

Supplementary Material

Figure S1. WG1. Chromatograms (A) and fragmentation spectra (B) of the substances identified and confirmed by the UHPLC-HRMS/MS method. (a) 4-FMC metabolite, (b) methoxyacetyl norfentanyl, (c) 2-CMC, (d) 2-MMC, (e) 3-CMC, (f) 3-MMC, (g) 4-CMC, (h) 5-methoxy AMT, (i) 2-FDCK, (l) 4-MEC metabolite, (m) 4-BMC, (n) methodesnitazene.

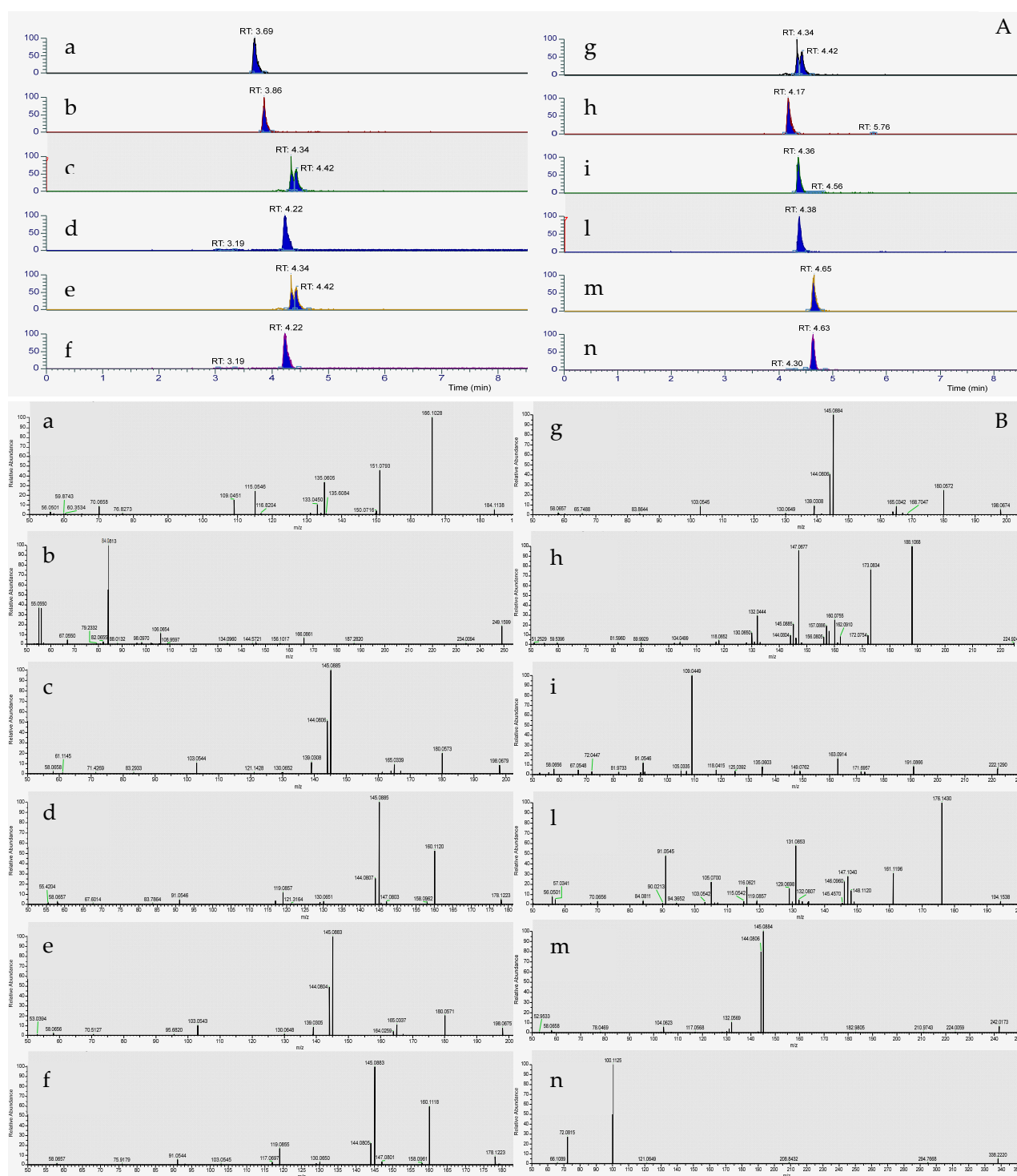


Figure S2. WG2. Chromatograms (A) and fragmentation spectra (B) of the substances identified and confirmed by the UHPLC-HRMS/MS method. (a) deschloro N ethyl ketamine, (b) 6-MAPB, (c) 2-methyl- α -PPP, (d) β -Pentedrone, (e) 5-methoxy MiPT, (f) furanyl norfentanyl, (g) trans 3-methyl norfentanyl, (h) cis 3-methyl norfentanyl, (i) etodesnitazene, (l) 2C-B, (m) N-ethyl pentylone, (n) 4 – EEC, (o) butyryl norfentanyl.

