, J. Ramsey, R. Archer, D.W. Holt, P.I. Dargan, Purchasing “legal highs” on the Internet-is there consistency in what you get? Qjm. 103 (2010) 489–493. doi: 10.1093/qjmed/hcq056
4. W. Zukiewicz-Sobczak, J. Zwoliński, J. Chmielewska-Badora, E. Krasowska, J. Piątek, P. Sobczak, A. Wojtyła, E. Fornal, A. Kuczumow, P. Billiński, Analysis of psychoactive and intoxicating substances in legal highs. Ann. Agric. Environ. Med. 19 (2012) 309–314. PMID: 22742807

5. N. Katz, G.J. Fanciullo, Role of urine toxicology testing in the management of chronic opioid therapy. Clin. J. Pain. 18 (4 Suppl) (2002) 76-82. doi:10.1097/00002508-200207001-00009

6. I.L.Tsai, T.I. Weng, Y.J. Tseng, H.K.L. Tan, H.J. Sun, C.H. Kuo, Screening and confirmation of 62 drugs of abuse and metabolites in urine by ultra-high-performance liquid chromatography-quadrupole time-of-flight mass spectrometry. J. Anal. Toxicol. 37 (2013) 642–651.doi: 10.1093/jat/bkt083

7. J.S. Tsai, G.L. Lin, Drug-Testing Technologies and Applications. Drugs of Abuse: Body Fluid Testing (2005) 29–69.

8. A. Helander, O. Beck, R. Hägerkvist, P. Hulten, Identification of novel psychoactive drug use in Sweden based on laboratory analysis-initial experiences from the STRIDA project. Scand. J. Clin. Lab. Invest. 73 (2013) 400–406. doi:10.3109/00365513.2013.793817

9. Australian/New Zealand Standard ™ Procedures for specimen collection and the detection and quantitation of drugs of abuse in urine; (2008).

10. A.Hb. Wu, R. Gerona, P. Armenian, D. French, M. Petrie, K.L. Lynch, Role of liquid chromatography-high-resolution mass spectrometry (LC-HR/MS) in clinical toxicology. Clin. Toxicol. 50 (2012) 733–742.doi: 10.3109/15563650.2012.713108

11. R.L. Fitzgerald, T.L. Griffin, Y.M. Yun, R.A. Godfrey, R. West, A. J. Pesce, D.A. Herold, Dilute and shoot: Analysis of drugs of abuse using selected reaction monitoring for quantification and full scan product ion spectra for identification. J. Anal. Toxicol. 36 (2012) 106–111. doi: 10.1093/jat/bkr024

12. L. Fattore, W. Fratta, Beyond THC: The new generation of cannabinoid designer drugs. Front. Behav. Neurosci. 5 (2011) 1–12. doi: 10.3389/fnbeh.2011.00060

13. K.A. Seely, J. Lapoint, J.H. Moran, L. Fattore, Spice drugs are more than harmless herbal blends: A review of the pharmacology and toxicology of synthetic cannabinoids. Prog. Neuro-Psychopharmacology Biol. Psychiatry. 39 (2012) 234–243. doi: 10.1016/j.pnpbp.2012.04.017

14. Z. Davey, F. Schifano, O. Corazza, P. Deluca, E-Psychonauts: Conducting research in online drug forum communities. J. Ment. Heal. 21 (2012) 386–394.

doi: 10.3109/09638237.2012.682265

15. A. Kjellgren, C. Soussan, Heaven and hell-a phenomenological study of recreational use of 4-HO-MET in Sweden. J. Psychoactive Drugs. 43 (2011) 211–219. doi: 10.1080/02791072.2011.605699

16. C.M. Murphy, A.R. Dulaney, M.C. Beuhler, S. Kacinko, "Bath Salts" and "Plant Food" Products: The Experience of One Regional US Poison Center. J. Med. Toxicol. 9 (2013) 42–48. doi: 10.1007/s13181-012-0243-1

17. C. Bell, C. George, A.T. Kicman, A. Traynor, Development of a rapid LC-MS/MS method for direct urinalysis of designer drugs. Drug Test. Anal. 3 (2011) 496–504. doi: 10.1002/dta.306

18. K. Björnstad, O. Beck, A. Helander, A multi-component LC-MS/MS method for detection of ten plant-derived psychoactive substances in urine. J. Chromatogr. B Anal. Technol. Biomed. Life Sci. 877 (2009) 1162–1168. doi: 10.1016/j.jchromb.2009.03.004

19. Scientific Working Group for Forensic Toxicology (SWGTOX) Standard Practices for Method Validation in Forensic Toxicology; (2013) 452–474. doi: 10.1093/jat/bkt054

Table 1. Summary of operating parameters LC-MS/MS and MRM pairs for each compound studied.

ANALYTE	Precursor Ion (Q1)	Product Ion (Q3)	DP	EP	CE for 1stMRM/ 2nd MRM	CXP for 1stMRM/ 2nd MRM	ANALYTE	Precursor Ion (Q1)	Product Ion (Q3)	DP	EP	CE for 1stMRM / 2nd MRM	CXP for 1stMRM / 2 MRM
4-CHLORO-ALPHA-PVP	266.300	125.1; 126.1	101	10	33/37	10/18	bk-2C-B	274.896	163.0; 178.1	81	10	39/21	39/21
1-(2-METHOXYPHENYL)PIPERAZINE	193.263	120.1; 150.1	106	10	43/25	8/18	bk-MDA	194.195	146.0; 118.1	56	10	19/31	14/14
1-(3-TRIFLUOROMETHYLPHENYL)PIPERAZINE (TFMPP)	231.278	188; 118.0	141	10	31/51	22/16	BMPEA	136.133	91.0; 119.1	46	10	25/11	10/16
1-(4-CHLOROPHENYL)PIPERAZINE (pCPP)	197.469	119.1; 118.1	121	10	33/45	14/16	BROMO-DRAGON-FLY	293.977	276.9	71	10	15	42
1,4-DIBENZYLPIPERAZINE (DBZP)	267.107	91.0; 65.1	111	10	47/91	12/10		296.128	278.9	81	10	17	12
1-AMINOINDAN	134.019	117.1; 115.1	56	10	15/33	14/14	BUPRENORPHINE	468.189	55.0; 152.0	116	10	95/117	12/10
1-METHYL-4-BENZYLPIPERAZINE (MBZP)	191.061	91.0; 65.0	86	10	31/63	12/10	BUPROPION	239.672	184.0; 131.1	66	10	17/37	24/16
1-METHYLAMINO-1-(3,4-METHYLENEDIOXYPHENYL)PROPANE	194.261	163.0; 105.1	61	10	13/33	22/16	BUTYLONE (bk-MBDB)	222.185	174.1; 204.1	66	10	25/17	20/10
2,3-DICHLOROPHENYLPIPERAZINE (DCPP)	230.937	188; 152.0	91	10	27/45	24/20	CAMFETAMINE	202.289	91.0; 67.0	76	10	43/25	14/14
2,3-DIMETHYLETHCATHINONE (2,3-DMEC)	206.062	188.1; 158.1	91	10	17/39	24/20	CANNABIDIOL	315.323	193.0; 123.0	121	10	29/43	10/16
2,3-DIMETHYLMETHCATHINONE (2,3-DMMC)	192.202	174.0; 159.1	66	10	17/27	20/20	CARBAMAZEPINE	237.209	194.1; 192.1	111	10	27/45	24/24
2,3-ETHYLONE ISOMER	222.247	174.1; 146.1	86	10	23/35	8/8	CATHINE	152.256	134.1; 117.1	51	10	13/23	22/14
2,3-MDMA	194.351	135.0; 77.0	91	10	25/53	18/12	CATHINONE	150.030	132.1; 117.1	56	10	17/31	18/14
2,3-MDPV	276.236	135.0; 126.1	91	10	31/37	16/14	CB-13	369.100	127.0; 170.7	151	10	61/39	20/24
2,4,5-TRIMETHOXYAMPHETAMINE	226.297	209.1; 179.1	76	10	15/35	10/10	CBL-018	358.214	214.1; 144.1	76	10	21/49	10/20
2,4-DIMETHYLMETHCATHINONE (2,4-DMMC)	192.190	174.1; 159.0	76	10	17/27	20/18	CI2201	394.203	188.9	151	10	37/35	24/24
2,4-DMEC	206.063	188.1; 158.1	41	10	17/47	12/20		396.214	191.0				
2,5-DMMA	210.264	151.1; 121.1	56	10	23/35	20/16	CLOBAZAM	301.995	260.0; 225.0	151	10	29/45	12/26

25B-NBF	368.124	243.0	106	10	27	12	CLOMIPRAMINE	315.043	86.1; 58.0	106	10	23/65	12/8
	370.116	245.0	131	10	27	12	CLONAZEPAM	316.097	270.1; 214.3	151	10	35/45	12/22
25C-NBF	324.164	199.0; 184.0	111	10	25/37	10/10	COCAETHYLENE	318.094	196.1; 82.0	101	10	27/39	24/12
25C-NBOH	322.138	199.0; 77.0	101	10	27/85	24/12	COCAINE	304.198	182.1; 77.1	106	10	27/79	22/12
25C-NBOMe	336.160	121.1; 91.1	96	10	25/59	14/12	CODEINE	300.058	152.0; 115.1	136	10	85/95	18/16
25D-NBOMe	316.169	91.0; 121.0	81	10	57/25	12/16	CUMYL-PICA	349.217	231.1; 91.0	86	10	21/73	12/12
25E-NBOMe	330.231	91.0; 121.1	106	10	61/27	12/16	D2PM	254.299	236.2; 130.1	81	10	19/39	12/8
25G-NBOMe	330.142	91.0; 121.1	81	10	61/27	12/14	DEMOXEPAM	286.956	179.9; 269.0	131	10	31/37	22/12
25H-NBOMe	302.346	91.0; 121.1	81	10	55/23	12/18	DESALKYLFLURAZEPAM	289.917	140.0; 141.0	116	10	39/39	18/18
25-I-NB2OMe	428.183	91.0; 121.0	121	10	75/27	12/16	DESCHLOROETIZOLAM	310.255	281.0; 356.0	151	10	33/31	12/12
25I-NB3OMe	428.176	121.1; 91.1	131	10	33/75	14/12	DESCHLORO-N-ETHYL-KETAMINE	218.287	91.0; 145.1	96	10	39/23	10/8
25I-NB4OMe	428.177	121.1; 78.0	91	10	21/113	16/10	DESIPRAMINE	267.085	72.1; 44.1	71	10	21/63	10/8
25I-NBF	416.016	290.8; 276.0	121	10	29/43	12/14	DESMETHYLDIAZEPAM (NORDIAZEPAM)	271.978	209.1; 140.0	141	10	39/39	26/18
25I-NBMD	442.154	135.1; 77.0	116	10	31/93	16/12	DESMETHYLFLUNITRAZEPAM	299.977	254.1; 198.0	116	10	35/53	12/24
25I-NBOH	414.121	291.0; 307.9	101	10	31/23	12/14	DESOMORPHINE	272.254	167.1; 152.1	126	10	49/73	20/18
25N-NBOMe	347.200	91.0; 121.1	86	10	59/23	12/16	DESOXY-D2PM	238.301	91.0; 117.1	101	10	33/23	12/8
25T2-NBOMe	362.264	91.0; 121.1	121	10	59/27	10/14	DESOXYPIPRADROL (2-DPMP)	252.331	91.1; 65.0	91	10	49/85	12/10
25T-NBOMe	348.035	91.1; 121.1	96	10	63/27	14/16	DEXTROMETHORPHAN	272.289	128.1; 171.0	126	10	81/51	16/20
2-AMINO-1-PHENYLBUTANE	150.209	91.0; 65.0	61	10	23/49	12/10	DIAZEPAM	285.397	154.0; 193.0	166	10	37/43	20/24
2-AMINOINDANE	134.257	117.1; 115.1	51	10	19/33	14/14	DICLAZEPAM	320.306	228.0; 89.0	166	10	43/103	28/12
2-BROMOAMPHETAMINE	214.186	169.0	61	10	27	8	DICLOFENSINE	322.115	121.1; 279.0	151	10	33/29	16/14
	216.192	170.9	56	10	27	20	DIETHYLCATHINONE (AMFEPRAMONE)	206.061	105.1; 100.1	81	10	31/29	12/14
2-BROMOMETHAMPHETAMINE	228.188	169.0	71	10	29/27	20/10	DIHYDROCODEINE	302.062	199.0; 128.1	121	10	43/81	26/16
	230.177	171.0					DIMETHOCAINE	279.175	120.1; 65.0	106	10	31/81	14/10

2C-B	259.957	243.0; 227.9	51	10	17/29	12/10	DIMETHYLONE (bk-MDDMA)	222.209	72.2; 91.0	86	10	25/49	10/12
2C-B_FLY	283.976	267.0; 188.1	106	10	21/33	12/24	DIPHENHYDRAMINE	256.071	167.1; 165.1	56	10	17/57	22/22
2C-C	216.441	199.0; 184.0	76	10	15/27	24/22	DIPHENIDINE	266.099	181.1; 103.1	76	10	25/47	22/12
2C-D	195.583	179.0; 164.1	71	10	15/25	24/20	DiPT	244.891	114.2; 144.1	81	10	21/31	14/20
2C-G	210.052	178.0; 163.0	76	10	23/37	22/20	DL-4662	266.292	248.1; 188.0	86	10	19/35	12/22
2-CHLOROAMPHETAMINE	170.196	125.0; 89.0	61	10	25/51	16/14	DOI	322.068	304.9; 277.0	61	10	17/27	12/12
2C-I	307.947	291.0; 276.0	66	10	19/31	12/12	DOTHIEPIN	296.089	202.0; 220.9	86	10	75/61	26/28
2C-P	224.065	207.1; 192.1	66	10	15/25	10/24	DOXEPIN	279.918	107.1; 77.0	101	10	31/73	14/10
2C-T-7	256.022	239.1; 91.1	71	10	17/63	10/12	DOXYLAMINE	271.067	167.1; 182.0	61	10	49/23	22/22
2C-TFM	250.269	233.1; 218.0	91	10	17/29	10/12	EAM-2201	388.297	183.1; 153.0	81	10	35/65	10/20
2-FEC	196.255	148.1; 135.1	76	10	41/37	18/10	EDDP	278.507	234.2; 249.1	86	10	41/33	10/10
2-FIC	168.199	123.1; 103.1	61	10	21/33	14/14	EG-2201	410.225	155.0; 127.1	181	10	33/71	22/16
2-FLUOROAMPHETAMINE	154.130	109.0; 137.1	61	10	23/13	14/16	ERGOMETRINE	326.400	223.1; 208.1	116	10	31/39	10/10
2-FLUOROMETHAMPHETAMINE (2-FMA)	168.247	109.1; 83.1	61	10	25/53	12/12	ESTAZOLAM	295.921	268.0; 206.0	101	10	33/55	12/24
2-FLUOROMETHCATHINONE (2-FMC)	182.187	164.1; 149.0	81	10	19/29	22/16	ETAQUALONE	264.918	146.1; 77.0	116	10	37/89	18/12
2-IODOAMPHETAMINE	262.178	216.9; 90.0	81	10	27/47	12/12	ETHCATHINONE METABOLITE	180.064	162.1; 115.1	76	10	17/39	20/14
2-MAPB	190.239	58.0; 91.1	51	10	19/47	8/14	ETHYLONE (bk-MDEA)	222.228	174.1; 204.1	71	10	25/19	20/10
2-MeOMC	194.219	176.1; 161.1	61	10	17/27	10/16	ETHYLPHENIDATE	248.328	84.1; 56.0	111	10	25/69	12/8
2-METHOXY-2-PHENYLETHYLAMINE	152.214	120.1; 77.0	61	10	15/45	14/12	ETIZOLAM	343.910	315.0; 224.1	121	10	35/65	14/10
2-METHOXYAMPHETAMINE (2-MA)	166.068	121.1; 149.0	56	10	21/13	16/18	EUTYLONE (bk-EBDB)	236.294	188.1; 189.1	96	10	25/29	24/22
2-METHOXYMETHAMPHETAMINE (2-MeOMA)	180.322	120.9; 91.1	66	10	23/39	14/8	FENFLURAMINE	232.018	159.0; 109.0	86	10	31/57	20/14
2-METHYLAMINO-1-PHENYLBUTANE	164.237	91.0; 65.0	71	10	25/55	14/8	FENTANYL	337.171	188.0; 105.0	131	10	29/57	10/12
2-METHYLMETHCATHINONE (2-MMC)	178.060	160.1; 145.1	76	10	17/27	22/18	FLUBROMAZEPAM	334.716	226.1; 186.0	161	10	39/41	10/22

2-METHYL-PBP	232.265	105.1; 91.0	116	10	33/53	12/12	FLUDIAZEPAM	303.922	212.0; 89.0	141	10	43/93	26/12
2-METHYL-PPP	218.291	98.1; 119.1	116	10	31/31	16/8	FLUMAZENIL	303.986	258.1; 217.0	81	10	23/35	12/26
3,4-DICHLOROMETHYLPHENIDATE (3,4-CTMP)	303.454	84.1; 56.0	121	10	27/77	12/8	FLUNITRAZEPAM	313.814	268.0; 239.0	136	10	35/47	12/12
3,4-DIMETHOXY-ALPHA-PVP	292.246	151.0; 126.1	116	10	35/33	22/12	FLUOXETINE	310.021	44.1; 148.1	51	10	43/11	8/18
3,4-DIMETHYLMETHCATHINONE (3,4-DMMC)	192.031	174.1; 159.2	81	10	17/27	20/18	FLURAZEPAM	388.023	315.0; 107.0	91	10	31/111	14/14
3,4-DMEC	206.146	158.1; 115.1	86	10	43/67	14/6	FUB-144	350.227	109.1; 125.1	111	10	61/29	14/14
3,4-DMMA	210.063	179.1; 151.1	61	10	17/29	22/20	FUB-JWH-018	380.203	155.1; 109.0	176	10	33/63	8/18
3,4-EDMA	208.248	177.1; 149.1	61	10	19/29	10/20	FUB-NPB-22	398.186	253.0; 109.1	86	10	23/47	12/8
3,4-EDMC	222.191	204.0; 189.1	61	10	19/29	10/10	FURANYLFENTANYL (Fu-F)	375.290	105.1; 188.1	136	10	55/29	14/20
3,4-MDMA (ECSTAZY)	194.025	163.1; 105.1	76	10	17/33	20/14	GHB	102.935	85.0; 57.0	-75	-10	-10/-10	-12/-18
3,4-MDPA	222.051	163.0; 105.1	81	10	19/35	20/14	HARMALINE	215.051	174.0; 171.9	61	10	29/37	10/18
3,4-MDPHP	290.285	135.1; 140.2	131	10	35/35	16/18	HARMINE	212.795	170.1; 198.0	121	10	41/31	20/26
3,4-METHYLENDIOXYPYROVALERONE	276.144	126.1;135.1	76	10	31/41	12/8	HYDROCODONE	300.050	199.0; 128.1	131	10	39/77	24/16
3,4-METHYLENEDIOXY_PV9	318.230	135.1; 168.2	166	10	35/39	8/20	IBOGAINE	312.288	122.1; 77.0	281	10	43/119	14/12
30C-NBOMe	396.257	181.1; 148.1	61	10	23/59	10/18	IMIPRAMINE	281.078	86.1; 58.1	66	10	21/59	12/8
3-BROMOAMPHETAMINE	214.192	168.9	46	10	25/25	20/14	ISOPENTEDRONE	192.055	91.0; 161.0	71	10	33/17	12/22
	216.189	171.1					JWH 018 BENZIMIDAZOLE ANALOG	343.221	126.6; 155.1	121	10	109/41	16/20
3-BROMOMETHAMPHETAMINE	228.180	169.0	86	10	27/27	22/20	JWH-011	384.202	155.1; 127.1	151	10	37/71	16/14
	230.202	170.9					JWH-018 ADAMANTYL CARBOXAMIDE	365.291	135.1; 77.0	156	10	37/109	20/12
3-BROMOMETHCATHINONE (3-BMC)	244.143	145.0	86	10	23/25	20/22	JWH-022	340.223	155.1; 127.1	136	10	31/61	8/16
	242.128	145.1					JWH-031	306.155	127.1; 76.9	131	10	51/95	8/6
3-CAF	383.161	239.0; 210.0	101	10	19/65	12/24	JWH-071	300.220	127.1; 155.1	111	10	57/29	16/8
3C-B-FLY	298.069	280.9	66	10	21	12	JWH-080	358.107	185.0; 127.1	61	10	33/69	24/16

	300.079	283.0	46	10	17	16	JWH-116	370.219	155.2; 127.1	121	10	33/69	16/6
3-CHLOROAMPHETAMINE	170.206	125.1; 89.0	66	10	25/53	14/12	JWH-145	367.929	154.8; 127.1	91	10	35/69	22/18
3-CHLOROMETHCATHINONE (3-CMC)	198.231	145.1; 144.1	76	10	25/41	18/18	JWH-146	396.312	155.1; 127.0	141	10	27/71	18/22
3-CHLOROPHENYLPIPERAZINE (mCPP)	197.249	154.1; 118.1	101	10	27/47	18/14	JWH-149	370.172	169.1; 115.2	156	10	35/95	26/14
3C-P	254.286	195.1; 107.1	56	10	19/35	10/14	JWH-167	306.156	91.1; 214.2	86	10	31/35	12/30
3-DESOXY-3,4-MDPV	274.249	126.1; 133.1	126	10	31/37	18/16	JWH-175	328.281	141.1; 115.1	106	10	29/83	18/14
3-ETHYLMETHCATHINONE (3-EMC)	192.220	174.1; 144.1	66	10	17/43	22/18	JWH-182	384.268	197.0; 141.0	196	10	33/61	10/14
3-FEC	196.262	135.1; 148.1	81	10	39/41	18/18	JWH-193	399.123	169.1; 115.0	116	10	31/97	10/6
3-FLUORO-ALFA-PPP	222.280	123.1; 98.1	86	10	31/33	12/14	JWH-198	415.117	185.1; 114.2	181	10	33/35	22/10
3-FLUOROAMPHETAMINE	154.134	109.0; 137.1	76	10	25/13	14/16	JWH-201	336.263	121.1; 77.0	151	10	35/77	16/10
3-FLUOROMETHAMPHETAMINE (3-FMA)	168.223	109.1; 83.1	76	10	27/53	18/10	JWH-213	384.326	183.1; 153.1	181	10	35/61	22/18
3-FLUOROMETHCATHINONE (3-FMC)	182.014	164.1; 149.1	81	10	19/27	20/18	JWH-307	386.153	155.0; 127.1	66	10	27/81	24/16
3-HYDROXYBROMAZEPAM	331.895	286.9; 314.9	106	10	27/21	12/14	JWH-309	418.325	155.0; 127.1	141	10	29/77	20/16
3-HYDROXYFLUNITRAZEPAM	330.031	238.0; 284.0	96	10	43/27	12/12	JWH-368	386.132	155.1; 127.0	106	10	29/69	20/16
3-IODOAMPHETAMINE	262.179	217.0;117.1	66	10	25/43	10/14	JWH-369	402.279	155.1; 127.0	126	10	29/65	20/18
3-MEC	192.185	144.2; 91.1	86	10	39/47	16/14	JWH-412	360.213	173.0; 145.1	161	10	33/63	10/18
3-MeOMC	194.225	161.1; 118.1	81	10	25/47	20/12	JWH-424	422.179	235.0	131	10	37	12
3-METHOXYAMPHETAMINE (3-MA)	166.070	121.1; 91.0	41	10	21/37	16/14		420.174	233.0	111	10	37	12
3-METHOXYPHENCYCLIDINE	274.190	86.1; 121.1	46	10	17/37	10/14	KETAMINE	238.083	125.0; 89.0	61	10	37/73	16/12
3-METHYLMETHCATHINONE (3-MMC)	178.046	160.1; 145.1	86	10	17/27	20/18	LAMPA	324.164	223.0; 208.0	116	10	33/41	28/26
3-METHYL-PBP	232.266	105.1; 91.0	106	10	31/55	14/12	LIDOCAINE	235.081	86.1; 58.1	126	10	23/51	10/10
3-METHYL-PPP	218.209	119.3; 91.0	116	10	31/49	6/8	LOPRAZOLAM	464.983	252.0; 111.1	126	10	57/35	12/14
4,4'-DMAR	191.255	148.1; 91.0	61	10	17/39	18/12	LORAZEPAM	321.924	275.9; 303.9	111	10	29/21	12/14

4-AcO-DET	275.216	86.0; 160.0	81	10	23/35	12/20	LORMETAZEPAM	335.939	289.9; 177.9	86	10	29/45	14/12
4-AcO-DMT	247.314	58.1; 160.1	81	10	21/33	6/16	LSD	324.277	223.0; 207.0	101	10	33/57	28/26
4-AcO-MET	261.300	72.0; 160.0	76	10	21/35	10/22	MAPROTILINE	278.114	191.0; 189.0	116	10	47/83	24/22
4-APB	176.148	131.1; 91.0	66	10	25/39	16/12	MBDB	208.040	135.0; 77.0	51	10	27/55	18/10
4-APDB	178.238	161.1; 133.1	71	10	13/25	22/16	MDAT	192.204	175.1; 117.1	66	10	15/35	10/8
4-BROMO-2,5-DMMA	288.233	257.0	61	10	19	12	MDBP	221.272	135.0; 77.0	61	10	23/53	10/12
	290.240	259.0	56	10	19	12	MDEA	208.054	163.0; 105.0	66	10	19/35	20/14
4-BROMOAMPHETAMINE	214.182	169.0	76	10	25	20	MDMB-CHMINACA	386.303	241.1; 145.0	156	10	33/57	12/18
	216.181	170.9	56	10	25	22	MDPBP	262.024	161.0; 112.1	86	10	31/35	20/14
4-BROMOMETHAMPHETAMINE	228.205	168.9	91	10	29/27	20/20	MECLONAZEPAM	329.969	284.0; 238.0	91	10	37/57	14/12
	230.200	170.9					MEDAZEPAM	271.019	206.9; 165.1	126	10	37/61	26/20
4-BROMOMETHCATHINONE (BREFEDRONE)	243.495	145.1; 144.1	101	10	23/45	18/18	MEMANITINE	180.261	163.2; 107.2	56	10	19/33	8/10
4-CAB	184.174	125.1; 89.0	46	10	25/57	16/14	MEPERIDINE	248.140	220.1; 91.1	121	10	31/59	20/8
4-CEC	212.210	159.3; 144.1	66	10	25/39	8/18	MEPHTETRAMINE (MTTA)	190.139	44.0; 147.1	101	10	31/13	8/18
4-CHLORO-ALPHA-PPP	238.267	139.1; 98.1	111	10	33/33	16/12	MEPIRAPIM	314.241	214.1; 144.1	66	10	21/47	10/8
4-CHLOROAMPHETAMINE	170.197	125.0; 89.0	51	10	25/53	12/12	MEPROBAMATE	219.029	158.1; 55.1	66	10	11/31	20/8
4-CHLOROMETHCATHINONE (4-CMC)	198.000	145.1; 144.1	76	10	25/41	18/18	MESCALINE	212.183	195.1; 77.0	76	10	13/63	24/12
4-CMA	184.235	125.1; 89.0	81	10	29/57	14/12	METHADONE	310.094	265.1; 105.0	66	10	21/35	12/14
4-EAPB	204.264	131.1; 91.0	76	10	29/45	10/12	METHAMPHETAMINE	150.063	91.0; 119.1	51	10	25/15	12/16
4-ETHYL-N,N-DMC	206.207	133.2; 105.2	61	10	27/35	14/18	METHANDIENONE	301.060	121.2; 149.1	131	10	35/21	14/18
4-FEC	196.260	148.1; 135.1	71	10	41/37	18/16	METHAQUALONE	251.007	132.1; 91.0	131	10	37/57	18/12
4-FLUORO BUPHEDRONE	196.234	149.1; 148.1	76	10	31/47	18/18	METHCATHINONE	164.056	131.1; 130.1	61	10	27/41	18/16
4-FLUORO PENTEDRONE	210.264	109.0; 74.0	86	10	33/111	14/10	METHEDRONE (bk-PMMA)	193.998	176.0; 161.0	56	10	15/31	10/6