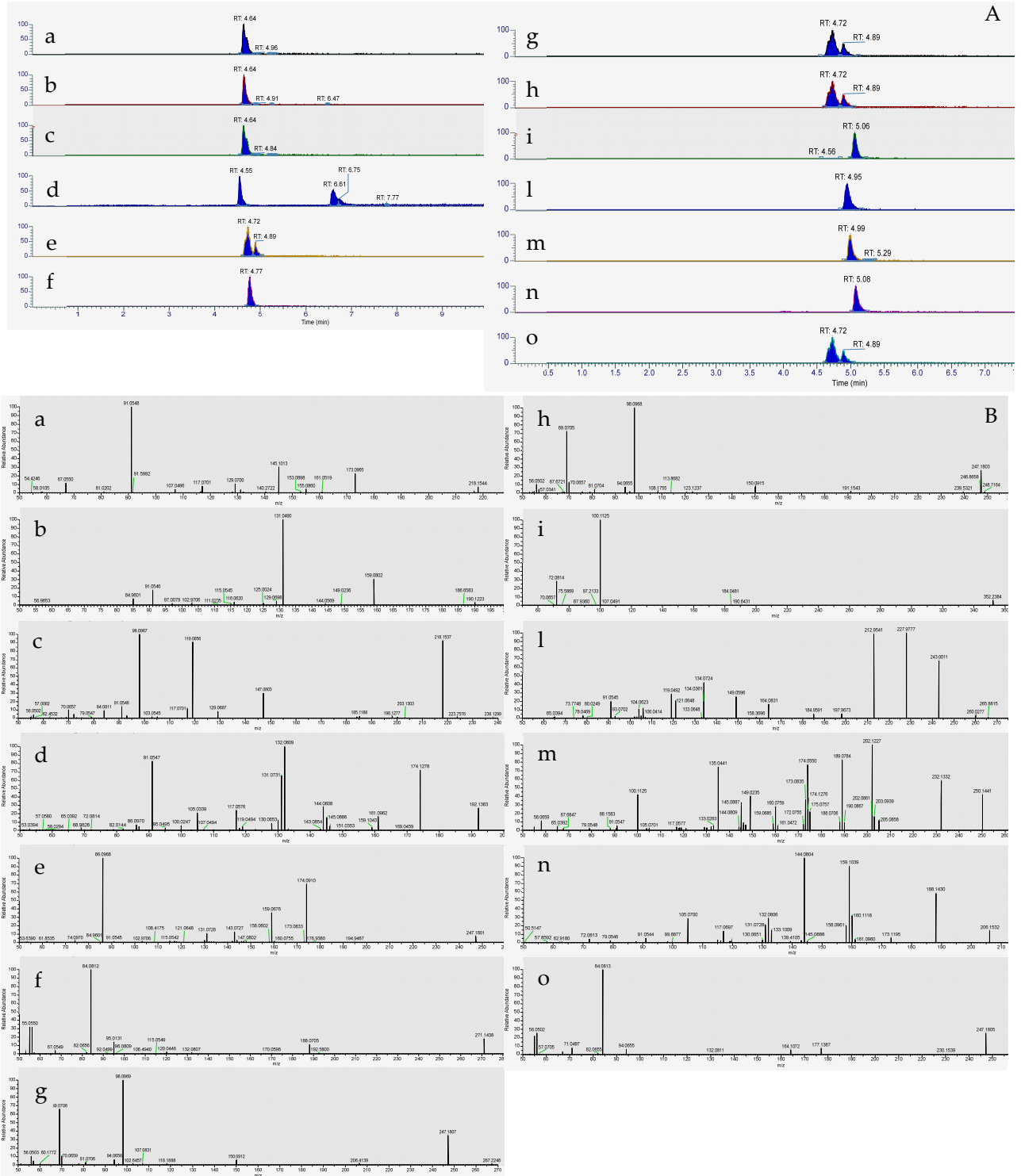


Figure S3. WG3. Chromatograms (A) and fragmentation spectra (B) of the substances identified and confirmed by the UHPLC-HRMS/MS method. (a) 3-F α -PVP, (b) AP-237, (c) 3-HO-PCP, (d) 5-methoxy DALT, (e) AP-238, (f) 2-methyl AP-237, (g) methoxyacetyl fentanyl, (h) α – PiHP, (i) β hydroxythiofentanyl, (l) α -PHP, (m) acetyl fentanyl, (n) 3-methoxy-PCE, (o) 4-Cl- α -PVP.

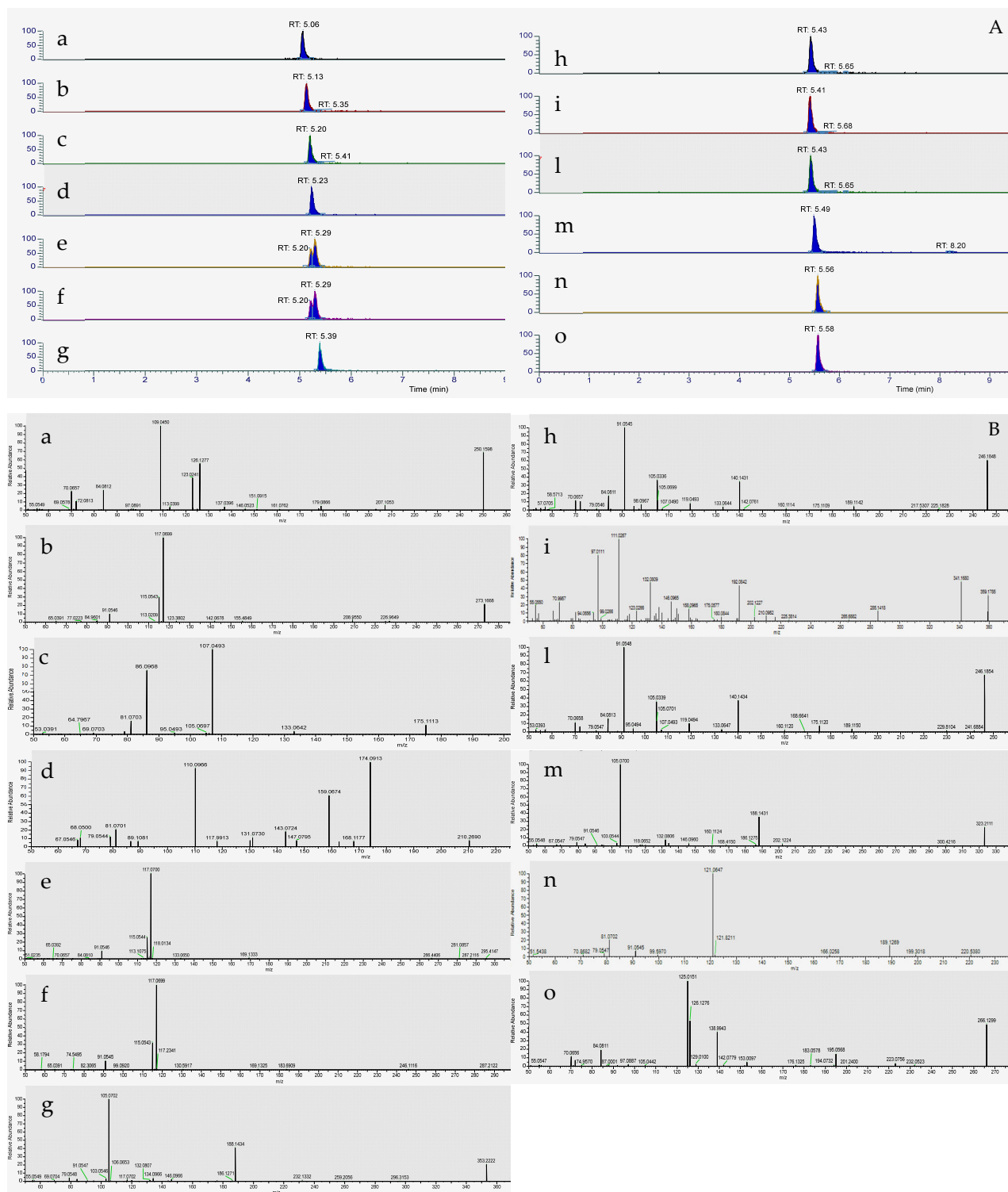


Figure S4. WG4. Chromatograms (A) and fragmentation spectra (B) of the substances identified and confirmed by the UHPLC-HRMS/MS method. (a) 4-f α PHP, (b) MDPiHP, (c) ethyleneoxynitazene, (d) β hydroxyfentanyl, (e) α -PHP metabolite, (f) N-cyclohexyl butylone, (g) N-pyrrolidino etonitazene, (h) N-ethyl heptedrone, (i) brorphine, (l) MPHP, (m) 1-naphyrone, (n) N-piperidinyl etonitazene.