4-FLUORO PV8	278.165	109.0; 95.1	126	10	33/71	16/12	METHOHEXITAL	263.072	221.0; 77.1	116	10	19/67	10/10
4-FLUORO PV9	292.257	109.1. 95.0	116	10	35/71	14/14	METHOXETAMINE	248.059	121.1. 203.0	76	10	37/19	16/26
4-FLUORO-ALFA-PPP	222.267	123.1; 98.1	86	10	31/33	8/14	METHOXPHENIDINE	297.324	129.1; 117.1	101	10	27/31	16/14
4-FLUOROMETHAMPHETAMINE (4-FMA)	168.214	109.1; 137.0	81	10	27/15	12/18	METHYLHEXANAMINE	116.066	57.0; 41.1	71	10	17/31	8/6
4-FLUOROMETHCATHINONE (4-FMC)	182.011	164.1; 149.0	71	10	19/29	22/20	METHYLONE (bk-MDMA)	208.272	160.0; 132.1	86	10	25/37	20/14
4F-PVP	250.250	109.0; 126.1	91	10	31/35	12/16	METHYLPHENIDATE	234.300	84.1; 56.0	71	10	23/65	10/8
4-HYDROXY DiPT	262.005	161.1; 114.1	171	10	31/21	20/14	MEXEDRONE	208.300	91.0; 119.0	76	10	47/29	16/6
4-HYDROXYMIDAZOLAM	341.932	325.0; 297.0	121	10	31/41	14/14	MIANSERIN	265.493	208.1; 58.1	146	10	29/45	24/10
4-IODOAMPHETAMINE	262.177	245.0; 216.9	56	10	15/27	12/12	MIDAZOLAM	326.065	291.1; 248.9	136	10	37/51	12/30
4-MAPB	190.254	131.1; 91.0	76	10	27/41	18/10	MITRAGYNINE	399.094	174.0; 159.1	136	10	41/63	22/20
4-MEAP	220.297	144.1; 105.1	66	10	43/29	18/12	MMAI	178.131	161.0; 103.0	61	10	15/53	22/14
4-MEO-ALPHA-PVP	262.212	121.1; 191.2	91	10	33/25	12/18	MMB018	345.251	214.1; 144.0	66	10	19/51	10/20
4-MeOPBP	248.282	112.1; 121.1	101	10	31/37	14/16	MMB2201	363.251	232.1; 144.1	81	10	21/53	10/16
4-METHOXY PHENCYCLIDINE	274.176	121.1; 189.1	61	10	39/17	14/10	MN-25	440.336	114.1;261. 1	141	10	41/33	12/12
4-METHOXY PV8	290.295	121.1; 154.2	126	10	35/33	16/8	MN-25-2-METHYL DERIVATIVE	454.347	114.1; 275.1	151	10	41/31	18/14
4-METHOXY PV9	304.286	121.1; 168.2	101	10	35/35	14/8	MO-CHMINACA	387.261	241.1; 145.1	121	10	27/47	22/8
4-METHOXYMETHAMPHETAMINE (PMMA)	180.289	149.0; 121.1	66	10	15/27	20/14	MORPHINE	286.043	152.1; 128.1	176	10	79/77	20/16
4-METHYL PENTEDRONE	206.274	144.1; 105.1	86	10	47/29	18/14	MPBP	232.059	105.1; 91.1	116	10	33/57	14/12
4-METHYL-ALPHA-ETHYLAMINOBUTIOPHENONE	206.110	188.3; 144.2	56	10	19/43	22/10	MT-45	349.380	181.0; 77.0	176	10	37/93	24/12
4-METHYLAMPHETAMINE	150.227	105.1; 133.1	56	10	23/11	16/8	N-(3-METHYLBENZYL)PIPERAZINE	191.273	105.1; 77.0	81	10	27/55	14/10
4-METHYLCATHINONE	164.232	146.1; 131.0	71	10	15/27	18/16	N,N-DIETHYLPHENETHYLAMINE	178.273	105.1; 77.0	101	10	25/55	10/12
4-METHYLMETHAMPHETAMINE (4-MMA)	164.250	105.1; 133.1	66	10	25/15	14/16	N,N-DIMETHYLPENTYLONE (bk-DMBDP)	250.302	100.1; 135.0	101	10	27/31	12/14
4-METHYLMETHCATHINONE (4-MMC)	178.066	160.1; 145.1	71	10	17/27	20/18	N,N-DMT	189.572	58.0; 144.1	116	10	19/23	8/18

4-METHYL-N,N-DMC	192.249	119.1; 72.1	101	10	27/33	16/12	N-ACETYL-3,4-MDMC	250.245	208.1; 160.1	76	10	19/35	22/18
4-METHYL-N-METHYLBUPHEDRONE	206.209	105.0; 90.9	51	10	29/47	16/12	NAPHYRONE	282.065	140.9; 17.0	51	10	37/59	10/24
4-METHYL-N-METHYLHEXANOPHENONE	220.287	144.1; 105.1	86	10	47/29	16/14	NAPHYRONE-1-NAPHTYL ISOMER	282.125	127.0; 141.0	51	10	57/37	22/10
4-METHYL-PBP	232.310	105.1; 91.0	81	10	33/55	14/12	N-BENZYLNORBUTYLONE	298.241	91.1; 65.0	96	10	41/91	14/16
4-METHYL-PHP	260.347	105.1; 91.1	131	10	33/63	14/10	N-ETHYL-4-METHOXYAMPHETAMNE	194.253	121.0; 91.0	66	10	29/45	16/14
4-METHYL-α-ETHYLTRYPTAMINE	203.040	144.1; 186.0	56	10	29/13	20/24	N-ETHYLBUPHEDRONE	192.296	130.1; 91.0	66	10	39/35	10/14
5-APB	176.082	44.0; 91.0	46	10	23/47	8/10	N-ETHYL-N-METHYLCATHINONE	192.099	105.0; 77.2	76	10	29/57	6/14
5-APDB	178.290	161.0; 133.1	56	10	13/27	22/18	N-ETHYLNORDAZEPAM	299.364	165.1; 77.0	216	10	59/89	20/10
5-APDI	176.173	159.2; 131.2	71	10	13/27	22/10	N-ETHYLNORKETAMINE	252.180	125.0;89.1	71	10	41/75	16/14
5-CHLORO AB-PINACA	365.216	320.1	91	10	21	14	N-ETHYLOXAZEPAM	315.994	270.0; 242.0	116	10	29/47	12/12
	367.248	322.2	86	10	21	14	N-ETHYLPENTYLONE	250.269	232.2; 202.0	71	10	21/27	22/12
5-CHLORO-NNEI	391.226	247.9; 144.1	86	10	31/55	12/8	NIMETAZEPAM	296.187	250.1; 221.0	171	10	35/45	12/26
5-EAPB	204.961	132.1; 131.6	86	10	29/29	16/16	NITRACAINE	309.822	92.0; 76.0	216	10	57/91	12/12
5F-ABICA	348.070	232.1; 144.1	71	10	29/53	12/18	NITRAZEPAM	281.974	236.0; 180.1	141	10	33/51	30/24
5-F-JWH-018 ADAMANTYL ANALOG	368.294	135.1; 77.0	171	10	39/113	10/12	NM2201	376.276	232.0; 144.1	131	10	21/51	12/18
5-FLUORO THJ	377.255	233.1; 145.1	91	10	29/53	12/14	N-METHYL-2AI	148.043	117.1; 115.1	81	10	23/37	14/14
5-FLUORO-2-ADB-PINACA_ISOMER_2	363.254	145.1; 318.1	116	10	47/29	10/14	N-METHYL-PEA	136.182	105.1; 77.0	51	10	19/43	18/12
5-FLUORO-CUMYL-PICA	367.233	249.1; 91.0	96	10	21/77	12/14	N-METHYLTRYPTAMINE	175.508	144.1; 117.1	66	10	17/37	18/14
5-FLUORO-SDB-006	339.222	91.0; 232.0	141	10	63/31	14/10	NN-DMC	178.233	105.0; 72.1	91	10	29/29	14/10
5-F-PENTYL-3-PYRIDINOYLINDOLE	311.223	144.1. 89.0	136	10	51/99	18/12	NORCLOBAZAM	286.954	245.1; 210.0	141	10	27/43	12/26
5F-SDB-005	377.212	233.1; 145.1	121	10	15/51	10/10	NORCLOMIPRAMINE	301.026	72.1; 44.1	101	10	21/65	10/8
5-HYDROXY DMT	205.058	58.1; 160.1	81	10	17/25	8/20	NORKETAMINE	224.176	125.1; 207.2	51	10	13/21	12/12
5-IT	175.275	158.1; 130.1	61	10	13/31	18/18	NORTRIPTYLINE	264.066	91.1; 105.1	81	10	29/27	12/14

5-MAPB	190.252	159.1; 131.1	56	10	15/29	16/20	N-PROPYLAMPHETAMINE	178.103	119.1; 65.0	86	10	17/61	16/10
5-MAPDB	192.202	161.1; 133.1	56	10	17/31	18/14	NRG-3	242.250	181.1; 180.1	81	10	35/53	8/16
5-MeO-ALPHA-ET	219.295	160.1; 117.1	71	10	27/55	18/14	o-CPP	197.229	154.1; 118.1	121	10	27/45	20/8
5-MeO-DALT	271.063	110.1; 174.1	86	10	21/27	14/22	OCTACAINE	235.279	100.1; 72.1	81	10	23/51	14/10
5-METHOXY AMT	205.050	188.0; 147.1	56	10	15/27	24/20	ORG-28611	384.309	270.2; 174.0	71	10	25/47	12/22
5-METHOXY DiPT	275.078	114.2; 174.1	91	10	21/29	14/22	OXAZEPAM	288.031	242.1; 269.9	91	10	31/21	12/12
5-METHOXY DMT	219.968	58.1; 175.0	146	10	21/21	8/22	OXYMORPHONE	302.251	284.0; 227.1	151	10	25/37	14/12
5-METHOXY METHYLONE	238.277	190.1; 147.1	96	10	21/37	24/16	PARACETAMOL	152.016	110.0; 65.0	81	10	21/39	14/10
5-METHOXY MiPT	247.988	86.1; 87.1	156	10	19/19	10/10	PAROXETINE	330.014	70.0; 44.1	111	10	49/71	10/8
6-APB	176.049	159.1; 131.1	66	10	13/25	20/18	PCEEA	248.346	91.0; 90.1	56	10	45/13	12/12
6-APDB	178.157	161.0; 132.9	36	10	15/29	22/8	PCMPA	248.342	91.0; 90.1	66	10	43/15	14/12
6-BROMO-MDMA	272.170	240.9	86	10	19	12	PCPr	218.345	91.0; 159.1	46	10	39/15	6/22
	274.156	242.8	76	10	19	12	PENTEDRONE	192.062	91.0; 132.1	81	10	31/25	12/16
6-CHLORO-MDMA	228.238	169.0; 77.0	61	10	29/53	12/12	PENTEDRONE METABOLITE	194.308	176.1; 91.0	81	10	17/43	22/12
6-EAPB	204.150	131.1; 159.1	56	10	29/17	16/8	PENTYLONE (bk-MBDP)	235.658	188.1; 218.1	136	10	25/19	24/10
6-IT	175.258	158.1; 130.1	51	10	15/31	8/18	PHENAZEPAM	350.845	206.0; 179.0	131	10	49/63	26/22
6-MAM	328.010	165.0;43.0	141	10	51/95	20/8	PHENCYCLIDINE (PCP)	244.103	86.1; 91.0	56	10	17/43	12/12
6-MAPB	190.239	131.1; 91.0	71	10	27/43	10/10	PHENOBARBITAL	231.014	42.0; 188.0	-100	-10	-10/-10	-44/-14
7-AMINOCLONAZEPAM	286.241	121.1; 222.1	111	10	39/33	14/26	PHENTERMINE	150.067	91.0; 133.1	41	10	27/13	12/16
7-AMINODESMETHYLFLUNITRAZEPAM	270.396	121.1; 77.0	146	10	37/75	14/10	PHENYTOIN	253.004	182.1; 104.1	116	10	25/45	24/12
7-AMINOFLUNITRAZEPAM	283.767	135.1; 77.1	121	10	37/87	18/12	PRAVADOLINE	379.060	135.1; 77.1	76	10	23/89	14/12
7-AMINONITRAZEPAM	252.005	121.1; 77.1	111	10	35/73	16/10	PRAZEPAM	325.365	271.0; 140.0	126	10	31/49	12/18
7-APB	176.239	131.1; 77.0	46	10	25/53	14/10	PREGABALIN	160.078	142.1; 55.0	116	10	15/29	18/8

7-APDB	178.233	161.1; 133.1	61	10	15/25	10/18	PROCAINE	237.063	100.1; 120.1	81	10	21/37	12/14
A-834735	340.308	125.1; 55.0	156	10	29/61	16/10	PROLINTANE	218.162	91.1; 72.1	86	10	33/23	12/10
A-836339	311.150	187.1; 125.2	101	10	23/33	12/10	PROMETHAZINE	285.029	86.1; 71.1	76	10	21/63	12/10
AB-FUBINACA	369.130	352.0; 109.1	81	10	13/47	14/14	PROPAFENONE	342.045	116.1; 72.1	86	10	29/47	14/10
AB-FUBINACA 2-FLUOROBENZYL ISOMER	369.269	253.0; 324.2	86	10	33/19	12/14	PROPRANOLOL	260.069	56.0; 58.1	86	10	45/45	8/10
AB-FUBINACA 3-FLUOROBENZYL ISOMER	369.241	253.0; 324.1	66	10	35/21	12/14	PROPYLHEXEDRINE	155.882	69.1; 55.0	81	10	23/37	10/8
ADB-PINACA ISOMER_1	345.335	215.1; 300.2	86	10	33/21	10/14	PSB-SB-1202	367.248	259.1; 121.1	121	10	23/23	12/8
ADB-PINACA ISOMER_2	345.304	215.1; 300.1	71	10	35/19	10/14	PTI-1	356.299	283.0; 213.1	106	10	29/47	14/10
ADB-PINACA ISOMER_3	345.292	215.1; 300.2	71	10	33/19	10/14	PTI-2	400.341	283.0; 213.1	116	10	31/51	14/10
ADB-PINACA ISOMER_4	345.305	215.1; 300.1	81	10	33/19	10/14	PV-8	260.116	91.1; 77.1	96	10	33/73	12/10
AH-7921	329.174	284.0; 173.0	91	10	23/35	12/18	PV9	274.307	91.0; 77.0	126	10	33/73	12/12
AKB48_N-(4-FLUOROBENZYL)_ANALOG	404.265	135.1; 77.0	136	10	29/121	16/14	PX-2	397.253	233.0; 352.2	86	10	33/21	12/14
ALFA-ETHYLAMINOPENTIOPHENONE	206.323	188.1; 91.0	86	10	17/39	22/12	PYRAZOLAM	353.943	167.1; 206.0	151	10	47/41	20/26
ALFA-PROPYLAMINOPENTIOPHENONE	220.315	202.1; 91.1	91	10	19/33	10/10	QUETIAPINE	384.090	253.1; 221.0	116	10	31/51	12/28
ALLYLESCALINE	238.321	221.1; 77.0	51	10	13/67	10/12	RH-34	326.300	121.1; 91.1	91	10	25/57	14/10
ALPHA-DIMETHYLAMINOPENTIOPHENONE	206.291	91.1; 77.1	101	10	27/57	14/12	R-MMC	236.144	188.2;218.1	61	10	25/17	10/18
ALPHA-ETHYLAMINOHEXANOPHENONE	220.312	91.0; 130.1	106	10	33/47	12/14	SCOPOLAMINE	303.805	138.1; 156.1	96	10	29/23	18/20
ALPHA-ETHYLTRYPTAMINE	188.767	130.1; 172.1	76	10	27.lis	16/20	SDB-005	359.177	215.2; 145.0	51	10	21/45	10/20
ALPHA-HYDROXYMIDAZOLAM	341.989	324.0; 203.0	121	10	29/37	14/26	SDB-006	321.153	91.0; 214.1	171	10	61/39	12/10
ALPHA-METHYLTRYPTAMINE	175.029	158.1; 143.1	56	10	15/35	20/16	SERTRALINE	306.988	276.0; 159.0	66	10	17/37	12/20
ALPHA-PHP	246.318	91.0; 77.0	76	10	33/65	10/10	SILDENAFIL	475.047	58.1;100.1	91	10	103/35	10/12
ALPHA-PHTALIMIDOPROPIOPHENONE	280.193	105.1; 77.0	116	10	31/79	14/12	STANOZOLOL	329.138	81.1; 95.1	241	10	79/51	12/12
ALPHA-PIPBP	232.294	91.1; 77.0	106	10	33/61	8/10	TAPENTADOL	222.343	107.1; 77.0	86	10	35/63	14/12
ALPHA-PPP	204.261	105.1; 98.1	71	10	31/33	14/8	TEMAZEPAM	301.993	256.0; 284.1	116	10	31/19	12/12

ALPHA-PVP	232.243	91.1; 126.1	71	10	39/57	8/6	TETRACAINE	265.226	176.1; 72.0	96	10	21/37	18/10
ALPHA-PVT	238.017	126.2; 97.0	91	10	29/31	16/12	THIOPROPAMINE	142.098	125.0; 97.0	51	10	13/25	8/12
ALPHA-PYRROLIDINOBUTHIOPHENONE	224.190	112.2; 97.0	81	10	29/39	12/12	THJ	359.247	215.2;145.0	121	10	29/49	10/16
ALPRAZOLAM	309.934	282.0; 206.0	171	10	37/57	12/26	TILETAMINE	224.246	179.0; 151.1	51	10	13/23	10/18
AM1220	383.315	98.0; 112.1	101	10	49/27	14/12	TRAMADOL	264.304	58.1; 42.1	96	10	47/113	8/8
AM2201 8-QUINOLINYL CARBOXAMIDE	376.237	232.1; 144.1	86	10	23/55	12/16	TRAZODONE	372.082	176.0; 148.0	126	10	33/45	24/20
AM2201 BENZIMIDAZOLE ANALOG	361.184	127.1; 155.1	131	10	73/41	16/20	TRIAZOLAM	343.990	309.1; 239.9	106	10	37/57	14/30
AM2232	353.245	155.1; 127.0	131	10	31/63	18/14	TRIMIPRAMINE	294.788	100.2; 58.1	81	10	23/61	12/8
AMITRIPTYLINE	278.073	91.0; 105.1	101	10	33/31	12/14	U-47700	329.037	284.0	56	10	25	14
AMPHETAMINE	136.030	91.0; 119.1	51	10	23/11	12/16		331.017	286.0	96	10	25	14
ATENOLOL	267.122	145.1; 56.1	101	10	35/43	20/8	W-15	377.154	105.1	141	10	33	16
ATRAZYNA	216.245	174.0; 104.0	126	10	23/39	24/14		379.165	105.2	166	10	33	12
AZACYCLONOL	268.279	250.1; 91.0	81	10	17/51	20/14	WIN 54,461	457.176	135.1; 77.0	126	10	29/95	12/12
BB-22	385.123	240.1; 144.0	101	10	19/51	16/18	WIN 55,212-2	427.117	155.1;27.2	161	10	33/75	18/12
BDB	194.030	135.0; 177.0	56	10	25/11	18/24	XLR12	352.216	125.1; 254.0	141	10	31/35	8/12
BENOCYCLIDINE	300.293	215.1; 147.0	66	10	17/39	10/18	YANGONIN	259.148	161.0; 89.0	121	10	29/93	22/10
BENZEDRONE	254.273	91.1; 65.1	111	10	31/77	12/10	ZALEPLON	305.911	264.0; 236.1	141	10	31/37	12/10
BENZOCAINE	166.030	120.0; 94.0	71	10	25/23	16/12	ZOLPIDEM	308.323	235.1; 236.0	111	10	47/37	10/30
BENZOYLECGONINE	290.034	168.1; 77.0	91	10	27/77	20/10	ZOPICLONE	389.014	244.9;112.0	81	10	23/79	12/16
BENZYDAMINE	310.213	86.1; 58.1	106	10	23/71	10/10	ZUCLOPENTHIXOL	401.024	221.0; 231.0	101	10	73/49	26/28

Table 2. The results of concentration, precision, BIAS, and limit of detection (LOD) and quantification (LOQ) for validated compounds.

Analyte	Concentration (ng/mL)	t_R (min)	Average recovery (%)	CV (%)	BIAS (%)	Range analysis (ng/mL)	LOD (ng/mL)	LOQ (ng/mL)
1-(2-METHOXYPHENYL)PIPERAZINE	10	5.34	119.94	4.39	19.94	10-100	0.5	10
	100		102.03	14.06	2.03			
	1000		52.73	6.37	-47.27			
	2000		48.49	6.68	-51.51			
	5000		60.06	5.68	-39.94			
1-(3-TRIFLUOROMETHYLPHENYL)PIPERAZINE (TFMPP)	100	7.99	108.80	11.58	8.80	100-5000	0.5	100
	1000		107.61	3.39	7.61			
	5000		105.00	8.67	5.00			
1-(4-CHLOROPHENYL)PIPERAZINE (pCPP)	100	6.79	96.84	14.76	-3.16	100-5000	0.5	100
	1000		92.65	7.70	-7.35			
	5000		108.74	8.18	8.74			
1-(4-FLUOROPHENYL)PIPERAZINE (FPP)	100	4.74	93.23	2.42	-6.77	100-5000	0.5	100
	1000		97.85	7.74	-2.15			
	5000		103.74	2.87	3.74			
1,4-DIBENZYLPIPERAZINE (DBZP)	100	7.83	106.18	7.31	6.18	100-5000	0.5	100
	1000		107.41	6.49	7.41			
	5000		110.88	3.75	10.88			
1-AMINOINDAN	100	4.12	112.00	5.24	12.00	100-5000	0.5	100
	1000		107.31	1.98	7.31			
	5000		97.14	10.45	-2.86			
1-METHYL-4-BENZYLPIPERAZINE (MBZP)	100	3.30	91.13	6.37	-8.87	100-5000	0.5	100
	1000		82.95	3.70	-17.05			
	5000		80.51	3.92	-19.49			
1-METHYLAMINO-1-(3,4-METHYLENEDIOXYPHENYL)PROPANE	10	6.07	93.73	13.11	-6.27	10-5000	0.5	10
	100		92.45	10.45	-7.55			
	1000		116.68	6.57	16.68			
AMITRIPTYLINE	100	10.93	98.64	4.23	-1.36	100-5000	0.5	100
	1000		108.51	5.53	8.51			
	5000		106.03	3.28	6.03			
AMPHETAMINE	100	4.76	98.95	15.13	-1.05	100-5000	0.5	100
	1000		83.17	11.70	-16.83			
	5000		90.43	10.86	-9.57			
ATENOLOL	100	4.00	106.15	6.69	6.15	100-5000	0.5	100
	1000		104.15	5.83	4.15			
	5000		92.26	6.26	-7.74			
AZACYCLONOL	10	8.70	100.37	13.34	0.37	10-5000	0.5	10
	100		115.13	7.26	15.13			
	1000		114.96	1.54	14.96			
	2000		108.17	6.59	8.17			
	5000		99.82	2.60	-0.18			
BB-22	10	15.12	86.48	15.38	-13.52	10-1000	0.5	10
	100		110.55	10.43	10.55			
	1000		119.04	8.52	19.04			
BDB	100	6.43	110.57	12.26	10.57	100-5000	0.5	100
	1000		111.41	6.19	11.41			
	5000		99.73	4.21	-0.27			
BENOCYCLIDINE	10	10.63	98.09	7.77	-1.92	10-5000	0.5	10
	100		101.48	8.04	1.48			
	1000		107.95	4.80	7.95			
	2000		97.98	6.24	-2.02			
	5000		97.75	6.30	-2.25			
BENZEDRONE	10	9.15	83.91	16.22	-16.10	10-5000	0.5	10

	2000		106.05	3.11	6.05					100		113.81	2.83	13.81			
	5000		116.87	4.03	16.87					1000		114.51	2.89	14.51			
	100		114.79	18.67	14.79					2000		115.88	2.18	15.88			
2,3-DICHLOROPHENYLPIPERAZINE (DCPP)	1000	8.58	115.14	6.67	15.14	100-5000	0.5	100		5000		102.15	4.50	2.15			
	5000		85.69	6.80	-14.31				BENZOCAINE	100	8.95	101.05	3.38	1.05	100-5000	0.5	100
	100		105.95	5.28	5.95					1000		114.84	6.60	14.84			
2,3-DIMETHYLETHCATHINONE (2,3-DMEC)	1000	7.52	117.22	6.21	17.22	100-5000	0.5	100		5000		98.12	4.28	-1.88			
	5000		105.26	2.37	5.26				BENZOYLECGONINE	100	6.71	105.46	10.38	5.46	100-5000	0.5	100
	100		103.10	5.28	3.10					1000		88.48	6.78	-11.52			
2,3-DIMETHYLMETHCATHINONE (2,3-DMMC)	1000	7.08	99.52	8.09	-0.48	100-5000	0.5	100		5000		105.89	2.82	5.89			
	5000		88.55	9.24	-11.45				BENZYDAMINE	100	10.29	108.14	6.18	8.14	100-5000	0.5	100
	10		106.83	11.29	6.83					1000		110.95	4.18	10.95			
	100		118.53	1.56	18.53					5000		102.18	2.61	2.18			
	1000		79.04	1.53	-20.96					100		113.66	14.66	13.66			
2,3-ETHYLONE ISOMER	2000	5.47	72.26	5.20	-27.74	10-5000	0.5	10	bk-2C-B	1000	7.04	103.45	14.46	3.45	100-5000	0.5	100
	5000		85.22	3.65	-14.78					5000		99.14	7.83	-0.86			
	100		112.14	11.32	12.14					10		112.70	8.59	12.70			
2,3-MDMA	1000	5.79	93.06	9.09	-6.94	100-5000	0.5	100		100		101.31	8.67	1.31			
	5000		81.07	5.19	-18.93				bk-MDA	1000	4.27	44.41	3.04	-55.59	10-100	0.5	10
	10		81.31	8.23	-18.69					2000		33.89	4.75	-66.11			
	100		98.21	4.46	-1.79					5000		37.22	6.56	-62.78			
2,3-MDPV	1000	7.59	98.53	4.65	-1.47	10-5000	0.5	10		10		100.33	11.10	0.33			
	2000		98.08	6.32	-1.92					100		113.92	6.51	13.92			
	5000		90.21	4.52	-9.79				BMPEA	1000	4.88	100.51	3.88	0.51	10-5000	0.5	10
	10		87.01	12.74	-12.99					2000		89.63	3.24	-10.37			
	100		91.64	10.37	-8.36					5000		81.84	1.96	-18.16			
	1000		112.15	2.96	12.15					10		96.19	8.22	-3.81			
2,4,5-TRIMETHOXYAMPHETAMINE	2000	5.54	88.03	5.42	-11.97	10-5000	0.5	10		100		105.29	8.65	5.29			
	5000		80.73	2.18	-19.27				BROMO-DRAGON-FLY	1000	10.05	114.47	6.09	14.47	10-5000	0.5	10
	100		112.86	3.70	12.86					2000		107.41	2.43	7.41			
2,4-DIMETHYLMETHCATHINONE (2,4-DMMC)	1000	7.53	109.74	13.01	9.74	100-5000	0.5	100		5000		100.08	4.79	0.08			
	5000		115.59	4.95	15.59				BUPRENORPHINE	10	9.64	105.66	6.31	5.66	10-5000	0.5	10