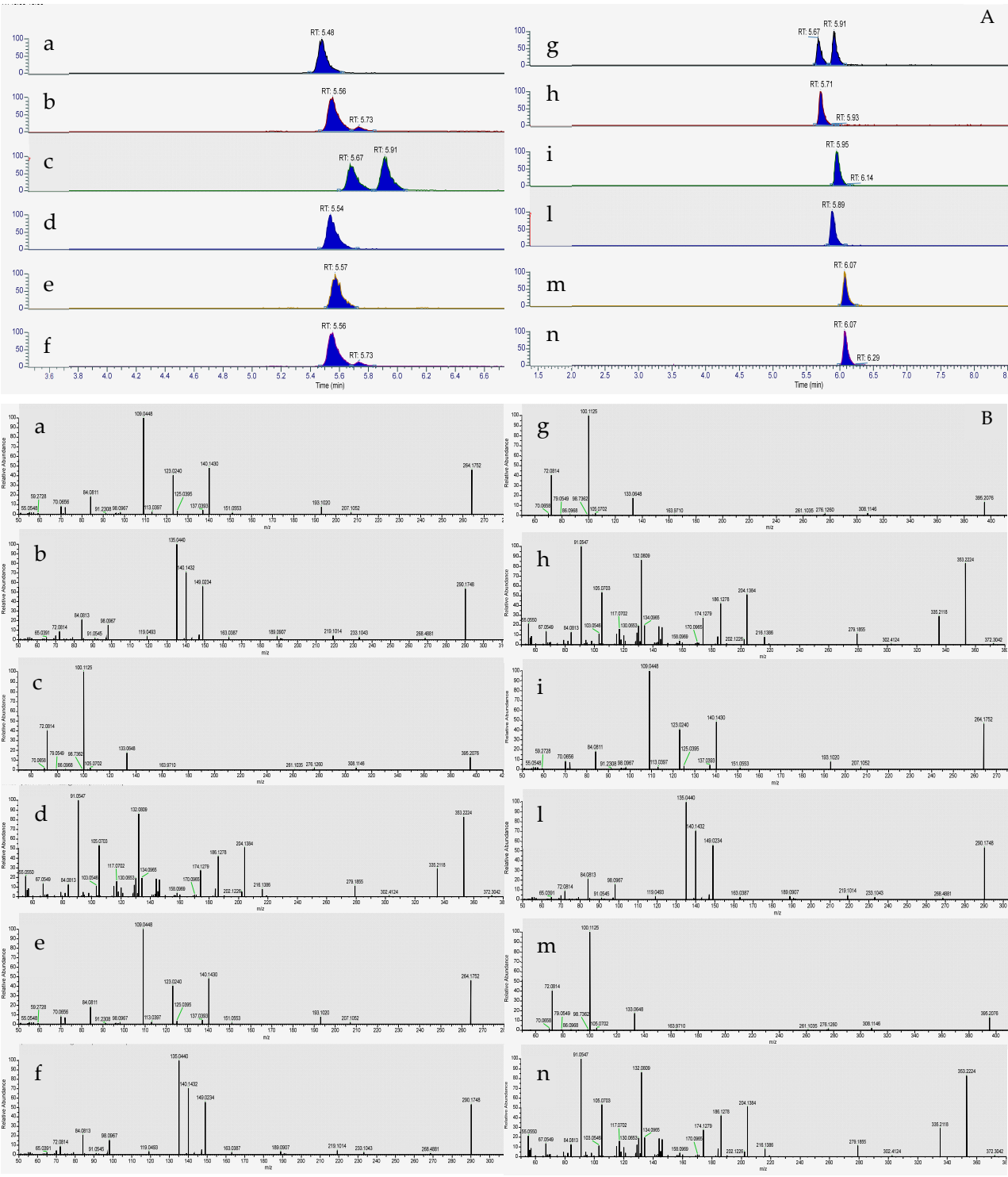


Figure S5. WG5. Chromatograms (A) and fragmentation spectra (B) of the substances identified and confirmed by the UHPLC-HRMS/MS method. (a) furanyl fentanyl, (b) pravadoline, (c) cyclopropyl fentanyl, (d) p-F-furanyl fentanyl, (e) 1CP-LSD, (f) butyryl fentanyl, (g) AM2233, (h) 3,4-Pr-PipVP, (i) 2'-F, o-F (±)-cis-3-methyl fentanyl, (l) protonitazene, (m) phenyl fentanyl, (n) ADB - 5Br – INACA, (o) butonitazene, (p) fluetizolam.

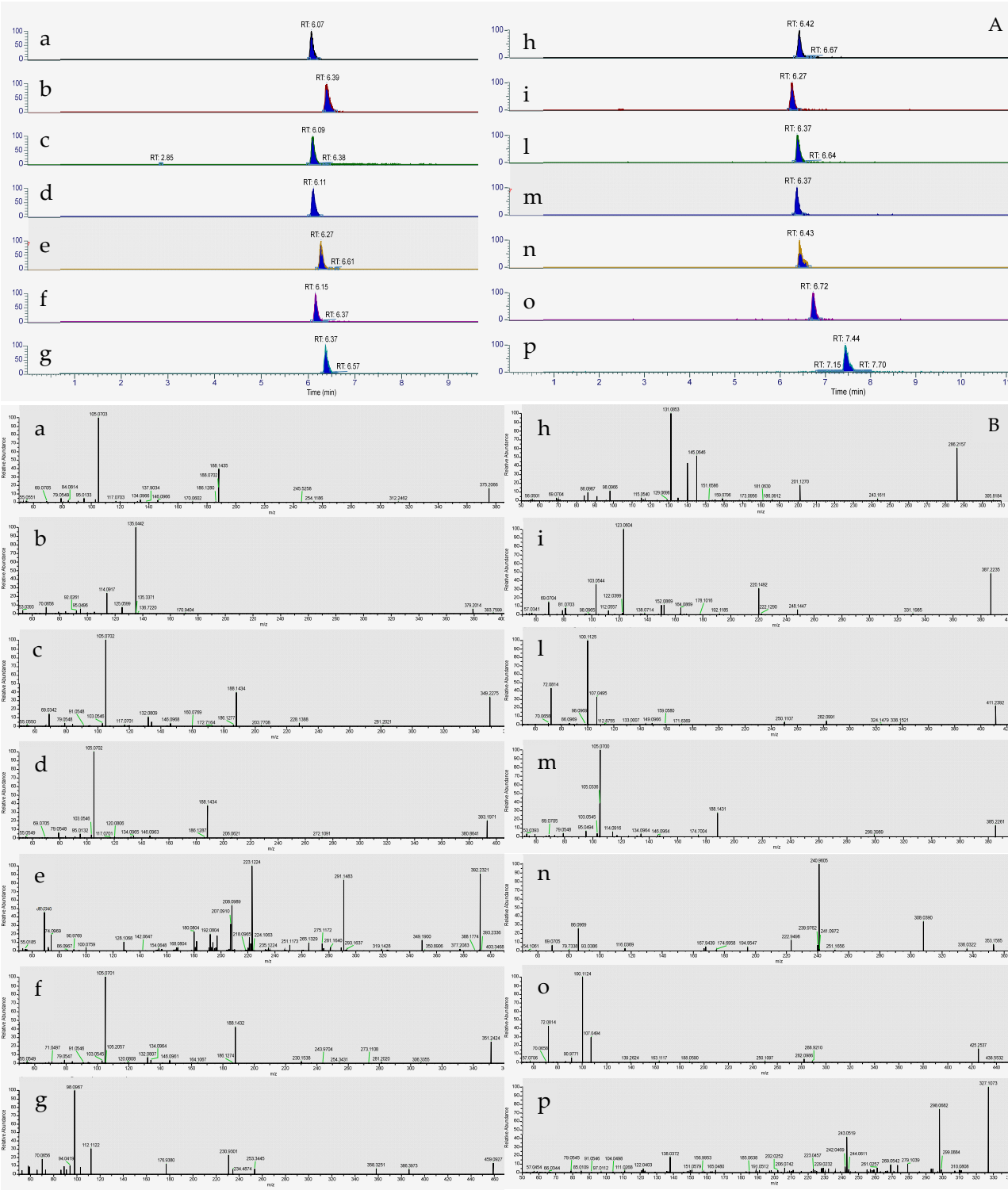


Figure S6. WG6. Chromatograms (A) and fragmentation spectra (B) of the substances identified and confirmed by the UHPLC-HRMS/MS method. (a) β -phenylfentanyl, (b) 5-fluoro-APP-PICA, (c) 5-fluoro-MDMB-7-PAICA, (d) ADB-BUTINACA, (e) APP FU-BINACA, (f) 5-fluoro-CUMYL-P7AICA, (g) ADB-4en-PINACA, (h) MMB2201, (i) 4-Fluoro- MDMB-BUTICA, (l) 4-fluoro MDMB-BUTINACA, (m) BZO-4en-POXIZID.