2,4-DMEC	10	8.3	83.20	18.31	-16.80	10-5000	0.5	10	BUPROPION	100	8.09	105.73	13.08	5.73	100-5000	0.5	100
	100		108.59	6.17	8.59					1000		104.70	7.01	4.70			
	1000		99.83	5.64	-0.17					2000		93.86	4.61	-6.14			
	2000		104.00	12.54	4.00					5000		88.99	4.70	-11.01			
	5000		94.67	11.52	-5.33				BUTYLONE (bk-MBDB)	100		106.54	4.96	6.54			
12,5-DMMA	10	6.73	86.04	11.61	-13.96	10-5000	0.5	10		1000		114.47	4.02	14.47			
	100		94.94	6.06	-5.06					5000		109.42	2.10	9.42			
	1000		92.75	6.45	-7.25					100		115.79	5.86	15.79	100-5000	0.5	100
	2000		87.73	4.67	-12.27					1000		105.38	11.46	5.38			
	5000		83.93	4.49	-16.07					5000		92.96	9.04	-7.04			
25B-NBF	10	10.16	95.48	7.30	-4.52	10-5000	0.5	10	CAMFETAMINE	10	8.23	104.53	19.14	4.53	10-5000	0.5	10
	100		103.74	8.19	3.74					100		104.45	11.56	4.45			
	1000		108.32	3.99	8.32					1000		111.86	9.29	11.86			
	2000		103.24	4.78	3.24					2000		105.89	4.67	5.89			
	5000		90.45	4.65	-9.55					5000		101.28	15.19	1.28			
25C-NBF	10	9.9	21.43	38.51	-78.57	100-5000	0.5	100	CANNABIDIOL	10	15.07	85.00	14.41	-15.00	10-1000	0.5	10
	100		117.58	8.08	17.58					100		100.36	14.81	0.36			
	1000		115.75	2.02	15.75					1000		113.49	2.39	13.49			
	2000		108.40	4.94	8.40				CARBAMAZEPINE	100	10.57	114.54	2.67	14.54	100-5000	0.5	100
	5000		96.07	4.18	-3.93					1000		119.47	5.29	19.47			
25C-NBOH	100	9.79	108.48	3.93	8.48	100-5000	0.5	100		5000		92.85	3.74	-7.15			
	1000		98.02	2.95	-1.98				CATHINE	100	3.68	96.88	6.85	-3.12	100-5000	0.5	100
	5000		105.92	5.38	5.92					1000		90.58	6.42	-9.42			
25C-NBOMe	100	10.33	109.24	6.39	9.24	100-5000	0.5	100		5000		109.41	5.61	9.41			
	1000		112.20	4.26	12.20				CATHINONE	100	3.75	102.31	6.61	2.31	100-5000	0.5	100
	5000		97.32	4.23	-2.68					1000		105.61	2.76	5.61			
25D-NBOMe	100	10.52	117.75	8.22	17.75	100-5000	0.5	100		5000		96.55	5.00	-3.45			
	1000		115.53	4.01	15.53				CB-13	10	16.51	48.58	13.54	-51.43	-	0.5	-
	5000		93.89	2.90	-6.11					100		23.41	44.87	-76.59			
25E-NBOMe	100	11.33	111.30	4.42	11.30	100-5000	0.5	100		1000		166.87	4.63	66.87			
	1000		118.37	3.86	18.37				CBL-018	10	15.82	13.76	78.19	-86.24	-	0.5	-
	5000		93.39	2.98	-6.61					100		64.57	18.02	-35.43			

25G-NBOMe	10	11.05	85.40	9.76	-14.60	10-2000	0.5	10
	100		100.53	4.49	0.53			
	1000		106.64	6.88	6.64			
	2000		95.22	3.94	-4.78			
	5000		78.31	2.90	-21.69			
25H-NBOMe	100	9.50	113.84	7.58	13.84	100-5000	0.5	100
	1000		117.57	5.70	17.57			
	5000		99.66	5.70	-0.34			
25-I-NB2OMe	10	10.89	103.28	8.89	3.28	10-5000	0.5	10
	100		103.62	5.51	3.62			
	1000		110.33	4.13	10.33			
	2000		103.65	2.35	3.65			
	5000		93.23	4.42	-6.77			
25I-NB3OMe	10	10.88	102.87	17.90	2.87	10-5000	0.5	10
	100		109.15	4.44	9.15			
	1000		110.36	5.05	10.36			
	2000		102.89	4.45	2.89			
	5000		96.93	3.14	-3.07			
25I-NB4OMe	10	10.81	113.08	6.73	13.08	10-5000	0.5	10
	100		107.92	4.15	7.92			
	1000		107.67	2.75	7.67			
	2000		96.87	5.34	-3.13			
	5000		92.63	2.70	-7.37			
25I-NBF	10	10.60	96.61	12.03	-3.39	10-5000	0.5	10
	100		102.89	6.83	2.89			
	1000		102.35	4.63	2.35			
	2000		96.11	3.28	-3.89			
	5000		91.17	3.58	-8.83			
25I-NBMD	10	10.72	91.29	12.09	-8.71	10-5000	0.5	10
	100		114.33	2.46	14.33			
	1000		116.91	3.82	16.91			
	2000		111.13	2.94	11.13			
	5000		107.04	2.69	7.04			
25I-NBOH	100	10.49	107.53	7.04	7.53	100-5000	0.5	100
	1000		114.49	5.90	14.49			
	5000		100.88	5.62	0.88			
	1000		166.61	5.54	66.61			
CI2201	10	14.96	29.91	44.72	-70.09	100-5000	0.5	100
	100		93.04	13.03	-6.96			
	1000		118.22	2.33	18.22			
	2000		115.43	2.57	15.43			
	5000		115.01	6.16	15.01			
CLOBAZAM	100	11.17	97.22	10.74	-2.78	100-5000	0.5	100
	1000		110.23	8.63	10.23			
	5000		110.15	7.60	10.15			
CLOMIPRAMINE	100	11.66	117.09	4.83	17.09	100-5000	0.5	100
	1000		114.54	7.56	14.54			
	5000		96.33	4.30	-3.67			
CLONAZEPAM	100	10.80	90.50	6.69	-9.50	100-5000	0.5	100
	1000		119.07	7.62	19.07			
	5000		103.21	6.12	3.21			
COCAETHYLENE	100	8.16	100.19	3.87	0.19	100-5000	0.5	100
	1000		117.01	4.39	17.01			
	5000		109.47	8.13	9.47			
COCAINE	100	7.22	108.70	2.51	8.70	100-5000	0.5	100
	1000		114.25	7.29	14.25			
	5000		106.19	4.31	6.19			
CODEINE	100	4.47	115.22	8.09	15.22	100-5000	0.5	100
	1000		85.49	3.42	-14.51			
	5000		85.97	4.74	-14.03			
CUMYL-PICA	10	14.69	115.76	6.91	15.76	10-1000	0.5	10
	100		99.62	6.46	-0.38			
	1000		97.18	3.58	-2.82			
D2PM	10	7.97	92.04	9.47	-7.96	10-5000	0.5	10
	100		109.97	7.18	9.97			
	1000		116.18	1.96	16.18			
	2000		102.07	10.12	2.07			
	5000		101.81	3.74	1.81			
DEMOXEPAM	100	10.27	100.86	6.55	0.86	100-5000	0.5	100
	1000		116.26	3.41	16.26			
	5000		106.05	3.67	6.05			
DESALKYLFLURAZEPAM	100	11.63	80.14	12.02	-19.86	100-5000	0.5	100

25N-NBOMe	100	9.15	111.42	4.60	11.42	100-5000	0.5	100	DESCHLOROETIZOLAM	1000	11.53	114.25	8.30	14.25	100-5000	0.5	100
	1000		116.87	4.19	16.87					5000		93.57	4.98	-6.43			
	5000		97.82	6.75	-2.18					100		99.31	10.92	-0.69			
25T2-NBOMe	10	10.79	102.56	7.01	2.56	10-2000	0.5	10		1000		115.35	6.53	15.35			
	100		100.52	5.06	0.52					5000		112.68	6.36	12.68			
	1000		106.04	3.75	6.04				DESCHLORO-N-ETHYL-KETAMINE	10	6.23	103.20	10.54	3.20	10-5000	0.5	10
	2000		92.21	5.54	-7.79					100		97.61	9.87	-2.39			
	5000		67.64	1.36	-32.36					1000		84.23	8.78	-15.77			
25T-NBOMe	100	10.14	106.43	5.11	6.43	100-5000	0.5	100		2000		86.79	7.80	-13.21			
	1000		112.56	6.59	12.56					5000		86.65	6.28	-13.35			
	5000		102.64	3.84	2.64				DESIPRAMINE	100	10.75	117.35	8.93	17.35	100-5000	0.5	100
2-AMINO-1-PHENYLBUTANE	10	6.10	107.75	9.65	7.75	10-5000	0.5	10		1000		116.14	4.69	16.14			
	100		108.92	6.56	8.92					5000		93.31	3.78	-6.69			
	1000		86.99	5.03	-13.01				DESMETHYLDIAZEPAM (NORDIAZEPAM)	100	11.96	102.06	11.00	2.06	100-5000	0.5	100
	2000		82.47	6.63	-17.53					1000		118.98	5.31	18.98			
	5000		85.94	4.59	-14.06					5000		103.58	8.96	3.58			
2-AMINOINDANE	100	3.89	109.04	3.91	9.04	100-5000	0.5	100	DESMETHYLFLUNITRAZEPAM	100	10.38	88.28	7.70	-11.72	100-5000	0.5	100
	1000		95.58	4.00	-4.42					1000		119.27	2.69	19.27			
	5000		87.01	4.24	-12.99					5000		117.22	4.07	17.22			
2-BROMOAMPHETAMINE	10	7.05	29.96	101.14	-70.04	100-5000	0.5	100	DESOMORPHINE	100	5.22	113.43	9.50	13.43	100-5000	0.5	100
	100		96.46	13.06	-3.54					1000		95.28	4.11	-4.72			
	1000		98.05	4.54	-1.95					5000		92.80	7.15	-7.20			
	2000		91.30	6.33	-8.70				DESOXY-D2PM	10	8.69	91.80	10.17	-8.20	10-5000	0.5	10
	5000		90.86	5.09	-9.14					100		106.49	8.11	6.49			
2-BROMOMETHAMPHETAMINE	100	7.21	110.08	8.04	10.08	100-5000	0.5	100		1000		99.68	13.83	-0.32			
	1000		111.06	6.29	11.06					2000		100.88	7.53	0.88			
	5000		86.42	12.60	-13.58					5000		92.24	3.36	-7.76			
2C-B	100	7.75	106.11	4.88	6.11	100-5000	0.5	100	DESOXYPIPRADROL (2-DPMP)	100	9.10	113.12	3.17	13.12	100-5000	0.5	100
	1000		118.78	7.10	18.78					1000		114.71	6.12	14.71			
	5000		104.67	5.22	4.67					5000		100.74	5.51	0.74			
2C-B FLY	100	8.06	101.98	6.88	1.98	100-5000	0.5	100	DEXTROMETHORPHAN	100	9.33	101.02	7.20	1.02	100-5000	0.5	100
	1000		112.82	8.10	12.82					1000		110.09	4.82	10.09			
	5000		104.47	2.27	4.47					5000		105.59	2.27	5.59			

2C-C	100	7.31	111.72	11.49	11.72	100-5000	0.5	100	DIAZEPAM	100	12.37	89.73	9.18	-10.27	100-5000	0.5	100
	1000		91.32	16.03	-8.68					1000		116.78	7.59	16.78			
	5000		104.11	8.79	4.11					5000		101.30	7.20	1.30			
2C-D	100	7.56	107.50	7.33	7.50	100-5000	0.5	100	DICLAZEPAM	100	12.40	99.30	9.45	-0.70	100-5000	0.5	100
	1000		105.12	6.89	5.12					1000		114.86	4.15	14.86			
	5000		113.36	3.51	13.36					5000		106.28	3.69	6.28			
2C-G	100	8.59	113.98	7.51	13.98	100-5000	0.5	100	DICLOFENSINE	10	11.04	93.94	10.90	-6.07	10-5000	0.5	10
	1000		116.96	4.40	16.96					100		104.57	4.37	4.57			
	5000		98.13	7.63	-1.87					1000		106.41	5.65	6.41			
2-CHLOROAMPHETAMINE	10	6.59	91.69	13.99	-8.31	10-5000	0.5	10		2000		99.40	6.22	-0.60			
	100		92.00	7.10	-8.00					5000		94.09	6.43	-5.91			
	1000		97.52	8.73	-2.48				DIETHYLCATHINONE (AMFEPRAMONE)	100	5.41	97.16	7.02	-2.84	100-5000	0.5	100
	2000		93.44	7.93	-6.56					1000		88.88	5.41	-11.12			
	5000		92.86	10.43	-7.14					5000		100.00	3.93	0.00			
2C-I	100	8.45	117.64	7.52	17.64	100-1000	0.5	100	DIHYDROCODEINE	100	4.41	108.69	8.13	8.69	100-5000	0.5	100
	1000		114.84	5.88	14.84					1000		86.85	4.66	-13.15			
2C-P	100	10.14	93.63	9.71	-6.37	100-5000	0.5	100		5000		81.87	8.46	-18.13			
	1000		109.77	11.26	9.77				DIMETHOCAINE	100	6.36	100.70	4.15	0.70	100-5000	0.5	100
	5000		101.56	6.85	1.56					1000		115.56	8.12	15.56			
2C-T-7	100	9.64	107.60	3.91	7.60	100-5000	0.5	100		5000		107.11	3.09	7.11			
	1000		99.12	43.43	-0.88				DIMETHYLONE (bk-MDDMA)	100	4.93	92.36	7.36	-7.64	100-5000	0.5	100
	5000		103.93	5.47	3.93					1000		92.61	7.95	-7.39			
2C-TFM	10	8.68	109.14	4.77	9.14	10-5000	0.5	10		5000		94.79	3.83	-5.21			
	100		117.56	6.32	17.56				DIPHENHYDRAMINE	100	9.34	106.22	3.51	6.22	100-5000	0.5	100
	1000		108.41	3.04	8.41					1000		109.92	6.35	9.92			
	2000		99.09	6.64	-0.91					5000		101.49	3.38	1.49			
	5000		93.76	4.00	-6.24				DIPHENIDINE	100	8.81	108.46	6.36	8.46	100-5000	0.5	100
2-FEC	10	4.99	80.30	4.58	-19.70	10-5000	0.5	10		1000		105.24	8.65	5.24			
	100		104.08	9.05	4.08					5000		90.35	4.71	-9.65			
	1000		90.54	3.90	-9.46				DiPT	100	7.79	107.69	4.15	7.69	100-5000	0.5	100
	2000		84.46	3.12	-15.54					1000		118.79	4.92	18.79			
	5000		92.11	3.99	-7.89					5000		107.84	5.14	7.84			
2-FIC	10	3.21	94.79	11.75	-5.21	10-100	0.5	10	DL-4662	10	7.34	101.43	7.29	1.43	10-5000	0.5	10
	100		101.92	5.02	1.92					100		113.60	9.75	13.60			
	1000		33.13	3.65	-66.87					1000		108.39	3.34	8.39			
	2000		28.23	1.65	-71.77					2000		97.71	6.02	-2.29			
	5000		27.82	4.75	-72.18					5000		89.19	3.62	-10.81			

2-FLUOROAMPHETAMINE	100	5.14	111.25	7.36	11.25	100-5000	0.5	100	DOI	100	8.98	104.78	8.77	4.78	100-5000	0.5	100
	1000		110.28	6.43	10.28					1000		112.29	7.85	12.29			
	5000		100.40	6.05	0.40					5000		99.72	3.71	-0.28			
2-FLUOROMETHAMPHETAMINE (2-FMA)	100	5.39	116.77	4.71	16.77	100-5000	0.5	100	DOTHIEPIN	100	10.24	107.85	7.14	7.85	100-5000	0.5	100
	1000		90.19	9.59	-9.81					1000		107.72	4.58	7.72			
	5000		80.53	12.17	-19.47					5000		99.38	5.27	-0.62			
2-FLUOROMETHCATHINONE (2-FMC)	100	4.10	90.71	10.20	-9.29	100-5000	0.5	100	DOXEPIN	100	9.59	105.52	3.67	5.52	100-5000	0.5	100
	1000		93.91	7.54	-6.09					1000		106.02	6.90	6.02			
	5000		89.74	8.07	-10.26					5000		102.31	4.64	2.31			
2-IODOAMPHETAMINE	10	7.77	119.06	8.38	19.06	10-5000	0.5	10	DOXYLAMINE	100	6.08	84.21	13.82	-15.79	100-5000	0.5	100
	100		104.32	3.46	4.32					1000		115.72	4.86	15.72			
	1000		101.21	9.53	1.21					5000		117.91	5.72	17.91			
	2000		96.55	11.74	-3.45				EAM-2201	10	14.95	84.10	11.51	-15.90	10-1000	0.5	10
	5000		99.19	7.92	-0.81					100		105.68	11.08	5.68			
										1000		115.93	5.23	15.93			
2-MAPB	10	7.07	94.83	7.33	-5.17	10-2000	0.5	10	EDDP	100	9.4	91.82	3.80	-8.18	100-5000	0.5	100
	100		94.95	3.87	-5.05					1000		105.84	5.30	5.84			
	1000		108.23	6.50	8.23					5000		95.99	9.00	-4.01			
	2000		91.76	24.40	-8.24												
	5000		74.33	38.19	-25.67				EG-2201	10	15.66	83.81	14.54	-16.19	10-1000	0.5	10
										100		45.03	9.25	-54.97			
2-MeOMC	10	5.33	95.75	14.11	-4.25	10-5000	0.5	10		1000		115.13	2.87	15.13			
	100		116.44	6.12	16.44				ERGOMETRINE	10	5.33	83.38	16.89	-16.62	10-100	0.5	10
	1000		75.34	5.13	-24.66					100		108.91	13.02	8.91			
	2000		73.62	5.14	-26.38					1000		42.38	6.47	-57.62			
	5000		87.74	5.14	-12.26					2000		36.38	8.96	-63.62			
										5000		37.97	13.99	-62.03			
2-METHOXY-2-PHENYLETHYLAMINE	10	4.98	91.37	10.39	-8.63	10-100	0.5	10	ESTAZOLAM	100	11.08	101.51	5.36	1.51	100-5000	0.5	100
	100		107.71	11.04	7.71					1000		114.08	4.52	14.08			
	1000		43.29	4.52	-56.71					5000		99.16	2.84	-0.84			
	2000		38.60	4.77	-61.40												
	5000		42.10	9.86	-57.90												
2-METHOXYAMPHETAMINE (2-MA)	100	6.21	106.43	8.52	6.43	100-5000	0.5	100	ETAQUALONE	100	11.99	108.55	5.15	8.55	100-5000	0.5	100
	1000		117.86	5.95	17.86					1000		113.61	6.40	13.61			
	5000		105.57	3.29	5.57					5000		99.44	6.41	-0.56			

2-METHOXYMETHAMPHETAMINE (2-MeOMA)	100	6.42	105.85	9.88	5.85	100-5000	0.5	100	ETHCATHINONE METABOLITE	100	4.77	103.95	8.12	3.95	100-5000	0.5	100
	1000		110.80	7.07	10.80					1000		91.30	4.54	-8.70			
	5000		108.34	3.95	8.34					5000		86.00	8.69	-14.00			
2-METHYLAMINO-1-PHENYLBUTANE	10	6.23	89.60	9.93	-10.40	10-5000	0.5	10	ETHYLONE (bk-MDEA)	100	5.26	104.12	9.49	4.12	100-5000	0.5	100
	100		91.85	8.60	-8.15					1000		88.29	6.39	-11.71			
	1000		106.30	2.98	6.30					5000		103.43	4.59	3.43			
	2000		88.66	4.49	-11.34				ETHYLPHENIDATE	100	8.22	113.87	2.97	13.87	100-5000	0.5	100
	5000		90.33	2.19	-9.67					1000		114.98	5.03	14.98			
2-METHYLMETHCATHINONE (2-MMC)	100	5.81	109.71	3.13	9.71	100-5000	0.5	100		5000		104.29	3.88	4.29			
	1000		104.71	3.10	4.71				ETIZOLAM	100	11.80	103.12	5.74	3.12	100-5000	0.5	100
	5000		107.21	12.43	7.21					1000		115.09	5.70	15.09			
2-METHYL-PBP	10	7.51	94.12	13.88	-5.88	10-5000	0.5	10		5000		113.61	2.24	13.61			
	100		103.20	3.68	3.20				EUTYLONE (bk-EBDB)	100	6.30	97.87	6.27	-2.13	100-5000	0.5	100
	1000		103.57	8.90	3.57					1000		103.91	4.95	3.91			
	2000		92.08	9.83	-7.92					5000		99.43	1.33	-0.57			
	5000		95.55	8.22	-4.45				FENFLURAMINE	100	8.38	114.16	8.58	14.16	100-5000	0.5	100
2-METHYL-PPP	10	6.52	114.60	12.10	14.60	10-5000	0.5	10		1000		116.76	4.69	16.76			
	100		88.47	9.08	-11.53					5000		94.53	4.55	-5.47			
	1000		98.49	8.69	-1.51				FENTANYL	10	8.82	83.82	11.85	-16.18	10-5000	0.5	10
	2000		102.05	8.15	2.05					100		115.08	5.17	15.08			
	5000		109.46	3.62	9.46					1000		115.75	2.76	15.75			
3,4-DICHLOROMETHYLPHENIDATE (3,4-CTMP)	100	10.02	102.75	5.74	2.75	100-5000	0.5	100		2000		107.33	4.86	7.33			
	1000		108.42	5.49	8.42					5000		103.69	3.88	3.69			
	5000		108.22	6.54	8.22				FLUBROMAZEPAM	100	11.84	81.57	16.86	-18.43	100-5000	0.5	100
3,4-DIMETHOXY-ALPHA-PVP	10	7.45	48.86	35.24	-51.14	100-5000	0.5	100		1000		114.95	6.16	14.95			
	100		116.96	4.30	16.96					5000		108.33	4.43	8.33			
	1000		118.37	4.45	18.37				FLUDIAZEPAM	100	12.07	95.20	7.11	-4.80	100-5000	0.5	100
	2000		106.81	3.01	6.81					1000		119.51	6.89	19.51			
	5000		92.69	6.07	-7.31					5000		103.56	5.35	3.56			
3,4-DIMETHYLMETHCATHINONE (3,4-DMMC)	100	7.39	109.02	4.40	9.02	100-5000	0.5	100	FLUMAZENIL	100	9.31	114.25	7.04	14.25	100-5000	0.5	100
	1000		90.93	15.66	-9.07					1000		117.46	4.09	17.46			
	5000		110.16	2.70	10.16					5000		99.70	4.53	-0.30			
3,4-DMEC	10	7.76	100.56	18.74	0.56	10-5000	0.5	10	FLUNITRAZEPAM	100	10.91	95.19	10.71	-4.81	100-5000	0.5	100
	100		96.15	5.69	-3.85					1000		116.63	3.20	16.63			
	1000		106.92	5.66	6.92					5000		103.63	5.85	3.63			
	2000		95.63	2.03	-4.37				FLUOXETINE	100	11.24	107.77	8.71	7.77		0.5	100

	5000		94.43	10.30	-5.57					1000		109.39	5.88	9.39	100-5000		
3,4-DMMA	100	5.35	115.81	2.49	15.81	100-5000	0.5	100		5000		101.90	5.72	1.90			
	1000		104.37	6.84	4.37				FLURAZEPAM	100	9.43	101.10	3.64	1.10	100-5000	0.5	100
	5000		93.68	8.05	-6.32					1000		115.41	5.63	15.41			
	10		82.93	13.01	-17.07					5000		99.24	6.61	-0.76			
	100		108.32	6.75	8.32					10		80.26	12.29	-19.74			
3,4-EDMA	1000	5.63	81.23	3.82	-18.77	10-5000	0.5	10	FUB-144	100	14.96	89.09	5.61	-10.91	10-1000	0.5	10
	2000		76.71	4.94	-23.29					1000		100.35	7.91	0.35			
	5000		84.64	3.99	-15.36				FUB-JWH-018	10	14.47	105.44	7.96	5.44	10-1000	0.5	10
	10		91.46	10.10	-8.55					100		93.91	4.83	-6.09			
	100		101.63	10.40	1.63					1000		118.61	4.32	18.61			
3,4-EDMC	1000	5.25	78.76	2.46	-21.24	10-5000	0.5	10	FUB-NPB-22	10	13.66	96.34	11.03	-3.66	10-1000	0.5	10
	2000		70.80	5.05	-29.20					100		87.73	10.10	-12.27			
	5000		88.08	3.96	-11.92					1000		119.02	2.80	19.02			
	100		116.10	4.76	16.10				FURANYLFENTANYL (Fu-F)	100	8.95	107.36	2.38	7.36	100-5000	0.5	100
3,4-MDMA (ECSTAZY)	1000	5.37	93.67	4.53	-6.33	100-5000	0.5	100		1000		119.27	8.06	19.27			
	5000		113.75	5.18	13.75					5000		100.59	5.28	0.59			
	100		113.80	7.84	13.80				GHB	100	1.41	119.46	8.68	19.46	100-5000	0.5	100
3,4-MDPA	1000	6.82	116.44	3.64	16.44	100-5000	0.5	100		1000		103.62	8.29	3.62			
	5000		106.42	3.90	6.42					10		102.06	17.73	2.06			
	10		56.00	20.18	-44.00				HARMALINE	100	7.47	109.72	9.76	9.72	10-5000	0.5	10
	100		94.36	7.95	-5.64					1000		101.91	6.29	1.91			
3,4-MDPHP	1000	8.68	98.81	3.99	-1.19	100-5000	0.5	100		2000		91.77	5.09	-8.23			
	2000		93.91	3.77	-6.09					5000		84.46	5.58	-15.54			
	5000		91.41	4.77	-8.59					100		98.51	6.39	-1.49			
	10		88.35	6.85	-11.66				HARMINE	1000	8.03	115.61	4.65	15.61	100-5000	0.5	100
	100		100.06	4.64	0.06					5000		101.96	2.60	1.96			
3,4-METHYLENDIOXYPYROVALERONE	1000	7.53	99.40	2.70	-0.60	10-5000	0.5	10		100		108.04	6.24	8.04			
	2000		93.15	4.22	-6.85				HYDROCODONE	1000	4.99	103.24	8.40	3.24	100-5000	0.5	100
	5000		89.27	3.72	-10.73					5000		92.87	6.59	-7.13			
	10		105.55	8.61	5.55					100		99.76	7.83	-0.24			
3,4-METHYLENEDIOXY_PV9	100	10.84	101.57	4.31	1.57	10-5000	0.5	10	IBOGAINE	1000	8.05	106.77	7.59	6.77	100-5000	0.5	100
	1000		102.88	4.45	2.88					5000		87.64	6.47	-12.36			

	2000		92.84	3.01	-7.16					100		111.54	5.26	11.54			
	5000		83.66	3.92	-16.34				IMIPRAMINE	1000	10.63	113.86	6.50	13.86	100-5000	0.5	100
	10		24.99	54.51	-75.01					5000		96.80	4.08	-3.20			
	100		117.48	16.21	17.48					100		112.39	3.43	12.39			
30C-NBOMe	1000	9.75	115.33	6.49	15.33	100-5000	0.5	100	ISOPENTEDRONE	1000	6.86	118.48	6.85	18.48	100-5000	0.5	100
	2000		109.09	4.36	9.09					5000		109.51	4.85	9.51			
	5000		95.92	7.92	-4.08												
	100		119.18	10.16	19.18				JWH 018 BENZIMIDAZOLE ANALOG	10		111.28	13.78	11.28			
	1000									100	15.44	88.44	8.98	-11.56	10-1000	0.5	10
3-BROMOAMPHETAMINE		7.34	104.10	10.86	4.10	100-5000	0.5	100		1000		84.27	11.13	-15.73			
	5000		104.22	15.32	4.22												
	100		109.88	4.95	9.88					10		32.14	46.45	-67.86			
3-BROMOMETHAMPHETAMINE	1000	7.45	107.19	13.43	7.19	100-5000	0.5	100	JWH-011	100	15.80	62.86	24.32	-37.14	-	0.5	-
	5000		106.26	8.93	6.26					1000		173.55	6.83	73.55			
	100		106.21	11.47	6.21					10		90.56	11.75	-9.44			
	1000		88.68	11.65	-11.32				JWH-018 ADAMANTYL CARBOXAMIDE	100	15.72	105.14	16.55	5.14	10-1000	0.5	10
3-BROMOMETHCATHINONE (3-BMC)		6.52				100-5000	0.5	100		1000		106.41	6.83	6.41			
	5000		84.03	8.80	-15.97												
	10		104.58	11.84	4.58					10		91.21	11.19	-8.80			
3-CAF	100	15.30	109.98	9.14	9.98	10-1000	0.5	10	JWH-022	100	14.75	96.01	8.37	-3.99	10-1000	0.5	10
	1000		118.30	8.66	18.30					1000		102.08	7.52	2.08			
	10		110.79	6.47	10.79					10		90.67	7.69	-9.33			
	100		114.75	5.41	14.75				JWH-031	100	14.85	98.56	5.93	-1.44	10-1000	0.5	10
3C-B-FLY	1000	8.55	106.96	7.01	6.96	10-5000	0.5	10		1000		105.10	7.72	5.10			
	2000		101.02	3.34	1.02					10		97.53	8.14	-2.47			
	5000		93.53	4.27	-6.47				JWH-071	100	13.64	104.64	6.56	4.64	10-1000	0.5	10
	10									1000		98.62	3.52	-1.38			
			119.51	5.84	19.51					10		86.50	17.59	-13.50			
	100		99.61	13.25	-0.39				JWH-080	100	14.97	103.92	11.06	3.92	10-1000	0.5	10
3-CHLOROAMPHETAMINE	1000	6.85	109.36	9.80	9.36	10-5000	0.5	10		1000		111.60	5.78	11.60			
	2000		114.98	6.61	14.98					10		38.22	22.91	-61.78			
	5000		104.62	5.17	4.62				JWH-116	100	15.66	80.23	16.53	-19.77	100-1000	0.5	100
3-CHLOROMETHCATHINONE (3-CMC)	100	6.02	119.79	7.58	19.79		0.5	100		1000		116.92	7.78	16.92			

	1000		99.08	6.60	-0.92	100-5000				10		22.42	68.93	-77.58			
	5000		84.68	10.20	-15.32				JWH-145	100	15.59	61.91	13.52	-38.09	-	0.5	-
	100		115.67	6.40	15.67					1000		142.05	6.75	42.05			
3-CHLOROPHENYLPIPERAZINE (mCPP)	1000	6.83	106.31	10.87	6.31	100-5000	0.5	100		10		83.40	3.93	-16.60			
	5000		105.67	4.46	5.67				JWH-146	100	16.21	18.43	32.10	-81.57	10-1000	0.5	10
	10		91.34	14.32	-8.66					1000		113.55	8.53	13.55			
	100		108.11	6.63	8.11					10		100.65	5.44	0.65			
	1000								JWH-149		15.65		14.15				
3C-P		8.43	108.97	3.95	8.97	10-5000	0.5	10		100		77.78		-22.22	10-1000	0.5	10
	2000		100.17	3.92	0.17					1000		116.12	5.43	16.12			
	5000		97.75	6.09	-2.25												
									JWH-167	10	14.55	94.05	10.93	-5.96	10-1000	0.5	10
	10		113.75	7.90	13.75					100		104.28	4.87	4.28			
	100		95.65	6.43	-4.35					1000		108.72	1.85	8.72			
	1000		96.94	2.71	-3.06					10		89.06	7.91	-10.94			
3-DESOXY-3,4-MDPV	2000	8.01				10-5000	0.5	10					25.79				
			90.36	3.58	-9.64				JWH-175	100	16.76	34.86		-65.14	10-1000	0.5	10
	5000		86.85	3.22	-13.15					1000		113.31	2.07	13.31			
	100		101.72	8.23	1.72					10		80.79	5.28	-19.21			
	1000								JWH-182		16.07		29.69				
3-ETHYLMETHCATHINONE (3-EMC)		7.39	105.76	8.15	5.76	100-5000	0.5	100		100		30.80		-69.20	10-1000	0.5	10
	5000		82.18	12.16	-17.82					1000		112.18	6.77	12.18			
	10		86.14	6.65	-13.86												
										10		89.68	10.35	-10.32			
	100		96.60	7.87	-3.40				JWH-193	100	11.79	101.08	6.58	1.08	10-1000	0.5	10
	1000				-10.57					1000		100.03	4.71	0.03			
3-FEC		4.99	89.43	4.42		10-5000	0.5	10									
	2000		81.25	3.70	-18.75												
										10		102.91	13.13	2.91			
	5000		93.63	6.30	-6.37				JWH-198	100	11.57	97.64	6.85	-2.36	10-1000	0.5	10
	10		92.87	12.49	-7.13					1000		102.99	2.93	2.99			
	100																
			100.00	3.74	0.00					10		93.40	12.85	-6.60			
	1000		82.27	4.26	-17.73				JWH-201	100	14.46	110.15	7.23	10.15	10-1000	0.5	10
3-FLUORO-ALFA-PPP	2000	5.36				10-5000	0.5	10									
			76.99	4.25	-23.01					1000		114.67	6.19	14.67			
	5000		82.05	2.61	-17.95												
									JWH-213	10	15.92	33.86	28.75	-66.15	-	0.5	-
3-FLUOROAMPHETAMINE	100	5.13	109.90	9.94	9.90	100-5000	0.5	100		100		42.39	26.06	-57.61			

	1000		105.58	6.00	5.58					1000		118.54	7.37	18.54			
	5000		94.86	2.73	-5.14					10		84.39	8.15	-15.61			
	100		107.90	7.44	7.90				JWH-307	100	15.50	86.54	18.11	-13.46	10-1000	0.5	10
3-FLUOROMETHAMPHETAMINE (3-FMA)	1000	5.41	118.13	3.75	18.13	100-5000	0.5	100		1000		111.35	7.64	11.35			
	5000		103.40	4.09	3.40					10		36.57	16.63	-63.43			
	100		112.34	5.35	12.34				JWH-309	100	16.09	19.85	43.93	-80.15	-	0.5	-
3-FLUOROMETHCATHINONE (3-FMC)	1000	4.43	91.06	12.95	-8.94	100-5000	0.5	100		1000		121.90	8.55	21.90			
	5000		82.11	12.65	-17.89					10		97.28	5.21	-2.72			
	100		87.18	2.08	-12.82				JWH-368	100	15.47	113.41	4.21	13.41	10-1000	0.5	10
3-HYDROXYBROMAZEPAM	1000	9.19	113.76	8.88	13.76	100-5000	0.5	100		1000		117.75	4.35	17.75			
	5000		101.32	5.70	1.32					10		53.82	16.22	-46.18			
	100		96.57	9.55	-3.43				JWH-369	100	15.69	43.08	24.90	-56.92	-	0.5	-
3-HYDROXYFLUNITRAZEPAM	1000	10.23	118.13	6.44	18.13	100-5000	0.5	100		1000		127.63	8.93	27.63			
	5000		83.75	5.10	-16.25					10		99.32	15.33	-0.68			
	10		103.17	16.32	3.17				JWH-412	100	15.42	91.01	9.42	-8.99	10-1000	0.5	10
	100		104.14	7.50	4.14					1000		118.70	9.67	18.70			
	1000		92.87	9.49	-7.13					10		54.51	20.66	-45.49			
3-IODOAMPHETAMINE	2000	8.06	101.48	12.53	1.48	10-5000	0.5	10	JWH-424	100	14.97	95.08	8.83	-4.92	100-1000	0.5	100
	5000		105.02	9.83	5.02					1000		104.39	4.06	4.39			
	10		108.01	15.32	8.01					100		107.09	6.48	7.09			
	100		95.06	10.79	-4.94				KETAMINE	1000	6.51	110.48	8.76	10.48	100-5000	0.5	100
	1000		92.25	5.45	-7.75					5000		100.64	5.34	0.64			
3-MEC	2000	6.47	89.73	5.00	-10.27	10-5000	0.5	10		100		86.25	8.89	-13.75			
	5000		84.27	2.99	-15.73				LAMPA	1000	8.31	100.35	7.46	0.35	100-5000	0.5	100
	10		79.96	8.89	-20.04					5000		101.43	7.61	1.43			
	100		114.30	4.03	14.30					100		108.60	5.57	8.60			
	1000		72.87	5.13	-27.13				LIDOCAINE	1000	5.77	115.76	4.84	15.76	100-5000	0.5	100
3-MeOMC	2000	5.33	68.01	5.96	-31.99	10-5000	0.5	10		5000		108.67	3.88	8.67			
	5000		82.38	4.99	-17.62					100		108.64	8.05	8.64			
3-METHOXYAMPHETAMINE (3-MA)	100	5.67	117.88	5.04	17.88		0.5	100	LOPRAZOLAM	1000	9.31	117.93	7.50	17.93	100-5000	0.5	100

	1000		101.82	15.86	1.82	100-5000		
	5000		92.49	10.49	-7.51			
3-METHOXYPHENCYCLIDINE	10	8.93	86.92	11.43	-13.09	10-5000	0.5	10
	100		102.06	8.62	2.06			
	1000		107.35	4.73	7.35			
	2000		101.59	5.82	1.59			
	5000		97.49	3.50	-2.51			
3-METHYLMETHCATHINONE (3-MMC)	100	6.01	110.03	5.98	10.03	100-5000	0.5	100
	1000		92.52	4.62	-7.48			
	5000		86.47	9.80	-13.53			
3-METHYL-PBP	10	7.5	97.82	11.28	-2.18	10-5000	0.5	10
	100		103.93	8.19	3.93			
	1000		108.04	9.64	8.04			
	2000		90.23	6.73	-9.77			
	5000		102.95	7.06	2.95			
3-METHYL-PPP	10	6.67	97.23	13.47	-2.77	10-5000	0.5	10
	100		99.72	8.91	-0.28			
	1000		70.20	8.62	-29.80			
	2000		102.72	5.53	2.72			
	5000		106.49	4.12	6.49			
4,4'-DMAR	100	7.38	103.64	4.23	3.64	100-5000	0.5	100
	1000		101.11	2.90	1.11			
	5000		91.24	1.77	-8.76			
4-AcO-DET	10	6.38	103.43	14.56	3.43	10-5000	0.5	10
	100		108.47	5.96	8.47			
	1000		101.65	3.19	1.65			
	2000		95.17	2.67	-4.83			
	5000		90.87	4.76	-9.13			
4-AcO-DMT	10	5.47	112.59	4.06	12.59	10-5000	0.5	10
	100		115.15	5.46	15.15			
	1000		96.14	2.46	-3.86			
	2000		86.08	2.79	-13.92			
	5000		93.51	4.88	-6.49			
4-AcO-MET	100	6.07	102.41	12.15	2.41		0.5	100
	5000		105.45	2.94	5.45			
LORAZEPAM	100	11.41	108.57	15.41	8.57	100-5000	0.5	100
	1000		108.73	9.60	8.73			
	5000		106.39	7.20	6.39			
LORMETAZEPAM	100	11.87	97.14	4.49	-2.86	100-5000	0.5	100
	1000		110.88	7.09	10.88			
	5000		97.83	5.90	-2.17			
LSD	100	8.15	97.13	8.78	-2.87	100-5000	0.5	100
	1000		113.34	5.29	13.34			
	5000		104.92	5.65	4.92			
MAPROTILINE	100	10.76	114.59	7.17	14.59	100-5000	0.5	100
	1000		110.10	4.80	10.10			
	5000		99.88	4.23	-0.12			
MBDB	100	6.47	104.88	5.24	4.88	100-5000	0.5	100
	1000		108.60	5.32	8.60			
	5000		94.17	1.87	-5.83			
MDAT	10	5.44	366.85	23.67	266.85	100-5000	0.5	100
	100		106.75	9.63	6.75			
	1000		83.80	1.56	-16.20			
	2000		82.65	5.71	-17.35			
	5000		82.55	3.36	-17.45			
MDBP	10	2.47	235.60	1.07	135.60	-	0.5	-
	100		117.98	4.04	17.98			
	1000		32.62	1.62	-67.38			
	2000		28.77	2.76	-71.23			
	5000		30.34	3.45	-69.66			
MDEA	100	5.90	112.87	5.34	12.87	100-5000	0.5	100
	1000		110.92	4.39	10.92			
	5000		103.21	4.07	3.21			
MDMB-CHMINACA	10	15.49	89.91	12.94	-10.09	10-1000	0.5	10
	100		99.40	14.82	-0.60			
	1000		112.13	2.25	12.13			
MDPBP	100	6.47	93.75	12.62	-6.25	100-5000	0.5	100
	1000		111.49	7.66	11.49			

	1000		81.85	6.60	-18.15	100-5000		
	5000		103.12	2.60	3.12			
4-APB	10	6.71	94.37	13.20	-5.63	10-5000	0.5	10
	100		94.44	6.01	-5.56			
	1000		97.26	6.31	-2.74			
	2000		89.83	4.58	-10.17			
	5000		94.72	4.31	-5.28			
4-APDB	10	5.58	103.02	14.00	3.02	10-5000	0.5	10
	100		110.11	12.49	10.11			
	1000		86.62	8.52	-13.38			
	2000		88.65	7.11	-11.35			
	5000		85.16	5.31	-14.84			
4-BROMO-2,5-DMMA	100	8.39	116.46	3.66	16.46	100-5000	0.5	100
	1000		108.66	3.08	8.66			
	5000		86.23	2.67	-13.77			
4-BROMOAMPHETAMINE	100	7.47	109.70	10.90	9.70	100-5000	0.5	100
	1000		81.86	4.41	-18.14			
	5000		104.54	17.28	4.54			
4-BROMOMETHAMPHETAMINE	100	7.43	104.26	6.05	4.26	100-5000	0.5	100
	1000		102.48	17.14	2.48			
	5000		105.99	9.92	5.99			
4-BROMOMETHCATHINONE (BREFEDRONE)	100	6.69	104.13	6.50	4.13	100-5000	0.5	100
	1000		95.19	10.78	-4.81			
	5000		86.23	14.74	-13.77			
4-CAB	10	8.00	104.44	13.85	4.44	10-5000	0.5	10
	100		102.31	6.50	2.31			
	1000		99.06	10.68	-0.94			
	2000		96.78	4.61	-3.22			
	5000		87.43	6.65	-12.57			
4-CEC	10	6.70	99.15	14.49	-0.85	10-5000	0.5	10
	100		93.48	5.09	-6.52			
	1000		96.03	5.65	-3.97			
	5000		115.68	3.01	15.68			
MECLONAZEPAM	10	11.41	89.89	18.11	-10.11	10-5000	0.5	10
	100		105.24	3.79	5.24			
	1000		112.94	2.39	12.94			
	2000		100.32	5.01	0.32			
	5000		96.55	6.62	-3.45			
MEDAZEPAM	100	9.48	88.78	7.08	-11.22	100-5000	0.5	100
	1000		95.69	2.10	-4.31			
	5000		117.36	4.46	17.36			
MEMANITINE	10	9.10	97.19	13.42	-2.82	10-5000	0.5	10
	100		90.15	9.52	-9.85			
	1000		98.26	5.81	-1.74			
	2000		91.27	6.07	-8.73			
	5000		88.67	5.49	-11.33			
MEPERIDINE	10	7.52	87.02	14.14	-12.98	10-5000	0.5	10
	100		108.18	7.26	8.18			
	1000		112.44	3.43	12.44			
	2000		100.28	4.75	0.28			
	5000		97.69	3.14	-2.31			
MEPHTETRAMINE (MTTA)	100	5.44	100.06	3.76	0.06	100-5000	0.5	100
	1000		109.74	4.08	9.74			
	5000		106.22	5.00	6.22			
MEPIRAPIM	10	10.14	118.36	4.87	18.36	10-1000	0.5	10
	100		102.64	6.10	2.64			
	1000		98.27	3.39	-1.73			
MEPROBAMATE	100	8.82	90.89	14.01	-9.11	100-5000	0.5	100
	1000		93.27	4.21	-6.73			
	5000		81.96	6.49	-18.04			
MESCALINE	100	5.23	109.90	12.73	9.90	100-5000	0.5	100
	1000		93.67	13.40	-6.33			
	5000		86.42	4.13	-13.58			
METHADONE	100	10.84	112.97	7.73	12.97		0.5	100

	2000		87.53	8.44	-12.47					1000		114.37	8.94	14.37	100-5000		
	5000		82.41	3.18	-17.59					5000		93.47	2.99	-6.53			
	10		92.23	15.49	-7.77					100		96.62	7.15	-3.38			
	100		95.54	11.29	-4.46				METHAMPHETAMINE	1000	5.05	96.92	4.22	-3.08	100-5000	0.5	100
	1000		93.13	7.65	-6.87					5000		97.65	4.70	-2.35			
4-CHLORO-ALPHA-PPP	2000	6.88	90.29	6.88	-9.71	10-5000	0.5	10		100		107.02	5.14	7.02			
	5000		88.56	3.21	-11.44				METHANDIENONE	1000	12.51	115.12	1.87	15.12	100-5000	0.5	100
	10		64.80	23.27	-35.20					5000		99.18	5.28	-0.82			
	100		98.42	7.78	-1.58					100		115.63	3.76	15.63			
4-CHLORO-ALPHA-PVP	1000	8.95	107.24	4.10	7.24	100-5000	0.5	100	METHAQUALONE	1000	11.11	105.60	5.75	5.60	100-5000	0.5	100
	2000		94.27	5.81	-5.73					5000		90.48	7.08	-9.52			
	5000		88.45	3.31	-11.55					100		117.11	6.16	17.11			
	10		115.96	5.69	15.96				METHCATHINONE	1000	4.13	89.73	4.92	-10.27	100-5000	0.5	100
	100		101.82	10.08	1.82					5000		86.50	5.66	-13.50			
	1000		42.47	10.63	-57.53								10.76				
4-CHLOROAMPHETAMINE	2000	6.96	59.08	16.65	-40.92	10-100	0.5	10		10		89.91		-10.10			
	5000		44.83	25.63	-55.17				METHEDRONE (bk-PMMA)	100	5.33	98.38	6.55	-1.62	10-100	0.5	10
	100		108.34	6.23	8.34					1000		57.10	5.38	-42.90			
	1000		93.42	15.12	-6.58					2000		52.33	6.00	-47.67			
4-CHLOROMETHCATHINONE (4-CMC)	5000	6.21	96.25	9.43	-3.75	100-5000	0.5	100		5000		61.27	3.22	-38.73			
	10		117.86	9.87	17.86								10.36				
	100		103.46	10.30	3.46				METHOHEXITAL	100	11.79	109.05		9.05	100-5000	0.5	100
	1000		87.75	9.48	-12.25					1000		113.97	7.52	13.97			
4-CMA	2000	7.07	85.68	6.65	-14.32	10-5000	0.5	10		5000		98.58	6.15	-1.42			
	5000		87.71	7.33	-12.29					100		101.25	5.85	1.25			
	10		85.96	17.19	-14.05				METHOXETAMINE	1000	7.15	104.73	12.85	4.73	100-5000	0.5	100
	100		115.62	6.95	15.62					5000		109.89	3.52	9.89			
4-EAPB	1000	7.36	96.37	7.15	-3.63	10-5000	0.5	10					10.83				
	2000		98.24	9.50	-1.76				METHOXPHENIDINE	100	9.36	97.64		-2.36	100-5000	0.5	100
	5000		92.52	11.10	-7.48					1000		110.82	8.34	10.82			
	10									5000		106.84	2.44	6.84			
										100		103.55	9.79	3.55			
									METHYLHEXANAMINE	1000	5.76	94.33	9.11	-5.67	100-5000	0.5	100
4-ETHYL-N,N-DMC		7.52	82.63	2.64	-17.37	10-5000	0.5	10					11.60				
										5000		103.15		3.15			

	100		98.92	3.92	-1.08				METHYLONE (bk-MDMA)	100	4.68	101.53	9.11	1.53	100-5000	0.5	100
	1000		99.31	10.54	-0.69					1000		85.14	4.93	-14.86			
	2000		95.98	9.81	-4.02					5000		81.90	4.40	-18.10			
	5000		91.28	11.72	-8.72												
	10		91.33	10.64	-8.67				METHYLPHENIDATE	100	7.17	114.73	7.21	14.73	100-5000	0.5	100
	100		103.23	7.07	3.22					1000		119.76	5.38	19.76			
	1000				-					5000		107.39	5.16	7.39			
4-FEC		5.01	82.28	11.82	17.72	10-5000	0.5	10									
	2000				-					10		116.95	7.55	16.95			
			84.46	5.26	15.54								12.7				
	5000		94.91	3.30	-5.09				MEXEDRONE	100	6.36	105.69	4	5.69	10-5000	0.5	10
	10		99.36	7.52	-0.64					1000		100.89	4.06	0.89			
	100		91.83	5.58	-8.17					2000		92.12	3.78	-7.88			
4-FLUORO BUPHEDRONE	1000	5.77	110.04	13.06	10.04	10-5000	0.5	10		5000		92.90	3.72	-7.10			
	2000		92.34	8.35	-7.66					100		107.65	6.60	7.65			
	5000		99.45	10.22	-0.55				MIANSERIN	1000	9.35	119.93	3.99	19.93	100-5000	0.5	100
	10		105.68	12.94	5.68					5000		93.77	7.83	-6.23			
	100		100.98	11.20	0.98					100		97.70	4.36	-2.30			
	1000		94.61	5.15	-5.39				MIDAZOLAM	1000	9.41	118.47	4.13	18.47	100-5000	0.5	100
	2000				-					5000		106.05	4.95	6.05			
4-FLUORO PENTEDRONE		7.2	88.64	4.10	11.36	10-5000	0.5	10									
	5000				-					100		103.95	6.63	3.95			
			83.87	5.48	16.13				MITRAGYNINE		9.26				100-5000	0.5	100
	10				-					1000		111.31	2.12	11.31			
			84.02	7.43	15.98					5000		106.68	3.05	6.68			
	100		104.64	5.18	4.64					10		105.52	9.12	5.52			
	1000												14.4				
4-FLUORO PV8		10.01	102.51	4.77	2.51	10-5000	0.5	10		100		99.16	4	-0.84			
	2000		98.38	6.92	-1.62				MMAI	1000	6.81	103.77	7.81	3.77	10-5000	0.5	10
	5000				-					2000		82.76	4.58	-17.24			
			89.36	4.09	10.64					5000		81.63	8.75	-18.37			
	10		106.39	7.24	6.39					10		111.43	3.57	11.43			
	100		114.83	5.33	14.83				MMB018	100	14.15	95.36	6.98	-4.64	10-1000	0.5	10
	1000		117.01	2.17	17.01					1000		89.82	7.95	-10.18			
4-FLUORO PV9	2000	11.04	97.31	3.83	-2.69	10-5000	0.5	10									
	5000				-					10		93.11	9.13	-6.89			
			88.24	3.06	11.76				MMB2201		13.10		12.0		10-1000	0.5	10
	10				-					100		105.42	8	5.42			
			86.69	6.02	13.31					1000		106.33	3.40	6.33			
	100		100.86	9.69	0.86								15.8				
4-FLUORO-ALFA-PPP	1000	5.35	83.58	3.27	-16.42	10-5000	0.5	10	MN-25	10	12.48	113.05	2	13.05	10-1000	0.5	10
	2000				-												
			74.96	4.51	25.04					100		83.67	8.94	-16.33			

	5000		81.21	2.90	-18.79					1000		109.56	4.25	9.56			
4-FLUOROMETHAMPHETAMINE (4-FMA)	100	5.4	88.42	7.82	-11.58	100-5000	0.5	100	MN-25-2-METHYL DERIVATIVE	10	13.22	98.36	9.04	-1.64	10-1000	0.5	10
	1000		87.35	8.46	-12.65					100		102.67	4.34	2.67			
	5000		85.14	8.60	-14.86					1000		97.76	8.97	-2.24			
4-FLUOROMETHCATHINONE (4-FMC)	100	4.44	106.59	4.93	6.59	100-5000	0.5	100	MO-CHMINACA	10	15.47	89.41	12.38	-10.59	10-1000	0.5	10
	1000		89.85	8.14	-10.15					100		84.67	18.67	-15.33			
	5000		93.23	4.22	-6.77					1000		112.54	5.71	12.54			
4F-PVP	100	7.66	101.37	7.04	1.37	100-5000	0.5	100	MORPHINE	100	2.45	110.11	10.79	10.11	100-5000	0.5	100
	1000		101.87	5.81	1.87					1000		101.68	4.07	1.68			
	5000		97.76	3.90	-2.24					5000		96.63	5.04	-3.37			
4-HYDROXY DiPT	100	6.47	103.53	4.40	3.53	100-5000	0.5	100	MPBP	100	7.59	105.14	5.89	5.14	100-5000	0.5	100
	1000		109.00	5.43	9.00					1000		107.37	4.33	7.37			
	5000		105.12	2.28	5.12					5000		104.64	4.17	4.64			
4-HYDROXYMIDAZOLAM	100	8.89	55.98	25.24	-44.02	-	0.5	-	MT-45	100	10.85	95.07	8.37	-4.93	100-5000	0.5	100
	1000		129.54	5.42	29.54					1000		113.39	7.91	13.39			
	5000		87.53	3.53	-12.47					5000		107.62	2.53	7.62			
4-IODOAMPHETAMINE	10	8.22	107.56	11.16	7.56	10-5000	0.5	10	N-(3-METHYLBENZYL)PIPERAZINE	10	4.00	223.68	4.10	123.68	-	0.5	-
	100		95.27	8.13	-4.73					100		116.14	3.88	16.14			
	1000		87.22	6.97	-12.78					1000		48.74	3.32	-51.26			
	2000		81.48	4.85	-18.52					2000		45.49	3.31	-54.51			
	5000		93.73	13.90	-6.27					5000		51.24	3.85	-48.76			
4-MAPB	10	6.86	95.76	10.10	-4.24	10-5000	0.5	10	N,N-DIETHYLPHENETHYLAMINE	10	5.37	89.59	10.39	-10.41	10-5000	0.5	10
	100		95.34	6.45	-4.66					100		95.05	7.54	-4.95			
	1000		64.45	3.51	-35.55					1000		100.79	8.44	0.79			
	2000		96.66	10.66	-3.34					2000		94.01	1.87	-5.99			
	5000		97.48	8.12	-2.52					5000		94.99	3.58	-5.01			
4-MEAP	10	8.57	116.41	6.20	16.41	10-5000	0.5	10	N,N-DIMETHYLPENTYLONE (bk-DMBDP)	100	7.31	109.69	7.05	9.69	100-5000	0.5	100
	100		107.02	6.84	7.02					1000		110.18	6.77	10.18			
	1000		96.00	15.02	-4.00					5000		110.66	5.99	10.66			
	2000		91.08	15.66	-8.92				N,N-DMT	100	4.88	89.92	18.70	-10.08	100-5000	0.5	100