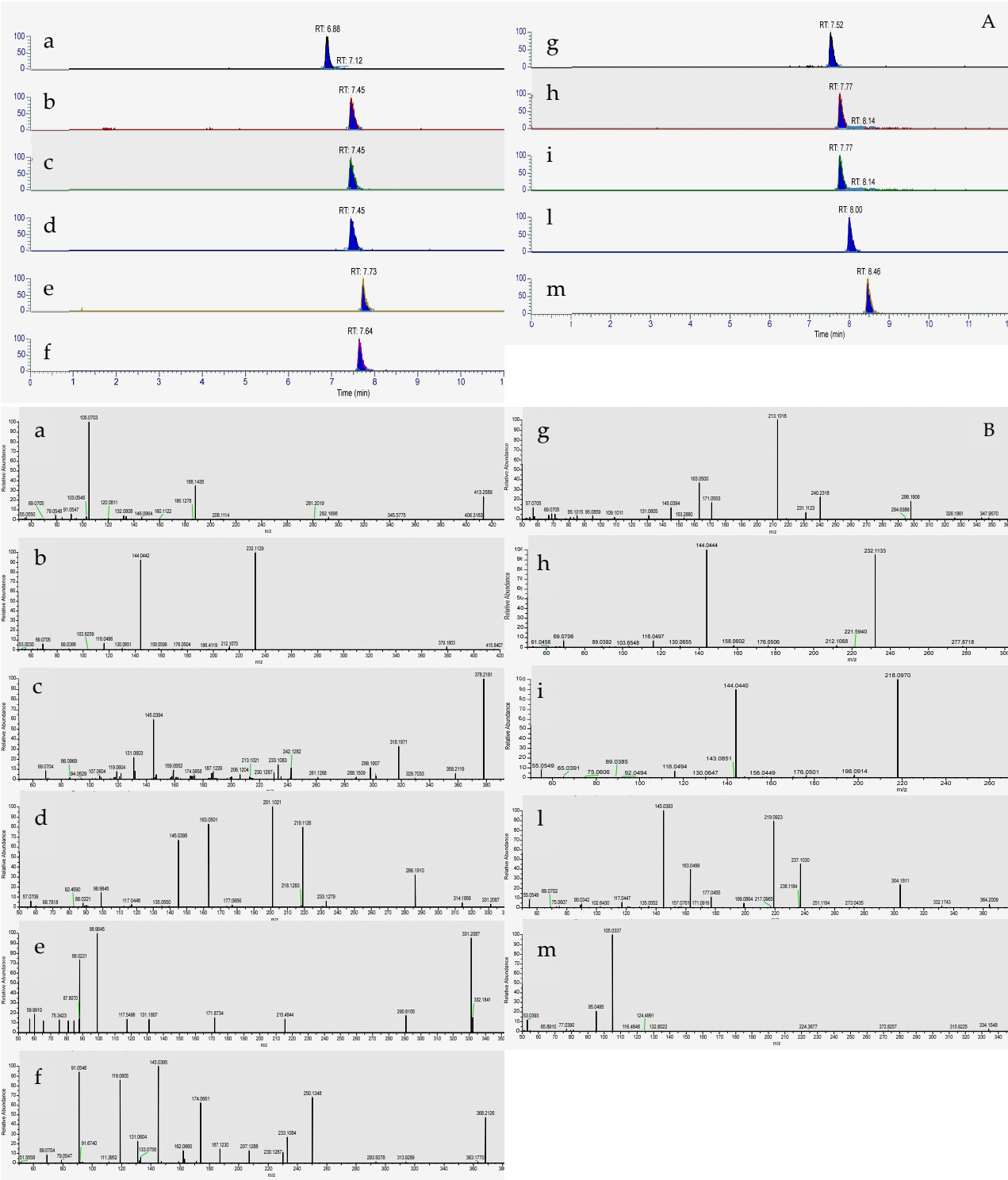


Figure S7. WG7. Chromatograms (A) and fragmentation spectra (B) of the substances identified and confirmed by the UHPLC-HRMS/MS method. (a) 5-fluoro-CUMYL-PICA, (b) 5-fluoro-CUMYL Pegaclone, (c) 5-fluoro NNEI 2'-naptyl isomer, (d) MDMB-4en-PINACA, (e) 5C-MDA-19, (f) 5-fluoro-CUMYL-PINACA, (g) MDMB-4en-PINACA metabolite, (h) MDMB-BUTINACA, (i) = JWH-016, (l) 5-chloro THJ 018, (m) EDMB-PINACA, (n) CUMYL-CH-MeGACLONE.