	5000		96.31	1.55	-3.69					1000		98.92	5.61	-1.08			
	10		112.35	5.23	12.35					5000		94.41	2.72	-5.59			
	100		97.44	8.69	-2.56					10		88.45	14.11	-11.55			
4-MEO-ALPHA-PVP	1000	8.04	99.82	3.25	-0.18	10-5000	0.5	10	N-ACETYL-3,4-MDMC	100		112.16	5.13	12.16			
	2000		93.33	5.21	-6.67					1000	9.24	110.78	4.36	10.78	10-5000	0.5	10
	5000		86.63	3.86	-13.37					2000		101.70	3.16	1.70			
	10		102.89	12.05	2.89					5000		93.77	3.47	-6.23			
	100		96.16	8.29	-3.84					10		97.24	9.74	-2.76			
	1000		89.59	7.30	-10.41					100		108.36	1.60	8.36			
4-MeOPBP	2000	6.93	81.63	2.40	-18.37	10-5000	0.5	10	NAPHYRONE	1000	10.08	111.02	4.69	11.02	10-5000	0.5	10
	5000		82.95	4.12	-17.05					2000		100.06	3.46	0.06			
	10		82.18	13.61	-17.82					5000		91.33	4.72	-8.67			
	100		107.51	5.04	7.51					10		101.56	18.53	1.56			
4-METHOXY PHENCYCLIDINE	1000	8.93	113.93	3.94	13.93	10-5000	0.5	10		100		111.72	5.24	11.72			
	2000		104.42	4.55	4.42				NAPHYRONE-1-NAPHTYL ISOMER	1000	9.61	113.29	2.96	13.29	10-5000	0.5	10
	5000		101.24	3.10	1.24					2000		108.51	3.26	8.51			
	10		88.91	7.39	-11.09					5000		98.14	3.88	-1.86			
	100		109.44	5.15	9.44					10		90.25	9.38	-9.75			
4-METHOXY PV8	1000	10.19	111.33	4.60	11.33	10-5000	0.5	10		100		111.51	7.15	11.51			
	2000		100.05	3.28	0.05				N-BENZYLNORBUTYLONE	1000	8.71	118.38	1.15	18.38	10-5000	0.5	10
	5000		90.84	5.61	-9.16					2000		111.24	5.23	11.24			
	10		84.42	8.29	-15.58					5000		101.34	3.28	1.34			
	100		113.48	6.57	13.48					10		91.97	6.65	-8.03			
4-METHOXY PV9	1000	11.13	118.17	3.76	18.17	10-5000	0.5	10		100		93.07	11.15	-6.93			
	2000		110.26	3.83	10.26				N-ETHYL-4-METHOXYAMPHETAMINE	1000	6.12	89.23	4.39	-10.77	10-5000	0.5	10
	5000		93.56	4.25	-6.44					2000		85.26	7.41	-14.74			
	100		105.15	8.15	5.15					5000		83.10	3.00	-16.90			
4-METHOXYMETHAMPHETAMINE (PMMA)	1000	5.69	105.31	10.18	5.31	100-5000	0.5	100		10		96.75	16.54	-3.25			
	5000		98.61	4.33	-1.39					100		102.31	7.11	2.31			
	10		81.31	13.46	-18.69				N-ETHYLBUPHEDRONE		5.82				10-5000	0.5	10
4-METHYL PENTEDRONE	100	8.30	93.27	6.74	-6.73	10-5000	0.5	10		1000		89.15	3.20	-10.85			
	1000		100.81	2.14	0.81					2000		85.77	5.07	-14.23			
										5000		87.75	5.41	-12.25			

	2000		92.22	5.99	-7.78												
	5000		86.51	4.54	-13.49												
4-METHYL-ALPHA-ETHYLAMINOBUTIOPHENONE	10	7.44	101.73	9.53	1.73	10-5000	0.5	10	N-ETHYL-N-METHYLCATHINONE	10	4.91	109.28	10.69	9.28	10-5000	0.5	10
	100		95.36	6.20	-4.64					100		111.15	6.84	11.15			
	1000		98.74	10.56	-1.26					1000		83.73	2.85	-16.27			
	2000		104.11	13.45	4.11					2000		79.58	5.11	-20.42			
	5000		90.86	7.49	-9.14					5000		87.05	4.31	-12.95			
4-METHYLAMPHETAMINE	10	6.71	100.60	11.50	0.60	10-5000	0.5	10	N-ETHYLNORDAZEPAM	100	12.89	100.52	7.60	0.52	100-5000	0.5	100
	100		95.14	12.28	-4.86					1000		117.70	3.58	17.70			
	1000		90.43	3.92	-9.57					5000		108.04	3.04	8.04			
	2000		84.95	2.26	-15.05				N-ETHYLNORKETAMINE	10	7.13	97.71	10.81	-2.30	10-5000	0.5	10
	5000		83.88	5.76	-16.12					100		95.86	8.04	-4.14			
4-METHYLCATHINONE	100	5.71	118.04	5.02	18.04	100-5000	0.5	100		1000		92.66	4.43	-7.34			
	1000		86.12	5.84	-13.88					2000		87.21	3.34	-12.79			
	5000		107.50	5.08	7.50					5000		87.03	7.71	-12.97			
4-METHYLMETHAMPHETAMINE (4-MMA)	100	6.88	80.08	6.56	-19.92	100-5000	0.5	100	N-ETHYLOXAZEPAM	100	12.25	94.36	6.73	-5.64	100-5000	0.5	100
	1000		91.70	5.75	-8.30					1000		116.62	3.10	16.62			
	5000		106.31	4.35	6.31					5000		111.99	5.74	11.99			
4-METHYLMETHCATHINONE (4-MMC)	100	6.01	116.89	6.36	16.89	100-5000	0.5	100	N-ETHYLPENTYLONE	100	7.51	108.63	1.62	8.63	100-5000	0.5	100
	1000		87.08	8.18	-12.92					1000		114.99	5.24	14.99			
	5000		81.26	12.40	-18.74					5000		103.47	4.59	3.47			
4-METHYL-N,N-DMC	10	6.04	92.86	10.44	-7.14	10-5000	0.5	10	NIMETAZEPAM	100	10.98	97.18	4.12	-2.82	100-5000	0.5	100
	100		91.79	5.29	-8.21					1000		114.50	6.83	14.50			
	1000		96.57	4.14	-3.43					5000		105.56	4.08	5.56			
	2000		90.86	4.56	-9.14				NITRACAINE	100	8.02	107.81	10.57	7.81	100-5000	0.5	100
	5000		91.95	5.04	-8.05					1000		115.46	7.67	15.46			
4-METHYL-N-METHYLBUPHEDRONE	10	7.10	91.67	10.92	-8.33	10-5000	0.5	10		5000		103.88	8.91	3.88			
	100		93.65	3.61	-6.35				NITRAZEPAM	100	10.62	82.78	9.40	-17.22	100-5000	0.5	100
	1000		97.15	6.77	-2.85					1000		117.69	3.47	17.69			
	2000		95.79	5.36	-4.21					5000		106.20	2.21	6.20			
	5000		101.63	15.94	1.63				NM2201	10	14.97	86.30	12.80	-13.70	10-1000	0.5	10
4-METHYL-N-METHYLHEXANOPHENONE	10	9.43	91.56	17.12	-8.44	10-5000	0.5	10		100		104.87	3.85	4.87			
	100		104.63	6.54	4.63					1000		118.73	4.29	18.73			
									N-METHYL-2AI	100	4.29	96.01	6.23	-3.99	100-5000	0.5	100
										1000		85.59	4.67	-14.41			

	1000		103.22	3.35	3.22			
	2000		97.18	3.57	-2.82			
	5000		94.72	2.93	-5.28			
4-METHYL-PBP	10	7.50	98.56	11.05	-1.44	10-5000	0.5	10
	100		100.20	7.58	0.20			
	1000		113.73	4.52	13.73			
	2000		118.50	3.17	18.50			
	5000		113.82	4.23	13.82			
4-METHYL-PHP	10	9.63	87.47	5.23	-12.53	10-5000	0.5	10
	100		100.73	7.57	0.73			
	1000		111.20	4.72	11.20			
	2000		100.00	2.02	0.00			
	5000		94.53	1.89	-5.47			
4-METHYL-α-ETHYLTRYPTAMINE	100	8.41	80.88	9.22	-19.12	100-5000	0.5	100
	1000		119.85	3.86	19.85			
	5000		112.13	4.67	12.13			
5-APB	100	7.03	105.00	9.03	5.00	100-5000	0.5	100
	1000		103.80	5.47	3.80			
	5000		89.13	2.68	-10.87			
5-APDB	100	5.66	115.00	10.40	15.00	100-5000	0.5	100
	1000		83.30	1.86	-16.70			
	5000		105.94	10.10	5.94			
5-APDI	10	8.73	89.59	10.21	-10.42	10-5000	0.5	10
	100		82.50	4.80	-17.50			
	1000		115.48	3.19	15.48			
	2000		105.44	3.38	5.44			
	5000		104.29	2.94	4.29			
5-CHLORO AB-PINACA	10	13.00	107.75	13.69	7.75	10-1000	0.5	10
	100		97.11	3.75	-2.89			
	1000		101.64	4.77	1.64			
5-CHLORO-NNEI	10	14.09	84.78	12.53	-15.22	10-1000	0.5	10
	100		107.12	8.70	7.12			
	1000		108.74	6.67	8.74			
5-EAPB	100	7.20	102.96	8.32	2.96	100-5000	0.5	100
	1000		108.36	11.05	8.36			
	5000		83.10	3.52	-16.90			
N-METHYL-PEA	10	3.73	115.26	1.90	15.26	10-100	0.5	10
	100		106.65	4.61	6.65			
	1000		42.25	1.61	-57.75			
	2000		39.30	1.51	-60.70			
	5000		43.90	3.25	-56.10			
N-METHYLTRYPTAMINE	100	4.82	110.75	5.30	10.75	100-5000	0.5	100
	1000		111.48	9.32	11.48			
	5000		97.58	4.78	-2.42			
NN-DMC	10	4.32	90.72	8.50	-9.28	10-5000	0.5	10
	100		97.27	4.83	-2.73			
	1000		103.23	7.04	3.23			
	2000		92.02	8.87	-7.98			
	5000		108.28	8.47	8.28			
NORCLOBAZAM	100	10.72	104.00	7.88	4.00	100-5000	0.5	100
	1000		109.35	2.10	9.35			
	5000		100.36	4.51	0.36			
NORCLOMIPRAMINE	100	11.77	110.55	4.95	10.55	100-5000	0.5	100
	1000		115.49	2.37	15.49			
	5000		100.35	6.55	0.35			
NORKETAMINE	100	6.45	109.21	11.01	9.21	100-5000	0.5	100
	1000		106.49	8.36	6.49			
	5000		94.10	4.87	-5.90			
NORTRIPTYLINE	100	11.06	117.35	5.49	17.35	100-5000	0.5	100
	1000		114.77	6.10	14.77			
	5000		109.00	4.11	9.00			
N-PROPYLAMPHETAMINE	100	6.69	105.67	6.06	5.67	100-5000	0.5	100
	1000		111.48	3.22	11.48			
	5000		109.62	5.73	9.62			
NRG-3	10	9.84	98.75	12.73	-1.25	10-5000	0.5	10
	100		108.82	9.16	8.82			
	1000		113.40	2.74	13.40			
	2000		106.53	3.00	6.53			
	5000		100.14	2.34	0.14			
o-CPP	10	6.80	147.17	9.29	47.17		0.5	1000

	5000		106.71	3.84	6.71					100		101.23	10.48	1.23			
5F-ABICA	10	12.12	81.39	18.49	-18.61	10-1000	0.5	10		1000		91.15	4.65	-8.85	1000-5000		
	100		95.68	7.08	-4.32					2000		83.26	4.14	-16.74			
	1000		95.99	7.75	-4.01					5000		82.68	2.48	-17.32			
5-F-JWH-018 ADAMANTYL ANALOG	10	15.31	84.84	5.55	-15.16	10-1000	0.5	10		10		82.98	2.21	-17.02			
	100		102.51	5.09	2.51				OCTACAINE	100	6.11	96.47	11.36	-3.53	10-5000	0.5	10
	1000		113.24	3.36	13.24					1000		96.44	2.79	-3.56			
5-FLUORO THJ	10	15.13	98.77	17.61	-1.23	10-1000	0.5	10		2000		93.11	3.31	-6.89			
	100		94.72	10.60	-5.28					5000		89.93	3.56	-10.07			
	1000		102.45	6.61	2.45					10		119.33	6.07	19.33			
5-FLUORO-2-ADB-PINACA ISOMER 2	10	12.30	88.09	10.32	-11.91	10-1000	0.5	10	ORG-28611	100	11.56	92.44	5.14	-7.56	10-1000	0.5	10
	100		103.32	6.06	3.32					1000		94.24	7.29	-5.76			
	1000		113.20	4.19	13.20					100		109.42	9.48	9.42			
5-FLUORO-CUMYL-PICA	10	13.78	88.29	10.30	-11.71	10-1000	0.5	10	OXAZEPAM	1000	11.37	117.47	5.67	17.47	100-5000	0.5	100
	100		106.06	7.51	6.06					5000		101.31	6.80	1.31			
	1000		106.85	6.54	6.85					10		5.65	169.40	-94.35			
5-FLUORO-SDB-006	10	13.05	95.74	13.20	-4.26	10-1000	0.5	10		100		147.73	72.88	47.73			
	100		96.52	3.92	-3.48				OXYMORPHONE	1000	2.65	35.12	46.60	-64.88	-	0.5	-
	1000		92.63	2.53	-7.37					2000		33.48	45.94	-66.52			
5-F-PENTYL-3-PYRIDINOYLINDOLE	10	12.12	95.28	10.58	-4.72	10-1000	0.5	10		5000		43.63	3.87	-56.37			
	100		103.95	5.81	3.95					100		117.86	3.72	17.86			
	1000		110.11	7.10	10.11				PARACETAMOL	1000	3.93	87.76	9.13	-12.24	100-5000	0.5	100
5F-SDB-005	10	14.79	90.33	11.99	-9.67	10-1000	0.5	10		5000		107.59	4.52	7.59			
	100		106.27	9.61	6.27					100		100.38	7.68	0.38			
	1000		100.72	7.57	0.72				PAROXETINE	1000	10.58	117.00	6.51	17.00	100-5000	0.5	100
5-HYDROXY DMT	100	2.99	116.19	4.59	16.19	-	0.5	-		5000		100.53	3.04	0.53			
	1000		60.52	4.81	-39.48					10		92.89	6.83	-7.11			
	5000		58.69	3.21	-41.31					100		104.36	6.53	4.36			
5-IT	100	5.08	99.99	6.72	-0.01	100-5000	0.5	100	PCEEA	1000	9.18	108.41	2.24	8.41	10-5000	0.5	10
	1000		97.99	7.59	-2.01					2000		100.90	5.03	0.90			
	5000		80.98	3.38	-19.02					5000		94.17	5.25	-5.83			
5-MAPB	100	6.71	111.27	6.02	11.27		0.5	100	PCMPA	10	8.96	87.59	2.62	-12.42	10-5000	0.5	10

	1000		99.04	6.52	-0.96	100-5000				100		96.51	7.48	-3.49			
	5000		107.91	2.76	7.91					1000		99.55	5.31	-0.45			
	10		76.41	13.27	-23.59					2000		94.67	8.91	-5.33			
	100		110.09	6.19	10.09					5000		89.00	6.51	-11.00			
5-MAPDB	1000	5.69	88.41	3.07	-11.59	100-5000	0.5	100		10		100.37	13.36	0.37			
	2000		84.51	6.11	-15.49				PCPr	100	9.06	92.95	5.11	-7.05	10-5000	0.5	10
	5000		93.31	3.05	-6.69					1000		92.12	3.00	-7.88			
	10		85.16	18.67	-14.84					2000		85.58	4.11	-14.42			
	100		98.61	11.88	-1.39					5000		86.58	4.01	-13.42			
5-MeO-ALPHA-ET	1000	7.09	106.65	5.97	6.65	10-5000	0.5	10		100		108.54	7.17	8.54			
	2000		99.27	2.50	-0.73				PENTEDRONE	1000	6.85	96.09	11.40	-3.91	100-5000	0.5	100
	5000		95.13	3.36	-4.87					5000		111.73	6.58	11.73			
	100		106.99	14.71	6.99					100		112.38	3.90	12.38			
5-MeO-DALT	1000	7.31	108.50	4.98	8.50	100-5000	0.5	100	PENTEDRONE METABOLITE	1000	6.90	113.73	3.13	13.73	100-5000	0.5	100
	5000		100.13	5.10	0.13					5000		100.12	7.15	0.12			
	100		113.40	4.37	13.40					100		111.26	4.77	11.26			
5-METHOXY AMT	1000	6.02	93.42	9.54	-6.58	100-5000	0.5	100	PENTYLONE (bk-MBDP)	1000	7.21	117.39	5.54	17.39	100-5000	0.5	100
	5000		110.80	4.11	10.80					5000		112.89	5.25	12.89			
	100		106.11	6.89	6.11					100		98.44	6.73	-1.56			
5-METHOXY DiPT	1000	7.32	112.44	7.31	12.44	100-5000	0.5	100	PHENAZEPAM	1000	12.14	117.39	1.09	17.39	100-5000	0.5	100
	5000		109.38	2.75	9.38					5000		110.47	2.59	10.47			
	100		102.40	11.28	2.40					100		100.69	7.29	0.69			
5-METHOXY DMT	1000	5.34	97.36	8.45	-2.64	100-5000	0.5	100	PHENCYCLIDINE (PCP)	1000	8.55	115.73	6.22	15.73	100-5000	0.5	100
	5000		96.67	6.05	-3.33					5000		103.66	3.46	3.66			
	10		113.16	8.84	13.16					100		104.58	7.71	4.58			
	100		115.83	2.97	15.83					1000		112.96	6.20	12.96			
	1000		79.77	4.00	-20.23				PHENOBARBITAL	5000	8.44	107.70	5.99	7.70	100-5000	0.5	100
5-METHOXY METHYLONE	2000	5.57	71.44	5.43	-28.56	10-5000	0.5	10									
	5000		82.75	4.57	-17.25					100		114.42	7.26	14.42			
	100		101.57	11.70	1.57				PHENTERMINE	1000	5.98	110.62	5.41	10.62	100-5000	0.5	100
5-METHOXY MiPT	1000	6.32	110.39	6.36	10.39	100-5000	0.5	100		5000		108.50	5.39	8.50			
	5000		103.42	4.49	3.42					100		95.37	6.41	-4.63			
	100		91.98	10.55	-8.02				PHENYTOIN	1000	10.21	117.96	4.32	17.96	100-5000	0.5	100
	1000									5000		103.63	5.34	3.63			
6-APB		6.51	107.58	11.02	7.58	100-5000	0.5	100		10		83.57	13.73	-16.43			
	5000		112.56	8.72	12.56				PRAVADOLINE	100	10.24	100.31	5.95	0.31	10-5000	0.5	10

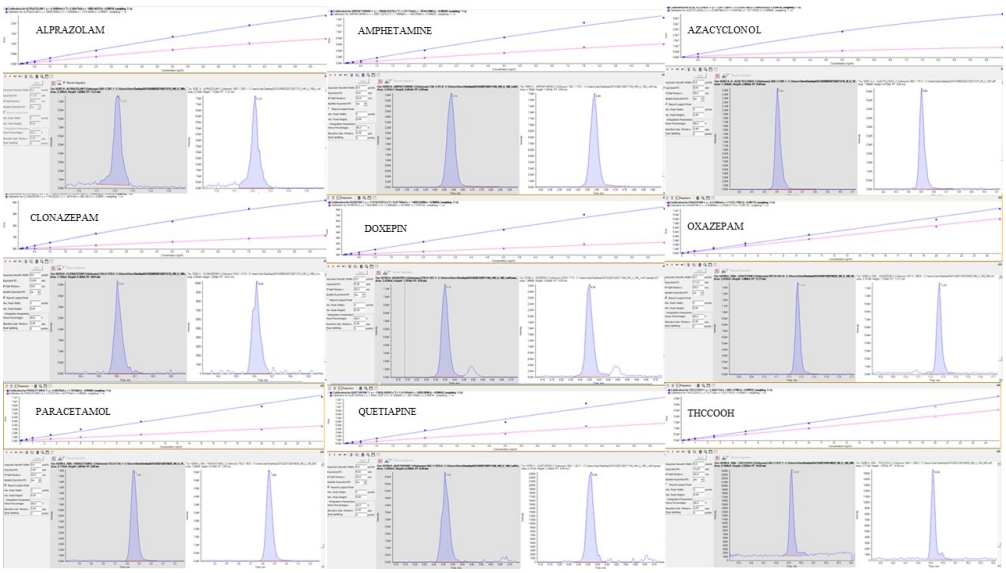
6-APDB	10	6.06	101.29	15.06	1.29	10-5000	0.5	10	PRAZEPAM	1000	13.52	105.43	8.76	5.43	100-5000	0.5	100
	100		108.44	12.18	8.44					2000		102.46	5.88	2.46			
	1000		91.30	17.97	-8.70					5000		92.26	5.79	-7.74			
	2000		96.56	6.52	-3.44					100		110.20	2.42	10.20			
	5000		94.17	10.36	-5.83					1000		113.83	4.77	13.83			
6-BROMO-MDMA	10	7.48	85.92	3.71	-14.08	10-5000	0.5	10	PREGABALIN	5000	4.62	94.23	2.21	-5.77	100-5000	0.5	100
	100		111.90	7.53	11.90					100		100.91	6.45	0.91			
	1000		111.65	4.41	11.65					1000		106.20	5.41	6.20			
	2000		100.93	4.12	0.93					5000		89.59	6.30	-10.41			
	5000		99.38	3.16	-0.62					100		101.57	7.15	1.57			
6-CHLORO-MDMA	10	7.08	82.67	9.88	-17.33	10-5000	0.5	10	PROCAINE	1000	4.20	84.87	5.66	-15.13	100-5000	0.5	100
	100		108.18	4.00	8.18					5000		82.94	5.28	-17.06			
	1000		104.70	4.27	4.70					100		101.12	6.74	1.12			
	2000		97.58	4.68	-2.42					1000		105.54	2.97	5.54			
	5000		94.20	2.75	-5.80					5000		105.36	4.85	5.36			
6-EAPB	10	7.03	99.06	9.71	-0.94	10-5000	0.5	10	PROMETHAZINE	100	10.22	108.21	5.76	8.21	100-5000	0.5	100
	100		107.52	11.50	7.52					1000		116.84	4.18	16.84			
	1000		110.57	7.70	10.57					5000		101.43	3.57	1.43			
	2000		94.46	8.54	-5.54					100		108.05	4.00	8.05			
	5000		90.09	5.44	-9.91				PROPAFENONE	1000	10.71	112.19	4.29	12.19	100-5000	0.5	100
6-IT	10	5.88	99.70	9.14	-0.30	10-5000	0.5	10		5000		98.15	5.61	-1.85			
	100		105.87	8.50	5.87					100		110.19	7.56	10.19			
	1000		86.17	5.69	-13.83				PROPRANOLOL	1000	9.12	105.71	6.54	5.71	100-5000	0.5	100
	2000		98.46	2.54	-1.54					5000		104.83	7.67	4.83			
	5000		93.30	5.60	-6.70					100		97.80	6.92	-2.20			
6-MAM	100	5.20	114.29	7.19	14.29	100-5000	0.5	100	PROPYLHEXEDRINE	1000	8.04	113.42	5.95	13.42	100-5000	0.5	100
	1000		98.84	5.78	-1.16					5000		111.16	3.02	11.16			
	5000		82.93	5.05	-17.07				PSB-SB-1202	10	15.97	91.11	7.57	-8.90	10-1000	0.5	10
6-MAPB	10	6.58	96.62	15.25	-3.38	10-5000	0.5	10		100		79.82	10.34	-20.18			
	100		92.41	16.31	-7.59					1000		119.68	2.35	19.68			
	1000		104.24	12.76	4.24				PTI-1	10	12.53	110.07	3.54	10.07	10-1000	0.5	10
	2000		99.41	15.80	-0.59					100		97.71	7.01	-2.29			
	5000		95.27	12.59	-4.73					1000		102.34	8.19	2.34			
7-AMINOCLONAZEPAM	100	6.68	108.53	7.03	8.53	100-5000	0.5	100	PTI-2	10	12.78	97.95	4.88	-2.05	10-1000	0.5	10
	1000		108.11	11.14	8.11					100		95.76	4.93	-4.24			
	5000		105.76	5.88	5.76					1000		101.06	3.39	1.06			
7-AMINODESMETHYLFLUNITRAZEPAM	100	5.71	93.53	9.85	-6.48	100-5000	0.5	100	PV-8	100	9.71	105.25	7.32	5.25	100-5000	0.5	100
	1000		116.37	7.36	16.37					1000		111.01	1.37	11.01			

	5000		99.36	11.60	-0.64					5000		102.80	3.76	2.80			
7-AMINOFLUNITRAZEPAM	100	7.72	81.75	6.26	-18.25	100-5000	0.5	100	PV9	10	10.70	81.33	19.03	-18.67	10-5000	0.5	10
	1000		118.25	3.85	18.25					100		110.02	4.96	10.02			
	5000		112.42	4.09	12.42					1000		115.64	3.98	15.64			
7-AMINONITRAZEPAM	100	4.74	103.17	9.18	3.17	100-5000	0.5	100		2000		107.84	3.54	7.84			
	1000		106.13	4.58	6.13					5000		90.93	7.68	-9.07			
	5000		102.03	4.88	2.03				PX-2	10	12.76	104.96	6.72	4.96	10-1000	0.5	10
7-APB	10	6.70	89.46	4.81	-10.54	10-5000	0.5	10		100		101.24	6.05	1.24			
	100		105.88	5.41	5.88					1000		109.39	4.70	9.39			
	1000		96.06	7.51	-3.94				PYRAZOLAM	100	9.50	92.36	3.30	-7.64	100-5000	0.5	100
	2000		86.69	5.83	-13.31					1000		116.40	3.41	16.40			
	5000		90.85	3.29	-9.15					5000		113.52	3.74	13.52			
7-APDB	10	5.99	92.60	14.66	-7.40	10-5000	0.5	10	QUETIAPINE	100	9.62	98.77	8.05	-1.23	100-5000	0.5	100
	100		100.21	11.41	0.21					1000		113.67	3.47	13.67			
	1000		89.11	8.02	-10.89					5000		101.31	3.71	1.31			
	2000		80.54	0.87	-19.46				RH-34	10	8.13	85.32	15.76	-14.68	10-5000	0.5	10
	5000		82.63	7.95	-17.37					100		106.34	8.24	6.34			
A-834735	10	14.21	95.17	5.06	-4.83	10-1000	0.5	10		1000		112.00	4.25	12.00			
	100		98.04	9.92	-1.96					2000		105.06	4.18	5.06			
	1000		100.87	5.65	0.87					5000		96.14	2.88	-3.86			
A-836339	10	12.46	105.15	6.14	5.15	10-1000	0.5	10	R-MMC	10	6.88	42.31	73.89	-57.70	100-5000	0.5	100
	100		104.57	5.47	4.57					100		100.86	14.64	0.86			
	1000		100.82	1.48	0.82					1000		103.67	6.70	3.67			
AB-FUBINACA	10	12.67	91.35	10.71	-8.65	10-1000	0.5	10		2000		94.44	6.08	-5.56			
	100		106.65	7.10	6.65					5000		89.34	5.21	-10.66			
	1000		115.66	3.78	15.66					100		109.16	9.75	9.16			
AB-FUBINACA 2-FLUOROBENZYL ISOMER	10	12.86	102.33	9.53	2.33	10-1000	0.5	10	SCOPOLAMINE	1000	4.80	92.60	6.73	-7.40	100-5000	0.5	100
	100		107.69	7.19	7.69					5000		82.01	8.44	-17.99			
	1000		101.93	5.66	1.93					10		95.00	14.03	-5.00			
AB-FUBINACA 3-FLUOROBENZYL ISOMER	10	12.76	100.00	8.11	0.00	10-1000	0.5	10	SDB-005	100	15.57	87.95	12.63	-12.05	10-1000	0.5	10
	100		100.83	4.38	0.83					1000		113.06	4.17	13.06			
	1000		102.16	7.06	2.16					10		100.19	7.73	0.19			
ADB-PINACA ISOMER 1	10	13.69	107.09	9.45	7.09	10-1000	0.5	10	SDB-006	100	14.09	103.88	6.08	3.88	10-1000	0.5	10
	100		104.71	8.04	4.71					1000		99.16	4.45	-0.84			

	1000		105.00	7.38	5.00					100		104.51	7.31	4.51			
	10		101.84	10.34	1.84				SERTRALINE	1000	11.57	106.81	6.82	6.81	100-5000	0.5	100
ADB-PINACA ISOMER 2	100	13.99	100.32	3.82	0.32	10-1000	0.5	10		5000		96.09	8.67	-3.91			
	1000		100.49	9.52	0.49					100		104.31	3.18	4.31			
	10		95.21	21.17	-4.79				SILDENAFIL	1000	10.34	114.91	6.00	14.91	100-5000	0.5	100
ADB-PINACA ISOMER 3	100	14.2	99.21	5.03	-0.79	10-1000	0.5	10		5000		101.54	6.80	1.54			
	1000		102.45	8.04	2.45					100		113.37	4.26	13.37			
	10		115.88	10.33	15.88				STANOZOLOL	1000	14.13	116.68	3.79	16.68	100-5000	0.5	100
ADB-PINACA ISOMER 4	100	13.99	90.15	9.00	-9.85	10-1000	0.5	10		5000		98.40	3.76	-1.60			
	1000		100.62	10.35	0.62					10		91.50	10.42	-8.50			
	100		102.40	7.44	2.40					100		108.05	8.23	8.05			
AH-7921	1000	9.79	104.79	4.52	4.79	100-5000	0.5	100	TAPENTADOL	1000	7.33	104.07	6.55	4.07	10-5000	0.5	10
	5000		105.38	3.65	5.38					2000		91.70	3.74	-8.30			
	10		88.67	4.44	-11.33					5000		86.99	2.63	-13.01			
AKB48_N-(4-FLUOROBENZYL) ANALOG	100	15.64	99.91	6.55	-0.09	10-1000	0.5	10		100		91.84	15.71	-8.16			
	1000		115.88	3.50	15.88				TEMAZEPAM	1000	11.68	116.15	7.32	16.15	100-5000	0.5	100
	100		98.00	8.49	-2.00					5000		97.65	3.86	-2.35			
ALFA-ETHYLAMINOPENTIOPHENONE	1000	7.14	108.63	4.46	8.63	100-5000	0.5	100		10		106.05	7.32	6.05			
	5000		105.60	3.97	5.60					100		104.31	10.13	4.31			
	100		99.57	4.26	-0.43				TETRACAINE	1000	9.03	110.46	2.96	10.46	10-5000	0.5	10
ALFA-PROPYLAMINOPENTIOPHENONE	1000	7.90	113.60	5.44	13.60	100-5000	0.5	100		2000		99.99	3.58	-0.01			
	5000		108.99	4.40	8.99					5000		89.32	6.07	-10.68			
	10		108.17	15.31	8.17					10		93.71	12.28	-6.29			
	100		93.92	14.22	-6.08					100		102.17	5.64	2.17			
ALLYLESCALINE	1000	7.40	86.48	5.90	-13.52	10-5000	0.5	10	THIOPROPAMINE	1000	3.76	33.28	3.80	-66.72	10-100	0.5	10
	2000		94.99	8.85	-5.01					2000		31.96	2.78	-68.04			
	5000		88.12	6.16	-11.88					5000		36.65	5.45	-63.35			
	10		100.07	12.03	0.07					10		86.72	9.37	-13.28			
	100		99.52	12.20	-0.48				THJ	100	15.97	88.48	6.42	-11.52	10-1000	0.5	10
	1000		98.12	8.30	-1.88					1000		119.02	2.71	19.02			
ALPHA-DIMETHYLAMINOPENTIOPHENONE	2000	6.87	92.07	9.97	-7.93	10-5000	0.5	10		10		103.09	14.74	3.09			
	5000		88.69	5.22	-11.31				TILETAMINE	100	5.70	99.14	15.19	-0.86	10-5000	0.5	10
	10		101.28	10.37	1.28					1000		73.38	3.24	-26.62			
ALPHA-ETHYLAMINOHEXANOPHENONE	100	8.42	107.36	7.85	7.36	10-5000	0.5	10		2000		70.12	6.13	-29.88			
	1000		112.51	4.69	12.51					5000		81.32	5.22	-18.68			

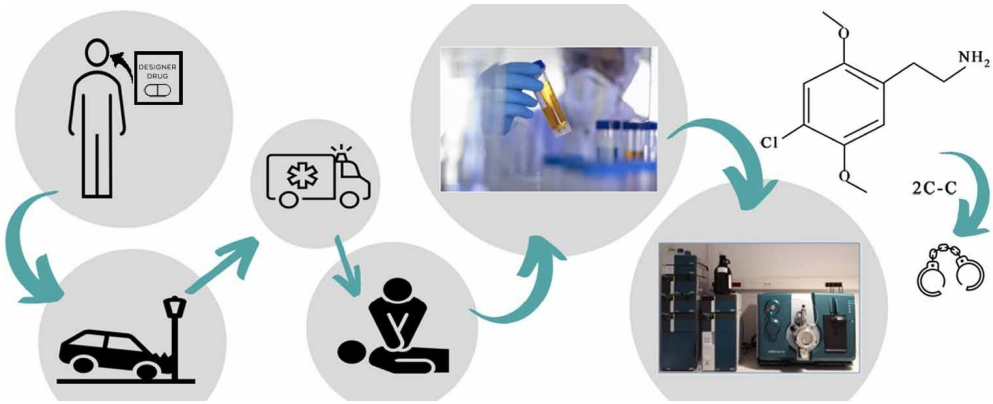
	2000		108.28	5.19	8.28					100		113.17	5.70	13.17			
	5000		100.04	4.73	0.04				TRAMADOL	1000	6.96	105.47	4.65	5.47	100-5000	0.5	100
	100		103.36	2.53	3.36					5000		106.85	6.29	6.85			
ALPHA-ETHYLTRYPTAMINE	1000	7.14	99.23	11.83	-0.77	100-5000	0.5	100		100		112.03	5.02	12.03			
	5000		106.06	2.38	6.06				TRAZODONE	1000	8.39	100.69	7.65	0.69	100-5000	0.5	100
	100		90.67	11.89	-9.33					5000		86.79	6.49	-13.21			
ALPHA-METHYLTRYPTAMINE	1000	5.77	104.08	7.57	4.08	100-5000	0.5	100		100		97.70	6.47	-2.30			
	5000		97.46	5.78	-2.54				TRIAZOLAM	1000	11.46	114.93	4.94	14.93	100-5000	0.5	100
	10		93.22	9.55	-6.78					5000		101.42	6.96	1.42			
	100		104.06	5.66	4.06					100		107.72	9.07	7.72			
ALPHA-PHP	1000	8.43	100.67	4.59	0.67	10-5000	0.5	10	TRIMIPRAMINE	1000	11.02	110.81	7.38	10.81	100-5000	0.5	100
	2000		95.54	2.03	-4.46					5000		100.68	2.54	0.68			
	5000		91.54	3.94	-8.46					10		78.52	2.60	-21.48			
	10		84.85	11.24	-15.15					100		113.25	4.22	13.25			
	100		114.19	5.01	14.19				U-47700	1000	9.13	111.77	5.67	11.77	10-5000	0.5	10
ALPHA-PHTALIMIDOPROPIOPHENONE	1000	11.76	114.06	3.59	14.06	10-5000	0.5	10		2000		102.48	6.93	2.48			
	2000		103.91	2.48	3.91					5000		95.35	2.57	-4.65			
	5000		89.53	3.32	-10.47					10		83.89	5.74	-16.11			
	10		92.70	6.30	-7.30					100		103.67	5.43	3.67			
	100		95.67	3.97	-4.33				W-15	1000	13.31	109.84	6.40	9.84	10-5000	0.5	10
	1000		94.28	5.17	-5.72					2000		98.01	5.34	-1.99			
ALPHA-PIPBP	2000	6.53	87.85	2.97	-12.15	10-5000	0.5	10		5000		98.68	8.19	-1.32			
	5000		83.12	4.35	-16.88					10		86.55	13.93	-13.45			
	10		93.49	11.39	-6.51				WIN 54,461	100	12.41	97.27	5.99	-2.73	10-1000	0.5	10
	100		97.85	9.59	-2.15					1000		99.27	3.84	-0.73			
	1000		66.80	3.50	-33.20					10		104.91	11.03	4.91			
ALPHA-PPP	2000	5.06	60.86	4.62	-39.14	10-100	0.5	10	WIN 55,212-2	100	13.65	95.03	4.94	-4.97	10-1000	0.5	10
	5000		57.78	43.31	-42.22					1000		91.09	7.43	-8.91			
	100		96.93	7.01	-3.07					10		93.26	17.46	-6.74			
ALPHA-PVP	1000	7.29	103.95	6.41	3.95	100-5000	0.5	100	XLR12	100	14.79	88.36	13.27	-11.64	10-1000	0.5	10
	5000		102.47	3.67	2.47					1000		102.64	7.70	2.64			
	100		104.43	4.50	4.43					10		103.43	11.54	3.43			
ALPHA-PVT	1000	6.39	108.04	7.41	8.04	100-5000	0.5	100	YANGONIN	100	11.88	93.63	7.51	-6.37	10-5000	0.5	10
	5000		105.33	5.04	5.33					1000		124.42	2.82	24.42			

ALPHA-PYRROLIDINOBUTHIOPHENONE	10	5.00	114.54	6.79	14.54	10-5000	0.5	10	ZALEPLON	2000	10.05	113.23	4.65	13.23	100-5000	0.5	100
	100		114.55	4.66	14.55					5000		117.56	3.14	17.56			
	1000		76.60	4.86	-23.40					100		93.55	10.23	-6.45			
	2000		71.51	5.06	-28.49					1000		110.49	5.04	10.49			
	5000		82.28	3.03	-17.72					5000		109.79	4.50	9.79			
ALPRAZOLAM	100	11.46	97.10	7.57	-2.90	100-5000	0.5	100	ZOLPIDEM	100	7.96	97.13	6.56	-2.87	100-5000	0.5	100
	1000		113.79	7.29	13.79					1000		115.31	10.06	15.31			
	5000		116.73	3.51	16.73					5000		111.64	2.68	11.64			
AM1220	10	10.52	116.60	5.87	16.60	10-1000	0.5	10	ZOPICLONE	100	6.84	111.10	4.25	11.10	100-5000	0.5	100
	100		97.82	3.75	-2.18					1000		115.86	5.11	15.86			
	1000		97.65	4.44	-2.35					5000		87.28	6.06	-12.72			
AM2201 8-QUINOLINYL CARBOXAMIDE	10	14.98	96.74	15.14	-3.26	10-1000	0.5	10	ZUCLOPENTHIXOL	100	12.20	100.16	7.08	0.16	100-5000	0.5	100
	100		95.26	6.36	-4.74					1000		118.63	2.39	18.63			
	1000		117.12	5.14	17.12					5000		107.20	5.84	7.20			
AM2201 BENZIMIDAZOLE ANALOG	10	14.45	119.43	6.98	19.43	10-1000	0.5	10	α-HYDROXYMIDAZOLAM	100	10.07	98.17	8.20	-1.83	100-5000	0.5	100
	100		94.22	5.78	-5.78					1000		116.20	3.82	16.20			
	1000		86.15	7.63	-13.85					5000		100.10	5.12	0.10			
AM2232	10	12.76	98.69	7.33	-1.31	10-1000	0.5	10									
	100		93.70	5.56	-6.30												
	1000		95.30	5.46	-4.70												



The calibration curves in matrix and chromatograms of substances detected in real samples.

338x190mm (96 x 96 DPI)



Graphical abstract

541x214mm (72 x 72 DPI)

6 Podsumowanie i wnioski

Badania przeprowadzone w ramach pracy doktorskiej umożliwiły opracowanie zaawansowanych metod analitycznych umożliwiających oznaczenie ponad 500 substancji psychoaktywnych, w tym nowych substancji psychoaktywnych (NPS), leków oraz ich metabolitów w matrycach biologicznych takich jak krew, mocz i włosy. Dzięki zastosowaniu techniki chromatografii cieczowej sprzężonej z tandemową spektrometrią mas (LC-MS/MS) możliwe było jednoczesne rozdzielenie i zidentyfikowanie tak dużej liczby analitów podczas jednej analizy. Opracowane metody cechują się nie tylko wysoką skutecznością, ale także elastycznością, umożliwiając łatwe przystosowanie do różnych matryc biologicznych. Wyniki badań wskazują na duży potencjał dalszego rozwoju tych metod, zarówno pod kątem zwiększenia liczby analizowanych substancji, jak i automatyzacji procesu analitycznego.

Na podstawie uzyskanych wyników można wysunąć następujące wnioski:

1. opracowane metodyki wyodrębniania i oznaczania wybranych analitów pozwalają na ich precyzyjną identyfikację - odpowiednio dobrane parametry pracy spektrometru mas, dostosowane do poszczególnych analitów, pozwoliły na skuteczną identyfikację wszystkich badanych związków. Wysoka czułość i selektywność spektrometru umożliwiły dokładne określenie obecności i stężenia substancji w analizowanych matrycach biologicznych,
2. optymalne rozdzielenie uzyskano badanych analitów w czasie 30 minut osiągnięto przy użyciu kolumny chromatograficznej Kinetex C18 (Phenomenex, 3,0 x 100 mm; 2,6 µm) przy fazie ruchomej składającej się z metanolu i wody z dodatkiem 2 mM mrówczanu amonu oraz 0,1% kwasu mrówkowego, co zapewniło odpowiednie warunki separacji dla szerokiego zakresu substancji psychoaktywnych,
3. opracowane metody analityczne pozwoliły na wyznaczenie zakresów liniowości w zależności od rodzaju matrycy:
    - krew: 0,05-50 ng/ml dla większości analitów, 1-200 ng/ml dla THC, 2-200 ng/ml dla kannabinoidów i syntetycznych kannabinoidów, oraz 10-1000 ng/ml dla pozostałych analitów.
    - mocz: 0,5-5000 ng/ml, co pozwala na wykrywanie substancji w szerokim zakresie stężeń.
    - włosy: 0,025-1,35 ng/mg dla kannabinoidów i 0,125-5 ng/mg dla pozostałych analitów, co umożliwia analizę nawet bardzo niskich stężeń substancji.

4. wyznaczone granice oznaczalności badanych analitów są na bardzo niskich poziomach stężeń, co jest kluczowe dla dokładnej analizy śladów substancji w próbkach biologicznych:
    - Krew: 1-200 ng/ml, umożliwiając wykrywanie zarówno niskich, jak i wysokich stężeń substancji.
    - Mocz: 10-100 ng/ml, co jest odpowiednie dla szerokiego zakresu badań toksykologicznych.
    - Włosy: 0,025-1,5 ng/mg, co jest szczególnie ważne w analizach retrospektywnych,
5. dzięki możliwości analizowania różnych matryc biologicznych (krew, mocz, włosy), opracowane metody pozwalają na weryfikację próbek pochodzących od jednej osoby. Umożliwia to badanie ścieżek metabolicznych substancji psychoaktywnych oraz prowadzenie badań retrospektywnych na podstawie próbek włosów, co jest szczególnie przydatne w kontekście długoterminowego monitorowania zażywania substancji,
6. opracowane metody analityczne zostały z sukcesem wdrożone do rutynowych analiz w Instytucie Genetyki Sądowej w Bydgoszczy. Wdrożenie to potwierdza praktyczną wartość opracowanych metod oraz ich zgodność z wymaganiami i standardami obowiązującymi w laboratoriach analitycznych. Potwierdzeniem skuteczności opracowanych metod jest również zgłoszenie patentowe, które dokumentuje innowacyjność i unikalność podejścia zastosowanego w ramach rozprawy doktorskiej.

7 Bibliografia

1. The European Parliament and the Council of the European Union Directive (EU) 2017/2103 of the European Parliament and of the Council of 15 November 2017 Amending Council Framework Decision 2004/757/JHA in order to Include New Psychoactive Substances in the Definition of 'Drug' and Repealing Council Decision 2005/387. Available online: http://data.europa.eu/eli/dir/2017/2103/oj (z dnia 30.04.2023).
2. Varì, M.R.; Mannocchi, G.; Tittarelli, R.; Campanozzi, L.L.; Nittari, G.; Feola, A.; Ronchi, F.U.; Ricci, G. New Psychoactive Substances: Evolution in the Exchange of Information and Innovative Legal Responses in the European Union. Int J Environ Res Public Health, 2020, 17, 8704.
3. United Nations Office on Drugs and Crime What are NPS? Available online: https://www.unodc.org/LSS/Page/NPS (z dnia 30.04.2023).
4. Nelson, M.E.; Bryant, S.M.; Aks, S.E. Emerging Drugs of Abuse. Emerg Med Clin N Am, 2014, 32, 1–28.
5. Graziano, S., Anzillotti, L, Mannocchi, G., Pichini, S., Busard`, F.P., Screening methods for rapid determination of new psychoactive substances (NPS) in conventional and non-conventional biological matrices, J Pharm Biomed Anal, 2019, 163, 170-179
6. Czarny, J.; Galant, N.; Raczkowski, M., Zbytniewski, R., Podgrudna, P., Herman, R., Michałowska, E., Czarny, Z., Kubiak, K., Powierska-Czarny, J. Comparison of screening with the use of Biochip Array Technology to the direct analysis of 521 psychoactive compounds and their residues with the use of LC-MS/MS method – does it mean the end of an era for immunochemical research? 2022, Toxicol Anal Clin 34(3):S104-S105
7. Szukalski, B. Analiza substancji psychoaktywnych w materiale biologicznym. Alkoholik Narkoman, 2001,14 (l): 151–163.
8. Maher, W.A., Pianca, D.J., Apollonio, L.G., Whittall, I.R., Kyd, J.M. Matrix effect and cross-reactivity of select amphetamine-type substances, designer analogues, and putrefactive amines using the bio-quant direct ELISA presumptive assays for amphetamine and methamphetamine. J Anal Toxicol, 2007, 31(4):208–213.
9. Kerrigan, S., Banuelos, S., Perrella, L., Hardy, B. Simultaneous detection of ten psychedelic phenethylamines in urine by gas chromatography-mass spectrometry. J Anal Toxicol, 2011, 35(7):459–469.
10. Kerrigan, S., Mellon, M.B., Banuelos, S., Arndt, C. Evaluation of commercial enzyme-linked immunosorbent assays to identify psychedelic phenethylamines. J Anal Toxicol, 2011, 35(7):444–451.
11. Nieddu, M., Trignano, C., Burrai L., Pirisi, M.A., Boatto, G. Cross-reactivities of 41 new amphetamine designer drugs to EMIT®immunoassays. Forensic Toxicol, 2013, 31(1):133–137.
12. Nieddu, M., Burrai, L., Trignano, C., Boatto, G. Cross-reactivities of 39 new amphetamine designer drugs on three abuse drugs urinary screening tests. Forensic Toxicol, 2014a, 32(1):132–138.
13. Nieddu, M., Burrai, L., Trignano, C., Boatto, G. Evaluation of commercial multi-drug oral fluid devices to identify 39 new amphetamine-designer drugs. Leg Med.,2014b, 16(2):106–109.
14. Swortwood, M.J., Hearn, W.L., Decaprio, A.P. Cross-reactivity of designer drugs, including cathinone derivatives, in commercial enzyme-linked immunosorbent assays. Drug Test Analysis, 2014, 6(7–8):716–727.
15. Nieddu, M.,, Burrai L., Baralla, E., Pasciu, V., Varoni, M.V., Briguglio, I., Demontis, M.P., Boatto, G. ELISA detection of 30 new amphetamine designer drugs in whole blood, urine and oral fluid using neogen® "amphetamine" and "methamphetamine/MDMA" kits. J Anal Toxicol, 2016, 40(7):492–497.

16. Scheidweiler, K.B., Jarvis, M.J.Y., Marilyn, A.H. Nontargeted SWATH acquisition for identifying 47 synthetic cannabinoid metabolites in human urine by liquid chromatography-high-resolution tandem mass spectrometry. Anal Bioanal Chem, 2015, 407(3):883–897.
17. Regester, L..E, Chmiel, J.D., Holler, J.M., Vorce, S.P., Levine, B., Bosy, T.Z.. Determination of designer drug cross-reactivity on five commercial immunoassay screening kits. J Anal Toxicol, 2015, 39(2):144–151.
18. O'Connor, L.C., Torrance, H..J, McKeown, D.A. ELISA detection of phenazepam, etizolam, pyrazolam, flubromazepam, diclazepam and delorazepam in blood using Immunalysis® Benzodiazepine kit. J Anal Toxicol, 2016, 40(2):159–161
19. Papoutsis, I.I., Athanaselis, S.A., Nikolaou, P.D., Pistos, C.M., Spiliopoulou, C.A.,, Maravelia s, C.P. Development and validation of an EI-GC-MS method for the determination of benzodiazepine drugs and their metabolites in blood: applications in clinical and forensic toxicology. J Pharm Biomed Anal, 2010, 52(4):609–614.
20. Kerrigan, S., Banuelos, S., Perrella, L., Hardy, B. Simultaneous detection of ten psychedelic phenethylamines in urine by gas chromatography-mass spectrometry. J Anal Toxicol, 2011, 35(7):459–469.
21. Tomczak, E., Woźniak, M.K., Kata, M., Wiergowski, M., Szpiech, B., Biziuk, M. Blood concentrations of a new psychoactive substance 4-chloromethcathinone (4-CMC) determined in 15 forensic cases. Forensic Toxicol, 2018, 36(2):476–485.
22. Alexandridou, A., Mouskeftara, T., Raikos, N., Gika, H.G. GC-MS anaysis of underivatised new psychoactivesubstances in whole blood and urine. J Chromatogr B, 2020, 1156:122308.
23. Institóris, L., Kovacs, K., Sija, E., Berkecz, R., Körmöczi, T., Nemeth, I., Elek, I., Bakos, A., Urban, I., Pap, C., Kereszty, E. Clinical symptoms and blood concentration of new psychoactive substances (NPS) in intoxicated and hospitalized patients in the Budapest region of Hungary (2018–19). Clin Toxicol, 2022, 60(1):18–24
24. Wohlfarth, A., Weinmann, W., Dresen, S. LC-MS/MS screening method for designer amphetamines, tryptamines, and piperazines in serum. Anal Bioanal Chem, 2010, 396(7):2403–2414.
25. Dalsgaard, P.W., Rasmussen, B.S., Muller, I.B., Linnet, K. Toxicological screening of basic drugs in whole blood using UPLC-TOF-MS. Drug Test Analysis, 2012, 4(5):313–319.
26. Kneisel, S., Auwärter, V. Analysis of 30 synthetic cannabinoids in serum by liquid chromatography-electrospray ionization tandem mass spectrometry after liquid-liquid extraction. J Mass Spectrom, 2012, 47(7):825–835.
27. Concheiro, M., Anizan, S., Ellefsen, K., Huestis, M.A. Simultaneous quantification of 28 synthetic cathinones and metabolites in urine by liquid chromatography-high resolution mass spectrometry. Anal Bioanal Chem, 2013, 405(29):9437–9448
28. Swortwood, M.J., Boland, D.M., Decaprio, A.P. Determination of 32 cathinone derivatives and other designer drugs in serum by comprehensive LC-QQQ-MS/MS Analysis. Anal Bioanal Chem, 2013, 405(4):1383–1397.
29. Tang, M.H.Y., Ching, C.K., Lee, C.Y.W., Lam, Y.,, Mak, T.W.L. Simultaneous detection of 93 conventional and emerging drugs of abuse and their metabolites in urine by UHPLC-MS/MS. J Chromatogr B Analyt Technol Biomed Life Sci, 2014, 969:272–284.
30. Wicka, M., Chołbiński, P., Kwiatkowska, D., Pokrywka, A. Wykrywanie substancji psychotropowych we krwi metodą LC/MS/MS. Problemy Kryminalistyki, 2014, 284(2):1–13.
31. Adamowicz, P., Tokarczyk, B. Simple and rapid screening procedure for 143 new psychoactive substances by liquid chromatography-tandem mass spectrometry. Drug Test Anal, 2016, 8(7):652–667.
32. Cannaert, A., Storme, J., Franz, F., Auwarter, V., Stove, C.P. Detection and activity profiling of synthetic cannabinoids and metabolites with a newly developed bio-assay. Anal Chem, 2016, 88(23):11476–11485.

33. Yeter, O. Determination of drugs in human blood via bidirectional solid phase extraction. LC-Tech Application Note 116. 2016
https://www.johnmorrisgroup.com/Content/Attachments/227518/LCTech-Application-Note-Drugs-Blood-en.pdf.
34. https://www.unodc.org/LSS/SubstanceGroup/GroupsDashboard?testType=NPS z dnia 12.06.2023 r godz. 11.31
35. Greenblatt, D.J. Pharmacology of benzodiazepine hypnotics. J Clin Psychiatry, 1992, 53(1), 7-13
36. Mandrioli, R., Mercolini, L., Raggi, M.A. Benzodiazepine Metabolism: An Analytical Perspective, Curr Drug Metab, 2008, 9, 827-844
37. Chouinard, G., Lefko-Singh, K., Teboul E. Metabolism of anxiolytics and hypnotics: benzodiazepines, buspirone, zoplicone, and zolpidem. Cell Mol Neurobiol, 1999, 19(4), 533-552.
38. Yasui, N., Otani, K., Kaneko, S., Ohkubo, T., Osanai, T., Sugawara, K., Chiba, K., Ishizaki, T. A kinetic and dynamic study of oral alprazolam with and without erythromycin in humans: In vivo evidence for the involvement of CYP3A4 in alprazolam metabolism. Clin Pharmacol Ther, 1996, 59(5), 514-519.
39. Williams, J.A., Ring, B.J., Cantrell, V.E., Jones, D.R., Eckstein, J., Ruterbories, K., Hamman, M.A., Hall, S.D., Wrighton, S.A. Comparative metabolic capabilities of CYP3A4, CYP3A5, and CYP3A7 Drug Metab Dispos, 2002, 30(8), 883-891.
40. Greenblatt, D.J., Divoll, M.K., Soong, M.H., Boxenbaum, H.G., Harmatz, J.S., Shader, R.I. Desmethyldiazepam pharmacokinetics: studies following intravenous and oral desmethyldiazepam, oral clorazepate, and intravenous diazepam. J Clin Pharmacol 1998, 28(9), 853-859.
41. Saito, K., Sakai, N., Kim, H.S., Ishizuka, M., Kazusaka, Akio., Fujita S. Strain differences in diazepam metabolism at its three metabolic sites in Sprague-Dawley, Brown Norway, Dark Agouti, and istar strain rats. Drug Metab Dispos *2004,* 32(9), 959-965
42. Gafni, I., Busto, U.E., Tyndale, R.F., Kaplan, H.L., Sellers, E.M. The role of cytochrome P450 2C19 activity in flunitrazepam metabolism *in vivo.* J Clin Psychopharmacol, 2003, 23(2), 169-175.
43. Coller, J.K., Somogyi, A.A., Bochner, F. Flunitrazepam oxidative metabolism in human liver microsomes: involvement of CYP2C19 and CYP3A4 Xenobiotica, 1999, 29(10), 973-986
44. Peng, F.C., Chaing, H.H., Tang, S.H., Chen, P.C., Lu, S.C. NADPH-Cytochrome P-450 Reductase is Involved in Flunitrazepam Reductive Metabolism in Hep G2 and Hep 3B Cells J Toxicol Environ Health, 2004, 67(2), 109-124.
45. Baselt, R.C., Cravey, R.H. in *Disposition of toxic drugs and chemicals in man, 4th ed.*, Chemical Toxicology Institute, Foster City, 1995, p. 211.
46. Židková, M., Linhart, I., Balíková M., Himl, M., Váňa, L. Vetýška, M., Páleníček, T., Lhotková, E., Dušek, M. Study on the metabolism of 5,6-methylenedioxy-2-aminoindane (MDAI) in rats: identification of urinary metabolites, Xenobiotica Early Online:2016, 1–10,
47. De la Torre, R., Farre,́ M., Roset, P.N., Pizarro, N., Abanades, S., Segura, M., Segura, J., Cami, J. Human pharmacology of MDMA: pharmacokinetics, metabolism, and disposition. Ther Drug Monit, 2004, 26:137–44
48. Hartman, R.L., Desrosiers, N.A., Barnes, A.J., Yun, K., Scheidweiler, K.B., Kolbrich-Spargo, E., Gorelick, D.A., Goodwin, R.S., Huestis, M.A. 3,4- Methylenedioxymethamphetamine (MDMA) and metabolites disposition in blood and plasma following controlled oral administration. Anal Bioanal Chem, 2014, 406:587–99.
49. Maurer, H.H. On the metabolism and the toxicological analysis of methylenedioxyphenylalkylamine designer drugs by gas chromatography mass spectrometry. Ther Drug Monit, 1996, 18:465–70.

50. Mestria, S., Odoardi, S., Federici, S., Bilel, S., Tirri, M., Marti, M., Rossi, S.S. Metabolism Study of N-Methyl 2-Aminoindane (NM2AI) and Determination of Metabolites in Biological Samples by LC–HRMS, J Anal Toxicol, 2021;45:475–483
51. Arbo, M.D., Bastos, M.L., Carmo, H.F. Piperazine compounds as drugs of abuse, Drug Alcohol Depen, 2012, 122, 174– 185
52. Maurer, H.H., Kraemer, T., Springer, D., Staack, R.F. Chemistry, pharmacology, toxicology and hepatic metabolism of designer drugs of the amphetamine (ecstasy), piperazine, and pyrrolidinophenone types. Ther Drug Monit, 2004, 26, 127–131.
53. Staack, R.F., Fritschi, G., Maurer, H.H. New designer drug 1-(3 trifluoromethylphenyl)piperazine (TFMPP): gas chromatography/mass spectrometry and liquid chromatography/mass spectrometry studies on its phase I and II metabolism and on its toxicological detection in rat urine. J Mass Spectrom, 2003, 38, 971–981.
54. Staack, R.F., Maurer, H.H. Metabolism of designer drugs of abuse. Curr Drug Metab, 2005, 6, 259–274.
55. Catherine, J. Lucas, P.G., Schneider, J. The pharmacokinetics and the pharmacodynamics of cannabinoids, Br J Clin Pharmacol, 2018, 84, 2477–2482
56. Zendulka, O., Dovrtelova, G., Noskova, K., Turjap, M., Sulcova, A., Hanus, L., Jurica, J. Cannabinoids and cytochrome P450 interactions. Curr Drug Metab, 2016, 17: 206–26.
57. Gaston, T.E., Friedman, D. Pharmacology of cannabinoids in the treatment of epilepsy. Epilepsy Behav, 2017, 70 (Pt B): 313–8.
58. Eichler, M., Spinedi, L., Unfer-Grauwiler, S., Bodmer, M., Surber, C., Luedi, M., Drewe, J. Heat exposure of Cannabis sativa extracts affects the pharmacokinetic and metabolic profile in healthy male subjects. Planta Med, 2012; 78: 686–91.
59. Su, M., Seely, K., Moran, J., Hoffman, R. Metabolism of classical cannabinoids and the synthetic cannabinoid JWH-018. Clin Pharmacol Ther, 2015, 97(6), 562–564.
60. Fantegrossia, W.E., Jeffery, H., Morana, C., Radominska-Pandyab, A., Prather, P.L. Distinct pharmacology and metabolism of K2 synthetic cannabinoids compared to Δ9-THC: Mechanism underlying greater toxicity? Life Sci, 2014, 97(1): 45–54.
61. Sobolevsky, T., Prasolov, I., Rodchenkov, G. Detection of JWH-018 metabolites in smoking mixturepost-administration urine. Forensic Sci Int, 2010, 200:141–7.
62. Grigoryev, A., Melnik, A., Savchuk, S., Simonov, A., Rozhanets, V. Gas and liquid chromatography-mass spectrometry studies on the metabolism of the synthetic phenylacetylindole cannabimimetic JWH-250, the psychoactive component of smoking mixtures. J Chromatogr B Analyt Technol Biomed Life Sci, 2011a, 879:2519–26.
63. Grigoryev, A., Savchuk, S., Melnik, A., Moskaleva, N., Dzhurko, J., Ershov, M., Nosyrev, A., Vedenin, A., Izotov, B., Zabirova, I., Rozhanets, V. Chromatography-mass spectrometry studies on the metabolism of synthetic cannabinoids JWH-018 and JWH-073,psychoactive components of smoking mixtures. J Chromatogr B, 2011b, 879:1126–36.
64. Dinis-Oliveira, R.J. Metabolism and metabolomics of opiates: A long way of forensic implications to unravel. J Forensic Leg Med, 2019, 61, 128–140.
65. Alexandridou, A., Mouskeftara, T., Raikos, N., Gika, H.G. GC-MS analysis of underivatised new psychoactive substances in whole blood and urine, Journal Chrom B, 2020, Volume 1156,122308,1570-0232,
66. Ferreira, A.B., Castro, A.L., Tarelho, S., Domingues, P., Franco, J.M. GC-MS – Still standing for clinical and forensic analysis: validation of a multidrug method to detect and quantify illicit drugs, Austr J For Sci, 2023, 55:1, 107-128
67. Giorgetti, A., Barone, R., Pelletti, G., Garagani, M., Pascali, J., Haschimi, B., Auwarter, V. Development and validation of a rapid LC-MS/MS method for the detection of 182 novel psychoactive substances in whole blood. Drug Test Anal, 2022, 14(2):202-223.
68. Bjornstad, K., Beck, O., Helander, A. A multi-component LC–MS/MS method for detection of ten plant-derived psychoactive substances in urine. J Chromatogr B, 2009, 877, 1162–1168

69. Cooman, T., Santos, H., Cox, J., Francisco Allochio Filho, J., Bastos Borges, K., Romão, W., Arroyo-Mora, L.E. Development, Validation And Evaluation Of a Quantitative Method For The Analysis Of Twenty-Four New Psychoactive Substances In Oral Fluid By LC-MS/MS. Forensic Chem, 2020, 100231.
70. Olesti, E., Pascual, J. A., Ventura, M., Papaseit, E., Farré, M., Torre, R., Pozo, Ó.J. LC-MS/MS method for the quantification of new psychoactive substances and evaluation of their urinary detection in humans for doping control analysis. Drug Test Anal, 2020, 12:785–797.
71. Chen, H-W., Liu, H-T., Kuo, Y-N., Yang, D-P., Ting, T-T., Chen, J-C., Chiu, J-Y., Jair, J-C., Li H-C., Chiang, P-J., Chen, W-R., Lin, M-C., Hsu, Y-H., Chen, P-S. Rapid and sensitive dilute-and-shoot analysis using LC-MS-MS for identification of multi-class psychoactive substances in human urine, J Pharm Biomed Anal, 2023, Volume 233, 115443, 0731-7085,
72. https://www.sciencedirect.com/science/article/abs/pii/S0731708523002121?via%3Dihub z dnia 10.07.2023
73. Yanes, E.G., Lovett D.P. High-throughput bioanalytical method for analysis of synthetic cannabinoid metabolites in urine using salting out sample preparation and LC–MS/MS. J Chromatogr B, 2012, 909:42–50.
74. Buszewski,. B, Szultka, M. Past, Present, and Future of Solid Phase Extraction: A Review. Crit Rev Anal Chem. 2012, 42(3):198–213.
75. Buszewski, B., Szultka, M., Gadzała-Kopciuch, R. Sorbent chemistry, evolution, in: Comprehensive Sampling and Sample Preparation. Analytical Techniques for Scientists. Ed J Pawliszyn. Elsevier, 2012, 2:243–256.
76. Aldlgan, A.A., Torrance, H.J. Bioanalytical methods for the determination of synthetic cannabinoids and metabolites in biological specimens. TrAC - Trends Anal Chem. 2016, 80:444–457.
77. Mueller, C.A., Weinmann, W., Dresen, S., Schreiber, A., Gergov, M. Development of a multi-target screening analysis for 301 drugs using a QTrap liquid chromatography/tandem mass spectrometry system and automated library searching. Rapid Commun Mass Spectrom, 2005, 19(10):1332–1338.
78. Scientific Working Group for Forensic Toxicology (SWGTOX) Standard Practices for Method Validation in Forensic Toxicology Journal of Analytical Toxicology 2013;37:452–474 doi:10.1093/jat/bkt054

8 Streszczenie

W ostatnich latach stale rośnie zainteresowanie substancjami psychoaktywnymi, a w szczególności dopalaczami, które stanowią często legalną alternatywę dla alkoholu czy klasycznych narkotyków. Powszechnie dostępne, sprzedawane jako sole do kąpieli czy inne preparaty oznaczane jako produkty nie do spożycia. Syntetyzowane w przydomowych laboratoriach nie mają jednoznacznie oznaczonego składu, co tylko potwierdza jak ogromne ryzyko dla zdrowia, a nawet życia stanowią te środki. Pojawiające się coraz to nowe struktury stanowią ogromne wyzwanie dla laboratoriów toksykologicznych i organów ścigania.

Celem niniejszej rozprawy doktorskiej było opracowanie i wdrożenie do rutynowych analiz metod analitycznych pozwalających na oznaczanie jak największej liczby substancji psychoaktywnych, leków i ich metabolitów w możliwie najkrótszym czasie w matrycach biologicznych (krwi, moczu i włosach) z zastosowaniem chromatografii cieczowej sprzężonej z tandemową spektrometrią mas. Bardzo istotnym elementem badań było opracowanie metody analitycznej, która umożliwi łatwe przystosowanie jej do innej matrycy, a także da się dalej rozwijać poprzez dodawanie kolejnych analitów, by móc podążać za oczekiwaniami rynku środków psychoaktywnych. Opracowane w ramach przeprowadzonych badań metody analityczne pozwoliły na jednoczesną analizę ponad 500 analitów w czasie pół godzinnej analizy za pomocą LC-MS/MS.

Oznaczanie substancji psychoaktywnych, leków i ich metabolitów w materiale biologicznym stanowi ogromne wyzwanie analityczne. Zastosowanie chromatografii cieczowej sprzężonej z tandemową spektrometrią mas daje duże możliwości analityczne do opracowania tak złożonej metody, jednakże nadal analiza takiej liczby substancji podczas jednej analizy stanowi ogromne wyzwanie analityczne. Analiza NPS wiąże się z trudnościami chromatograficznymi związanymi z dużą ilością izomerów czy też związków o bardzo podobnej strukturze. Każda z grup NPS zawiera podobnie strukturalnie anality, ponadto między innymi w przypadku katynonów wielokrotnie spotykamy się z izomerami i niewielkimi modyfikacjami struktur, które nie zmieniają masy związku chemicznego, ale według prawa nie są już substancjami zabronionymi. Fakty te pokazują, jak trudno uzyskać rozdzielenie chromatograficzne tak dużej liczby analitów. Dzięki zastosowaniu metody śledzenia par MRM, odpowiednio dobrane warunki spektrometru mas pozwoliły na jednoznaczną identyfikację badanych analitów.

Jako metodę przygotowania próbek zastosowano ekstrakcję ciecz-ciecz, która pozwoliła na wyizolowanie badanych analitów należących do różnych grup wśród NPS, co nie było możliwe przy zastosowaniu ekstrakcji do fazy stałej. Zastosowanie do badań ilościowych krzywej

wzorcowej w matrycy pozwoliło na uwzględnienie wpływu matrycy na wyniki uzyskiwane w przypadku poszczególnych analitów i matryc. Ponadto ostateczne rozcieńczenie próbek zamiast stosowanego zazwyczaj zatężania pozwoliło na zredukowanie jej wpływu na uzyskane wyniki. Opracowane metody analityczne pozwoliły na weryfikację próbek różnych matryc od jednego pacjenta, co daje możliwość badań nad metabolizmem NPS oraz przeprowadzaniu badań retrospektywnych.

Opracowane metody analityczne zostały poddane weryfikacji w badaniach biegłości następnie wdrożone do rutynowych analiz Instytutu Genetyki Sądowej w Bydgoszczy i poddane akredytacji przez Polskie Centrum Akredytacji. Metody te zostały także uwzględnione w zgłoszeniu patentowym.

9 Abstract

In recent years, there has been a growing interest in psychoactive substances, in particular legal highs, which are often a legal alternative to alcohol or classic drugs. Widely available, sold as bath salts or other preparations marked as not for consumption. Synthesized in home laboratories, they do not have a clearly marked composition, which only confirms the huge risk to health and even life these agents pose. The emerging new structures pose a huge challenge for toxicology laboratories and law enforcement agencies. The purpose of this doctoral dissertation was to develop and implement analytical methods for routine analyzes that allow the determination of the largest possible number of psychoactive substances, drugs and their metabolites in the shortest possible time in biological matrices - blood, urine and hair using liquid chromatography coupled with mass spectrometry. A very important element of the research was the development of an analytical method that would allow it to be easily adapted to a different matrix, and could be further developed by adding more analytes to be able to follow the expectations of the psychoactive substances market. The analytical methods developed as part of the research allowed for the simultaneous analysis of over 500 analytes during half an hour of analysis using LC-MS/MS.

Determination of psychoactive substances, drugs and their metabolites in biological material is a huge analytical challenge. The use of liquid chromatography coupled with tandem mass spectrometry gives great analytical possibilities to develop such a complex method, but still the analysis of such a number of substances during one analysis is a huge analytical challenge. The NPS analysis is associated with chromatographic difficulties due to the large number of isomers or compounds with a very similar structure. Each of the NPS groups contains structurally similar analytes, moreover, in the case of cathinones, we often encounter isomers and slight structural modifications that do not change the mass of the chemical compound, but are no longer prohibited substances by law. These facts show how difficult it is to achieve chromatographic separation of such a large number of analytes. Thanks to the use of the MRM pair tracking method, the properly selected conditions of the mass spectrometer allowed for the unambiguous identification of the analytes tested.

As a sample preparation method, liquid-liquid extraction was used, which allowed the isolation of the tested analytes belonging to different groups among NPS, which was not possible using solid phase extraction. The use of the standard curve in the matrix for quantitative research allowed to take into account the influence of the matrix on the results obtained for individual analytes and matrices. In addition, the final dilution of the samples instead of the usual concentration allowed to reduce the influence of the matrix on the obtained results. The

developed analytical methods allowed for the verification of samples of various matrices from one patient, which gives the opportunity to study the metabolism of NPS and to conduct retrospective studies.

The developed analytical methods were verified in proficiency tests, then implemented in routine analyzes of the Institute of Forensic Genetics in Bydgoszcz and accredited by the Polish Center for Accreditation. These methods have also been included in the patent application.

10 Dorobek naukowy

❖ Zgłoszenia patentowe

1. Jolanta Powierska-Czarny, Jakub Czarny, Radosław Zbytniewski, Michał Raczkowski, Natalia Galant, **Jadwiga Musiał**, Numer zgłoszenia P.441164 UPRP; Sposób wykrywania związków psychoaktywnych w próbkach biologicznych oraz zastosowanie tego sposobu do wykrywania substancji psychoaktywnych”**,** (MEiN = 70 pkt)

❖ Publikacje wchodzące w skład rozprawy doktorskiej

1. **Jadwiga Musiał**. Jakub Czarny, Renata Gadzała-Kopciuch, *Overview of analytical methods for determining novel psychoactive substances, drugs and their metabolites in biological samples*, Critical Reviews in Toxicology, 2022, 52:3, 239-258, https://doi.org/10.80/10408444.2022.2091424, IF=6,184 MeEiN = 100 pkt

2. **Jadwiga Musiał**, Jolanta Powierska-Czarny, Jakub Czarny, Michał Raczkowski, Natalia Galant, Bogusław Buszewski, Renata Gadzała-Kopciuch, *One-step extraction and determiantion of 513 psychoactive substances, drugs, and their metabolites from hair by LC-MS/MS*, Archives of Toxicology, 2022, 96:2927-2933, https://doi.org/10.1007/s00204-022-03343-w, IF=6,168 MEiN =140 pkt

3. Jakub Czarny, **Jadwiga Musiał**, Jolanta Powierska-Czarny, Natalia Galant, Michał Raczkowski, Bogusław Buszewski, Renata Gadzała-Kopciuch, *Validation of a simple and quick method for determination of psychoactive substances, drugs and their metabolites from human blood by LC-MS/MS*, Microchemical Journal, 2022, 182: 107922, https://doi.org/10.1016/j.microc.2022.107922, IF=5,304 MEiN =70 pkt

4. Jakub Czarny, **Jadwiga Musiał**, Jolanta Powierska-Czarny, Michał Raczkowski, Natalia Galant, Bogusław Buszewski, Renata Gadzała-Kopciuch, *Determination of 465 psychoactive substances, drugs and their metabolites in urine by LC-MS/MS*, Analytical Methods, 2024, https://doi.10.1039/D4AY00777H, IF= 2,7 MEiN = 70 pkt

❖ Konferencje naukowe:

a) Prezentacje ustne

1) **Jadwiga Musiał**, Jakub Czarny, Renata Gadzała-Kopciuch, *Oznaczenie 477 substancji psychoaktywnych w moczu za pomocą LC-MS/MS* – komunikat, XVI Wrocławskie Studenckie Sympozjum Chemiczne, Wrocław, 5-6.12.2020

b) Prezentacje posterowe

1) Katarzyna Kwaśniewska, **Jadwiga Szewczyk,** Renata Gadzała-Kopciuch, Bogusław Buszewski. *Opracowanie metody analitycznej rozdzielania i identyfikacji zearalenonu i jego metabolitów za pomocą LC/MS.* IX Poznańska Konferencja Naukowa: Chemia- nowe wyzwania dla nauki i przemysłu, Poznań 5.12.2014r.

2) **Jadwiga Musiał**, Natalia Galant, Jolanta Powierska-Czarny, Renata Gadzała-Kopciuch. *One-step extraction and determination of 513 psychoactive substances and drugs from hair by LC-MS/MS.* 25th International Symposium on Separation Sciences, Łódź, 15-18.09.2019r.

3) **Jadwiga Musiał**, Jakub Czarny, Natalia Galant, Michał Raczkowski, Barbara Przyjazna, Jolanta Powierska-Czarny, Renata Herman, Magdalena Chrostowska, Paulina Jerszyńska. *Development and validation of a simple and quick method for determination of 521 psychoactive substances, drugs and their metabolites from blood by LC-MS/MS.* The 57th Annual Meeting of The International Association of Forensic Toxicologists (TIAFT), Birmingham 2-6.09.2019r.

4) Natalia Galant, Jakub Czarny, **Jadwiga Musiał**, Renata Herman, Paulina Jerszyńska, Jolanta Powierska-Czarny, Michał Raczkowski. *Multiplex determination of psychoactive substances, drugs and their metabolites in urine by LC-MS/MS.* The 57th Annual Meeting of The International Association of Forensic Toxicologists (TIAFT), Birmingham 2-6.09.2019r.

5) Natalia Galant, Jakub Czarny, Michał Raczkowski, **Jadwiga Musiał**, Magdalena Chrostowska, Renata Herman, Jolanta Powierska-Czarny, Paulina Jerszyńska, Barbara Przyjazna. *One-step extraction and detection of 513 drugs from hair by LC-MS/MS.* The 57th Annual Meeting of The International Association of Forensic Toxicologists (TIAFT), Birmingham 2-6.09.2019r.

6) **Jadwiga Musiał**, Renata Gadzała-Kopciuch. *Driving under the influence-analysis of urine samples of drivers for 465 psychoactive substances and their metabolites by LC-MS/MS.* 26th International Symposium on Separation Sciences, Ljubljana 28.06-01.07.2022r.

7) **Jadwiga Musiał**, Renata Gadzała-Kopciuch, Jakub Czarny, Jolanta Powierska-Czarny, Michał Raczkowski, Natalia Galant, Bogusław Buszewski. *Jazda na podwójnym gazie - czyli analiza substancji psychoaktywnych, ich metabolitów i leków za pomocą LC-MS/MS w próbkach moczu pochodzących od kierowców.* 64 Zjazd Naukowy

Polskiego Towarzystwa Chemicznego, Lublin, 11-16.09.2022r.

11 Oświadczenia współautorów

Toruń, dnia 3 czerwca 2024 r.

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Oświadczenie o współautorstwie

Niniejszym oświadczam, że w pracach:

1. Jadwiga Musiał, Jakub Czarny, Renata Gadzała-Kopciuch, 2022, *Overview of analytical methods for determination of psychoactive substances, drugs and their metabolites in biological samples,* Critical Reviews in Toxicology, 52:239-258. Mój udział w powstaniu pracy wynosi 20 %.
2. Jadwiga Musiał, Jolanta Powierska-Czarny, Jakub Czarny, Michał Raczkowski, Natalia Galant, Bogusław Buszewski, Renata Gadzała-Kopciuch, 2022, *One-step extraction and determination of 513 psychoactive substances, drugs, and their metabolites from hair by LC-MS/MS,* Archives of Toxicology, 96: 2927-2933. Mój udział w powstaniu pracy wynosi 10 %.
3. Jakub Czarny, Jadwiga Musiał, Jolanta Powierska-Czarny, Natalia Galant, Michał Raczkowski, Bogusław Buszewski, Renata Gadzała-Kopciuch, 2022, *Validation of a simple and quick method for determination of psychoactive substances, drugs and their metabolites from human blood by LC-MS/MS*, Microchemical Journal,182:107922. Mój udział w powstaniu pracy wynosi 30 %.
4. Zgłoszenie patentowe: Numer zgłoszenia przed UPRP – P.441164; *Sposób wykrywania związków psychoaktywnych w próbkach biologicznych oraz zastosowanie tego sposobu do wykrywania substancji psychoaktywnych*, Jolanta Powierska-Czarny, Jakub Czarny, Radosław Zbytniewski, Michał Raczkowski, Natalia Galant, Jadwiga Musiał. Mój udział w powstaniu pracy wynosi 30 %.
5. Jakub Czarny, Jadwiga Musiał, Jolanta Powierska-Czarny, Michał Raczkowski, Natalia Galant, Bogusław Buszewski, Renata Gadzała-Kopciuch, *Determination of 465 psychoactive substances, drugs and their metabolites in urine by LC-MS/MS.* Praca wysłana do Analitycal Methods (RSC). Mój udział w powstaniu pracy wynosi 30 %.

   Mój wkład polegał na współudziale w opracowaniu metod analitycznych (ustawienia parametrów spektrometru mas, optymalizacja pracy spektrometru), konsultacji otrzymanych wyników, dyskusji eksperymentu naukowego, nadzorowaniu projektu badawczego oraz korekcie manuskryptów.

.....
(podpis)

Informacja o przetwarzaniu danych osobowych

Na podstawie Rozporządzenia Parlamentu Europejskiego i Rady (UE) 2016/679 z dnia 27 kwietnia 2016 r. w sprawie ochrony osób fizycznych w związku z przetwarzaniem danych osobowych i w sprawie swobodnego przepływu takich danych oraz uchylenia dyrektywy 95/46/WE, zwanego dalej „RODO", informujemy, że:

1. Administratorem Pana/~~Pani~~ danych osobowych będzie Uniwersytet Mikołaja Kopernika w Toruniu z siedzibą przy ul. Gagarina 11, 87-100 Toruń (dalej: Uczelnia, ADO).
2. Pana/~~Pani~~ dane osobowe w związku w związku z postępowaniem o nadanie stopnia naukowego będą przetwarzane:
   a. na podstawie art. 6 ust. 1 lit. c) RODO – obowiązek prawny wynikający z przepisów ustawy z dnia 20 lipca 2018 r. Prawo o szkolnictwie wyższym i nauce (Dz. U. z 2020, poz. 85);
   b. na podstawie art. 6 ust. 1 lit. f) RODO – prawnie uzasadniony interes ADO:
      - do ustalenia, obrony lub dochodzenia roszczeń – przez okres do przedawnienia roszczeń, lub przez okres prowadzenia postępowania przez właściwe organy lub sądy w przypadku dochodzenia roszczeń,
      - na potrzeby wewnętrzne tworzenia zestawień, analiz i statystyk – przez okres obowiązywania umowy,
      - na potrzeby prowadzenia ewidencji korespondencji przychodzącej i wychodzącej – wieczyście,
      - na potrzeby marketingu produktów i usług ADO.
3. Z zastrzeżeniem przepisów powszechnie obowiązującego prawa przysługują Panu/Pani prawa, które zrealizujemy na wniosek o:
   a. Żądanie dostępu do danych osobowych oraz prawo ich sprostowania,
   b. Żądanie usunięcia lub ograniczenia przetwarzania.
4. Przysługuje Panu/~~Pani~~ również prawo wniesienia sprzeciwu na przetwarzanie danych osobowych.
5. Podanie przez Pana/~~Panią~~ danych osobowych jest niezbędne do wykonania celu wymienionego w pkt 2 lit. a i b., a brak ich podania uniemożliwi otwarcie i przeprowadzenie postępowania.
6. Przysługuje Panu/~~Pani~~ prawo wniesienia skargi do Prezesa Urzędu Ochrony Danych Osobowych.
7. Pana/~~Pani~~ dane osobowe mogą być udostępnione recenzentom lub organom administracji publicznej, sądom, komornikom w zakresie sytuacji przewidzianych w przepisach prawa.
8. Na dzień zbierania Pana/~~Pani~~ danych osobowych nie planujemy przekazywać ich poza EOG (obejmujący Unię Europejską, Norwegię, Lichtenstein i Islandię), nie wykluczając tego w przyszłości, o czym zostanie Pan/~~Pani~~ poinformowania ze stosownym wyprzedzeniem.
9. W stosunku do Pana/~~Pani~~ nie będą prowadzone działania polegające na podejmowaniu decyzji w sposób zautomatyzowany, nie będą one również podlegały zautomatyzowanemu profilowaniu.
10. Jeżeli chce Pan/~~Pani~~ skontaktować się z Uczelnią w sprawach związanych z przetwarzaniem danych osobowych, w szczególności w związku z wniesieniem wniosku o realizację przysługujących praw prosimy o kontakt pod adresem e-mail: iod@umk.pl lub adresem korespondencyjnym: UMK w Toruniu, ul. Gagarina 11, 87-100 Toruń, z dopiskiem „IOD", dostępny jest również kontakt telefoniczny: 56 611 27 42.

.....
(podpis)

Załącznik nr 5 do uchwały Nr 38 Senatu UMK z dnia 26 września 2023 r.
w sprawie postępowania o nadanie stopnia doktora
na Uniwersytecie Mikołaja Kopernika w Toruniu

Toruń, dnia 3 czerwca 2024 r.

dr n. med. Jolanta Powierska-Czarny
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Uniwersytetu Mikołaja Kopernika w Toruniu

Oświadczenie o współautorstwie

Niniejszym oświadczam, że w pracach:

1. Jakub Czarny, Jadwiga Musiał, Jolanta Powierska-Czarny, Natalia Galant, Michał Raczkowski, Bogusław Buszewski, Renata Gadzała-Kopciuch, 2022, *Validation of a simple and quick method for determination of psychoactive substances, drugs and their metabolites from human blood by LC-MS/MS*, Microchemical Journal,182:107922. Mój udział w powstaniu pracy wynosi 10 %.
2. Jadwiga Musiał, Jolanta Powierska-Czarny, Jakub Czarny, Michał Raczkowski, Natalia Galant, Bogusław Buszewski, Renata Gadzała-Kopciuch, 2022, *One-step extraction and determination of 513 psychoactive substances, drugs, and their metabolites from hair by LC-MS/MS,* Archives of Toxicology, 96: 2927-2933. Mój udział w powstaniu pracy wynosi 20 %.
3. Jakub Czarny, Jadwiga Musiał, Jolanta Powierska-Czarny, Michał Raczkowski, Natalia Galant, Bogusław Buszewski, Renata Gadzała-Kopciuch, *Determination of 465 psychoactive substances, drugs and their metabolites in urine by LC-MS/MS.* Praca wysłana do Analitycal Methods (RSC). Mój udział w powstaniu pracy wynosi 10 %.
4. Zgłoszenie patentowe: Numer zgłoszenia przed UPRP – P.441164; *Sposób wykrywania związków psychoaktywnych w próbkach biologicznych oraz zastosowanie tego sposobu do wykrywania substancji psychoaktywnych*, Jolanta Powierska-Czarny, Jakub Czarny, Radosław Zbytniewski, Michał Raczkowski, Natalia Galant, Jadwiga Musiał. Mój udział w powstaniu pracy wynosi 30 %.

Mój wkład polegał na współudziale w opracowaniu metod analitycznych (ustawienia parametrów spektrometru mas, optymalizacja pracy spektrometru), konsultacji otrzymanych wyników, dyskusji eksperymentu naukowego, nadzorowaniu projektu badawczego oraz korekcie manuskryptów.

Jolanta Powierska-Czarny
.....
(podpis)

Informacja o przetwarzaniu danych osobowych

Na podstawie Rozporządzenia Parlamentu Europejskiego i Rady (UE) 2016/679 z dnia 27 kwietnia 2016 r. w sprawie ochrony osób fizycznych w związku z przetwarzaniem danych osobowych i w sprawie swobodnego przepływu takich danych oraz uchylenia dyrektywy 95/46/WE, zwanego dalej „RODO", informujemy, że:

1. Administratorem ~~Pana~~/Pani danych osobowych będzie Uniwersytet Mikołaja Kopernika w Toruniu z siedzibą przy ul. Gagarina 11, 87-100 Toruń (dalej: Uczelnia, ADO).
2. ~~Pana~~/Pani dane osobowe w związku w związku z postępowaniem o nadanie stopnia naukowego będą przetwarzane:
   a. na podstawie art. 6 ust. 1 lit. c) RODO – obowiązek prawny wynikający z przepisów ustawy z dnia 20 lipca 2018 r. Prawo o szkolnictwie wyższym i nauce (Dz. U. z 2020, poz. 85);
   b. na podstawie art. 6 ust. 1 lit. f) RODO – prawnie uzasadniony interes ADO:
      - do ustalenia, obrony lub dochodzenia roszczeń – przez okres do przedawnienia roszczeń, lub przez okres prowadzenia postępowania przez właściwe organy lub sądy w przypadku dochodzenia roszczeń,
      - na potrzeby wewnętrzne tworzenia zestawień, analiz i statystyk – przez okres obowiązywania umowy,
      - na potrzeby prowadzenia ewidencji korespondencji przychodzącej i wychodzącej – wieczyście,
      - na potrzeby marketingu produktów i usług ADO.
3. Z zastrzeżeniem przepisów powszechnie obowiązującego prawa przysługują Panu/Pani prawa, które zrealizujemy na wniosek o:
   a. Żądanie dostępu do danych osobowych oraz prawo ich sprostowania,
   b. Żądanie usunięcia lub ograniczenia przetwarzania.
4. Przysługuje ~~Panu~~/Pani również prawo wniesienia sprzeciwu na przetwarzanie danych osobowych.
5. Podanie przez ~~Pana~~/Panią danych osobowych jest niezbędne do wykonania celu wymienionego w pkt 2 lit. a i b., a brak ich podania uniemożliwi otwarcie i przeprowadzenie postępowania.
6. Przysługuje ~~Panu~~/Pani prawo wniesienia skargi do Prezesa Urzędu Ochrony Danych Osobowych.
7. ~~Pana~~/Pani dane osobowe mogą być udostępnione recenzentom lub organom administracji publicznej, sądom, komornikom w zakresie sytuacji przewidzianych w przepisach prawa.
8. Na dzień zbierania ~~Pana~~/Pani danych osobowych nie planujemy przekazywać ich poza EOG (obejmujący Unię Europejską, Norwegię, Lichtenstein i Islandię), nie wykluczając tego w przyszłości, o czym zostanie ~~Pan~~/Pani poinformowania ze stosownym wyprzedzeniem.
9. W stosunku do ~~Pana~~/Pani nie będą prowadzone działania polegające na podejmowaniu decyzji w sposób zautomatyzowany, nie będą one również podlegały zautomatyzowanemu profilowaniu.
10. Jeżeli chce ~~Pan~~/Pani skontaktować się z Uczelnią w sprawach związanych z przetwarzaniem danych osobowych, w szczególności w związku z wniesieniem wniosku o realizację przysługujących praw prosimy o kontakt pod adresem e-mail: iod@umk.pl lub adresem korespondencyjnym: UMK w Toruniu, ul. Gagarina 11, 87-100 Toruń, z dopiskiem „IOD", dostępny jest również kontakt telefoniczny: 56 611 27 42.

Jolanta Poniatko-Czarny
.....
(podpis)

Załącznik nr 5 do uchwały Nr 38 Senatu UMK z dnia 26 września 2023 r.
w sprawie postępowania o nadanie stopnia doktora
na Uniwersytecie Mikołaja Kopernika w Toruniu

Toruń, dnia 3 czerwca 2024 r

dr Michał Raczkowski
Instytut Genetyki Sądowej
ul. Aleje A. Mickiewicza 3/8
85-071 Bydgoszcz

Rada Dyscypliny Nauki Chemiczne
Uniwersytetu Mikołaja Kopernika w Toruniu

Oświadczenie o współautorstwie

Niniejszym oświadczam, że w pracach:

1. Jakub Czarny, Jadwiga Musiał, Jolanta Powierska-Czarny, Natalia Galant, Michał Raczkowski, Bogusław Buszewski, Renata Gadzała-Kopciuch, 2022, *Validation of a simple and quick method for determination of psychoactive substances, drugs and their metabolites from human blood by LC-MS/MS*, Microchemical Journal,182:107922. Mój udział w powstaniu pracy wynosi 10 %.
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3. Jakub Czarny, Jadwiga Musiał, Jolanta Powierska-Czarny, Michał Raczkowski, Natalia Galant, Bogusław Buszewski, Renata Gadzała-Kopciuch, *Determination of 465 psychoactive substances, drugs and their metabolites in urine by LC-MS/MS.* Praca wysłana do Analitycal Methods (RSC). Mój udział w powstaniu pracy wynosi 10 %.
4. Zgłoszenie patentowe: Numer zgłoszenia przed UPRP - P.441164; *Sposób wykrywania związków psychoaktywnych w próbkach biologicznych oraz zastosowanie tego sposobu do wykrywania substancji psychoaktywnych*, Jolanta Powierska-Czarny, Jakub Czarny, Radosław Zbytniewski, Michał Raczkowski, Natalia Galant, Jadwiga Musiał. Mój udział w powstaniu pracy wynosi 10 %.

Mój wkład polegał na współudziale w opracowaniu metod analitycznych (ustawienia parametrów spektrometru mas, optymalizacja pracy spektrometru), konsultacji otrzymanych wyników, dyskusji eksperymentu naukowego, nadzorowaniu projektu badawczego oraz korekcie manuskryptów.

M. Raczkowski

.....
(podpis)

Informacja o przetwarzaniu danych osobowych

Na podstawie Rozporządzenia Parlamentu Europejskiego i Rady (UE) 2016/679 z dnia 27 kwietnia 2016 r. w sprawie ochrony osób fizycznych w związku z przetwarzaniem danych osobowych i w sprawie swobodnego przepływu takich danych oraz uchylenia dyrektywy 95/46/WE, zwanego dalej „RODO", informujemy, że:

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2. Pana/~~Pani~~ dane osobowe w związku w związku z postępowaniem o nadanie stopnia naukowego będą przetwarzane:
   a. na podstawie art. 6 ust. 1 lit. c) RODO – obowiązek prawny wynikający z przepisów ustawy z dnia 20 lipca 2018 r. Prawo o szkolnictwie wyższym i nauce (Dz. U. z 2020, poz. 85);
   b. na podstawie art. 6 ust. 1 lit. f) RODO – prawnie uzasadniony interes ADO:
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      - na potrzeby wewnętrzne tworzenia zestawień, analiz i statystyk – przez okres obowiązywania umowy,
      - na potrzeby prowadzenia ewidencji korespondencji przychodzącej i wychodzącej – wieczyście,
      - na potrzeby marketingu produktów i usług ADO.
3. Z zastrzeżeniem przepisów powszechnie obowiązującego prawa przysługują Panu/Pani prawa, które zrealizujemy na wniosek o:
   a. Żądanie dostępu do danych osobowych oraz prawo ich sprostowania,
   b. Żądanie usunięcia lub ograniczenia przetwarzania.
4. Przysługuje Panu/~~Pani~~ również prawo wniesienia sprzeciwu na przetwarzanie danych osobowych.
5. Podanie przez Pana/~~Panią~~ danych osobowych jest niezbędne do wykonania celu wymienionego w pkt 2 lit. a i b., a brak ich podania uniemożliwi otwarcie i przeprowadzenie postępowania.
6. Przysługuje Panu/~~Pani~~ prawo wniesienia skargi do Prezesa Urzędu Ochrony Danych Osobowych.
7. Pana/~~Pani~~ dane osobowe mogą być udostępnione recenzentom lub organom administracji publicznej, sądom, komornikom w zakresie sytuacji przewidzianych w przepisach prawa.
8. Na dzień zbierania Pana/~~Pani~~ danych osobowych nie planujemy przekazywać ich poza EOG (obejmujący Unię Europejską, Norwegię, Lichtenstein i Islandię), nie wykluczając tego w przyszłości, o czym zostanie Pan/~~Pani~~ poinformowania ze stosownym wyprzedzeniem.
9. W stosunku do Pana/~~Pani~~ nie będą prowadzone działania polegające na podejmowaniu decyzji w sposób zautomatyzowany, nie będą one również podlegały zautomatyzowanemu profilowaniu.
10. Jeżeli chce Pan/~~Pani~~ skontaktować się z Uczelnią w sprawach związanych z przetwarzaniem danych osobowych, w szczególności w związku z wniesieniem wniosku o realizację przysługujących praw prosimy o kontakt pod adresem e-mail: iod@umk.pl lub adresem korespondencyjnym: UMK w Toruniu, ul. Gagarina 11, 87-100 Toruń, z dopiskiem „IOD", dostępny jest również kontakt telefoniczny: 56 611 27 42.

M. Rogalewska

.....

(podpis)

Załącznik nr 5 do uchwały Nr 38 Senatu UMK z dnia 26 września 2023 r.
w sprawie postępowania o nadanie stopnia doktora
na Uniwersytecie Mikołaja Kopernika w Toruniu

Toruń, dnia 3 czerwca 2024 r.

dr Natalia Galant
Instytut Genetyki Sądowej
ul. Aleje A. Mickiewicza 3/8
85-071 Bydgoszcz

Rada Dyscypliny Nauki Chemiczne
Uniwersytetu Mikołaja Kopernika w Toruniu

Oświadczenie o współautorstwie

Niniejszym oświadczam, że w pracach:

1. Jakub Czarny, Jadwiga Musiał, Jolanta Powierska-Czarny, Natalia Galant, Michał Raczkowski, Bogusław Buszewski, Renata Gadzała-Kopciuch, 2022, *Validation of a simple and quick method for determination of psychoactive substances, drugs and their metabolites from human blood by LC-MS/MS*, Microchemical Journal,182:107922. Mój udział w powstaniu pracy wynosi 10 %.
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3. Jakub Czarny, Jadwiga Musiał, Jolanta Powierska-Czarny, Michał Raczkowski, Natalia Galant, Bogusław Buszewski, Renata Gadzała-Kopciuch, *Determination of 465 psychoactive substances, drugs and their metabolites in urine by LC-MS/MS.* Praca wysłana do Analitycal Methods (RSC). Mój udział w powstaniu pracy wynosi 10 %.
4. Zgłoszenie patentowe: Numer zgłoszenia przed UPRP – P.441164; *Sposób wykrywania związków psychoaktywnych w próbkach biologicznych oraz zastosowanie tego sposobu do wykrywania substancji psychoaktywnych*, Jolanta Powierska-Czarny, Jakub Czarny, Radosław Zbytniewski, Michał Raczkowski, Natalia Galant, Jadwiga Musiał. Mój udział w powstaniu pracy wynosi 10 %.

Mój wkład polegał na współudziale w opracowaniu metod analitycznych (ustawienia parametrów spektrometru mas, optymalizacja pracy spektrometru), konsultacji otrzymanych wyników.

Galant Natalia
(podpis)

Informacja o przetwarzaniu danych osobowych

Na podstawie Rozporządzenia Parlamentu Europejskiego i Rady (UE) 2016/679 z dnia 27 kwietnia 2016 r. w sprawie ochrony osób fizycznych w związku z przetwarzaniem danych osobowych i w sprawie swobodnego przepływu takich danych oraz uchylenia dyrektywy 95/46/WE, zwanego dalej „RODO", informujemy, że:

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3. Z zastrzeżeniem przepisów powszechnie obowiązującego prawa przysługują Panu/Pani prawa, które zrealizujemy na wniosek o:
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4. Przysługuje ~~Panu~~/Pani również prawo wniesienia sprzeciwu na przetwarzanie danych osobowych.
5. Podanie przez ~~Pana~~/Panią danych osobowych jest niezbędne do wykonania celu wymienionego w pkt 2 lit. a i b., a brak ich podania uniemożliwi otwarcie i przeprowadzenie postępowania.
6. Przysługuje ~~Panu~~/Pani prawo wniesienia skargi do Prezesa Urzędu Ochrony Danych Osobowych.
7. ~~Pana~~/Pani dane osobowe mogą być udostępnione recenzentom lub organom administracji publicznej, sądom, komornikom w zakresie sytuacji przewidzianych w przepisach prawa.
8. Na dzień zbierania ~~Pana~~/Pani danych osobowych nie planujemy przekazywać ich poza EOG (obejmujący Unię Europejską, Norwegię, Lichtenstein i Islandię), nie wykluczając tego w przyszłości, o czym zostanie ~~Pan~~/Pani poinformowania ze stosownym wyprzedzeniem.
9. W stosunku do ~~Pana~~/Pani nie będą prowadzone działania polegające na podejmowaniu decyzji w sposób zautomatyzowany, nie będą one również podlegały zautomatyzowanemu profilowaniu.
10. Jeżeli chce ~~Pan~~/Pani skontaktować się z Uczelnią w sprawach związanych z przetwarzaniem danych osobowych, w szczególności w związku z wniesieniem wniosku o realizację przysługujących praw prosimy o kontakt pod adresem e-mail: iod@umk.pl lub adresem korespondencyjnym: UMK w Toruniu, ul. Gagarina 11, 87-100 Toruń, z dopiskiem „IOD", dostępny jest również kontakt telefoniczny: 56 611 27 42.

Gałat Natalia
(podpis)

Załącznik nr 5 do uchwały Nr 38 Senatu UMK z dnia 26 września 2023 r.
w sprawie postępowania o nadanie stopnia doktora
na Uniwersytecie Mikołaja Kopernika w Toruniu

Toruń, dnia 3 czerwca 2024 r.

prof. dr hab. Bogusław Buszewski
Katedra Chemii Środowiska i Bioanalityki
Wydział Chemii
Uniwersytet Mikołaja Kopernika w Toruniu
ul. Gagarina 7
87-100 Toruń

Rada Dyscypliny Nauki Chemiczne
Uniwersytetu Mikołaja Kopernika w Toruniu

Oświadczenie o współautorstwie

Niniejszym oświadczam, że w pracach:

1. Jakub Czarny, Jadwiga Musiał, Jolanta Powierska-Czarny, Natalia Galant, Michał Raczkowski, Bogusław Buszewski, Renata Gadzała-Kopciuch, 2022, *Validation of a simple and quick method for determination of psychoactive substances, drugs and their metabolites from human blood by LC-MS/MS*, Microchemical Journal,182:107922. Mój udział w powstaniu pracy wynosi 5 %.
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Mój wkład polegał na nadzorze merytorycznym oraz korekcie manuskryptów.

Podpis jest prawidłowy
Dokument podpisany przez
Bogusław Buszewski.
Data: 2024.06.05 07:38:21 CEST
(podpis)

Informacja o przetwarzaniu danych osobowych

Na podstawie Rozporządzenia Parlamentu Europejskiego i Rady (UE) 2016/679 z dnia 27 kwietnia 2016 r. w sprawie ochrony osób fizycznych w związku z przetwarzaniem danych osobowych i w sprawie swobodnego przepływu takich danych oraz uchylenia dyrektywy 95/46/WE, zwanego dalej „RODO", informujemy, że:

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8. Na dzień zbierania Pana/~~Pani~~ danych osobowych nie planujemy przekazywać ich poza EOG (obejmujący Unię Europejską, Norwegię, Lichtenstein i Islandię), nie wykluczając tego w przyszłości, o czym zostanie Pan/~~Pani~~ poinformowania ze stosownym wyprzedzeniem.
9. W stosunku do Pana/~~Pani~~ nie będą prowadzone działania polegające na podejmowaniu decyzji w sposób zautomatyzowany, nie będą one również podlegały zautomatyzowanemu profilowaniu.
10. Jeżeli chce Pan/~~Pani~~ skontaktować się z Uczelnią w sprawach związanych z przetwarzaniem danych osobowych, w szczególności w związku z wniesieniem wniosku o realizację przysługujących praw prosimy o kontakt pod adresem e-mail: iod@umk.pl lub adresem korespondencyjnym: UMK w Toruniu, ul. Gagarina 11, 87-100 Toruń, z dopiskiem „IOD", dostępny jest również kontakt telefoniczny: 56 611 27 42.

Podpis jest prawidłowy
Dokument podpisany przez
Bogusław Buszewski
Data: 2024.06.05 07:40:18 CEST

(podpis)

Załącznik nr 5 do uchwały Nr 38 Senatu UMK z dnia 26 września 2023 r.
w sprawie postępowania o nadanie stopnia doktora
na Uniwersytecie Mikołaja Kopernika w Toruniu

Toruń, dnia 3 czerwca 2024 r.

prof. dr hab. Renata Gadzała-Kopciuch
Katedra Chemii Środowiska i Bioanalityki
Wydział Chemii
Uniwersytet Mikołaja Kopernika w Toruniu
ul. Gagarina 7
87-100 Toruń

Rada Dyscypliny Nauki Chemiczne
Uniwersytetu Mikołaja Kopernika w Toruniu

Oświadczenie o współautorstwie

Niniejszym oświadczam, że w pracach:

1. Jadwiga Musiał, Jakub Czarny, Renata Gadzała-Kopciuch, 2022, *Overview of analytical methods for determination of psychoactive substances, drugs and their metabolites in biological samples,* Critical Reviews in Toxicology, 52:239-258. Mój udział w powstaniu pracy wynosi 20 %.
2. Jakub Czarny, Jadwiga Musiał, Jolanta Powierska-Czarny, Natalia Galant, Michał Raczkowski, Bogusław Buszewski, Renata Gadzała-Kopciuch, 2022, *Validation of a simple and quick method for determination of psychoactive substances, drugs and their metabolites from human blood by LC-MS/MS,* Microchemical Journal,182:107922. Mój udział w powstaniu pracy wynosi 5 %.
3. Jadwiga Musiał, Jolanta Powierska-Czarny, Jakub Czarny, Michał Raczkowski, Natalia Galant, Bogusław Buszewski, Renata Gadzała-Kopciuch, 2022, *One-step extraction and determination of 513 psychoactive substances, drugs, and their metabolites from hair by LC-MS/MS*, Archives of Toxicology, 96: 2927-2933. Mój udział w powstaniu pracy wynosi 10 %.
4. Jakub Czarny, Jadwiga Musiał, Jolanta Powierska-Czarny, Michał Raczkowski, Natalia Galant, Bogusław Buszewski, Renata Gadzała-Kopciuch, *Determination of 465 psychoactive substances, drugs and their metabolites in urine by LC-MS/MS.* Praca wysłana do czasopisma Analitycal Methods (RSC). Mój udział w powstaniu pracy wynosi 5 %.

Mój wkład polegał na omówieniu uzyskanych wyników, opiece merytorycznej, korekcie manuskryptów i odpowiedzi na recenzje.

R. Gadzała-Kopciuch
prof. dr hab. Renata Gadzała-Kopciuch
(podpis)

Informacja o przetwarzaniu danych osobowych

Na podstawie Rozporządzenia Parlamentu Europejskiego i Rady (UE) 2016/679 z dnia 27 kwietnia 2016 r. w sprawie ochrony osób fizycznych w związku z przetwarzaniem danych osobowych i w sprawie swobodnego przepływu takich danych oraz uchylenia dyrektywy 95/46/WE, zwanego dalej „RODO", informujemy, że:

1. Administratorem ~~Pana~~/Pani danych osobowych będzie Uniwersytet Mikołaja Kopernika w Toruniu z siedzibą przy ul. Gagarina 11, 87-100 Toruń (dalej: Uczelnia, ADO).
2. ~~Pana/~~Pani dane osobowe w związku w związku z postępowaniem o nadanie stopnia naukowego będą przetwarzane:
    a. na podstawie art. 6 ust. 1 lit. c) RODO – obowiązek prawny wynikający z przepisów ustawy z dnia 20 lipca 2018 r. Prawo o szkolnictwie wyższym i nauce (Dz. U. z 2020, poz. 85);
    b. na podstawie art. 6 ust. 1 lit. f) RODO – prawnie uzasadniony interes ADO:
        - do ustalenia, obrony lub dochodzenia roszczeń – przez okres do przedawnienia roszczeń, lub przez okres prowadzenia postępowania przez właściwe organy lub sądy w przypadku dochodzenia roszczeń,
        - na potrzeby wewnętrzne tworzenia zestawień, analiz i statystyk – przez okres obowiązywania umowy,
        - na potrzeby prowadzenia ewidencji korespondencji przychodzącej i wychodzącej – wieczyście,
        - na potrzeby marketingu produktów i usług ADO.
3. Z zastrzeżeniem przepisów powszechnie obowiązującego prawa przysługują Panu/Pani prawa, które zrealizujemy na wniosek o:
    a. Żądanie dostępu do danych osobowych oraz prawo ich sprostowania,
    b. Żądanie usunięcia lub ograniczenia przetwarzania.
4. Przysługuje ~~Panu/~~Pani również prawo wniesienia sprzeciwu na przetwarzanie danych osobowych.
5. Podanie przez ~~Pana~~/Panią danych osobowych jest niezbędne do wykonania celu wymienionego w pkt 2 lit. a i b., a brak ich podania uniemożliwi otwarcie i przeprowadzenie postępowania.
6. Przysługuje ~~Panu~~/Pani prawo wniesienia skargi do Prezesa Urzędu Ochrony Danych Osobowych.
7. ~~Pana~~/Pani dane osobowe mogą być udostępnione recenzentom lub organom administracji publicznej, sądom, komornikom w zakresie sytuacji przewidzianych w przepisach prawa.
8. Na dzień zbierania ~~Pana~~/Pani danych osobowych nie planujemy przekazywać ich poza EOG (obejmujący Unię Europejską, Norwegię, Lichtenstein i Islandię), nie wykluczając tego w przyszłości, o czym zostanie ~~Pan~~/Pani poinformowania ze stosownym wyprzedzeniem.
9. W stosunku do ~~Pana~~/Pani nie będą prowadzone działania polegające na podejmowaniu decyzji w sposób zautomatyzowany, nie będą one również podlegały zautomatyzowanemu profilowaniu.
10. Jeżeli chce ~~Pan~~/Pani skontaktować się z Uczelnią w sprawach związanych z przetwarzaniem danych osobowych, w szczególności w związku z wniesieniem wniosku o realizację przysługujących praw prosimy o kontakt pod adresem e-mail: iod@umk.pl lub adresem korespondencyjnym: UMK w Toruniu, ul. Gagarina 11, 87-100 Toruń, z dopiskiem „IOD", dostępny jest również kontakt telefoniczny: 56 611 27 42.

Renata Gadzińska-Kopciuch
.....
(podpis)

Załącznik nr 5 do uchwały Nr 38 Senatu UMK z dnia 26 września 2023 r.
w sprawie postępowania o nadanie stopnia doktora
na Uniwersytecie Mikołaja Kopernika w Toruniu

Toruń, dnia 3 czerwca 2024 r.

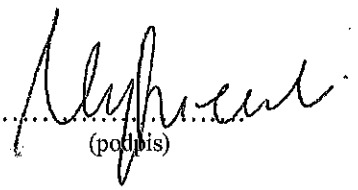
dr Radosław Zbytniewski
Instytut Genetyki Sądowej
ul. Aleje A. Mickiewicza 3/8
85-071 Bydgoszcz

Rada Dyscypliny Nauki Chemiczne Uniwersytetu Mikołaja Kopernika w Toruniu

Oświadczenie o współautorstwie

Niniejszym oświadczam, że w zgłoszeniu patentowym:

Numer zgłoszenia przed UPRP – P.441164; *Sposób wykrywania związków psychoaktywnych w próbkach biologicznych oraz zastosowanie tego sposobu do wykrywania substancji psychoaktywnych*, Jolanta Powierska-Czarny, Jakub Czarny, Radosław Zbytniewski, Michał Raczkowski, Natalia Galant, Jadwiga Musiał. Mój wkład polegał na dyskusji eksperymentu naukowego oraz konsultacji otrzymanych wyników w ramach projektu badawczego. Mój udział w powstaniu pracy wynosi 10 %.



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(podpis)

Informacja o przetwarzaniu danych osobowych

Na podstawie Rozporządzenia Parlamentu Europejskiego i Rady (UE) 2016/679 z dnia 27 kwietnia 2016 r. w sprawie ochrony osób fizycznych w związku z przetwarzaniem danych osobowych i w sprawie swobodnego przepływu takich danych oraz uchylenia dyrektywy 95/46/WE, zwanego dalej „RODO", informujemy, że:

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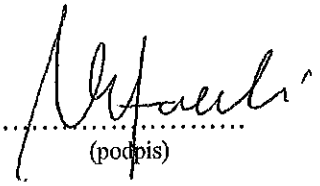

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(podpis)