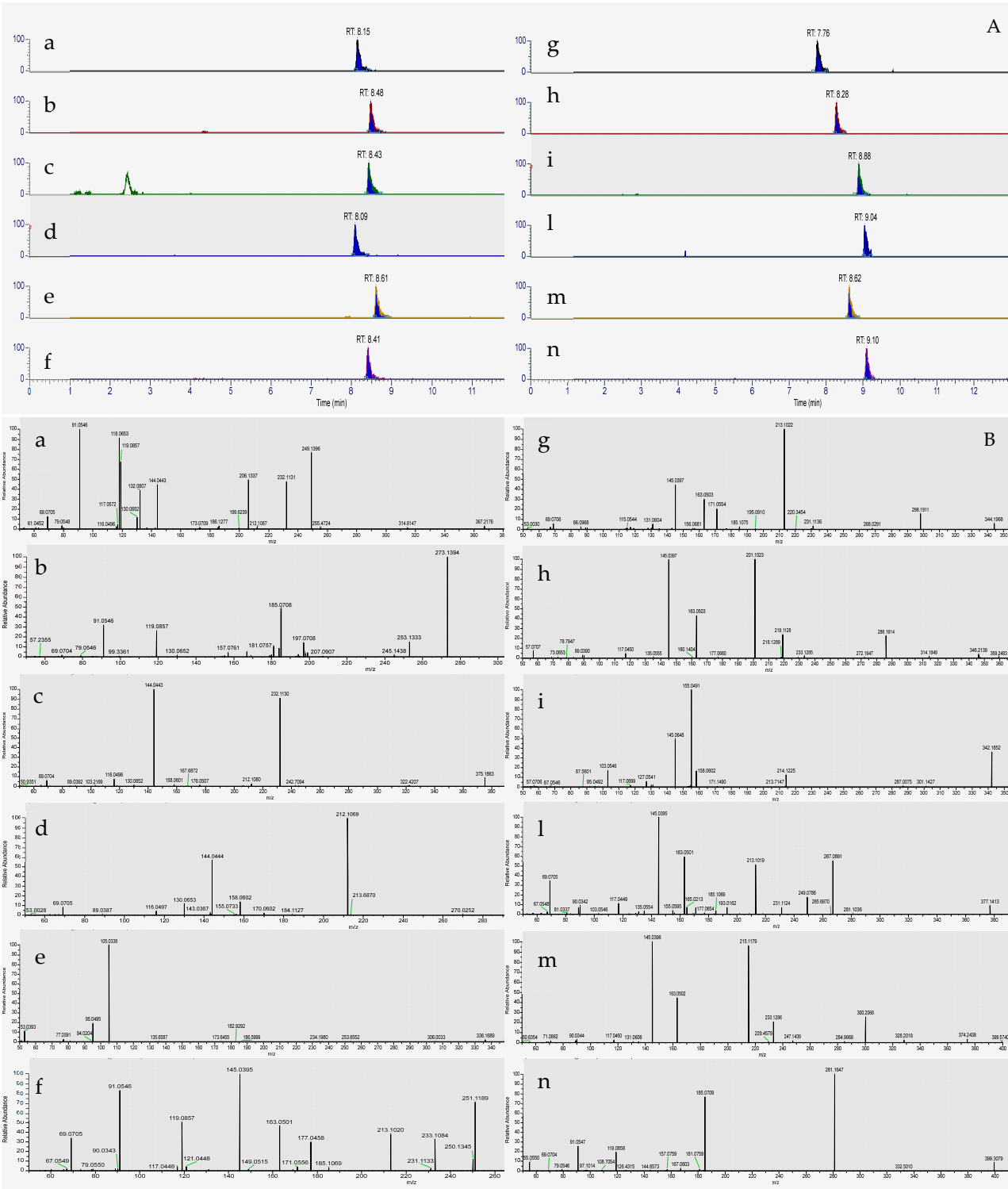


Figure S8. WG8 group. Chromatograms (A) and fragmentation spectra (B) of the substances identified and confirmed by the UHPLC-HRMS/MS method. (a) CUMYL-NBMINACA, (b) 9()-HHC, (c) JWH-147.

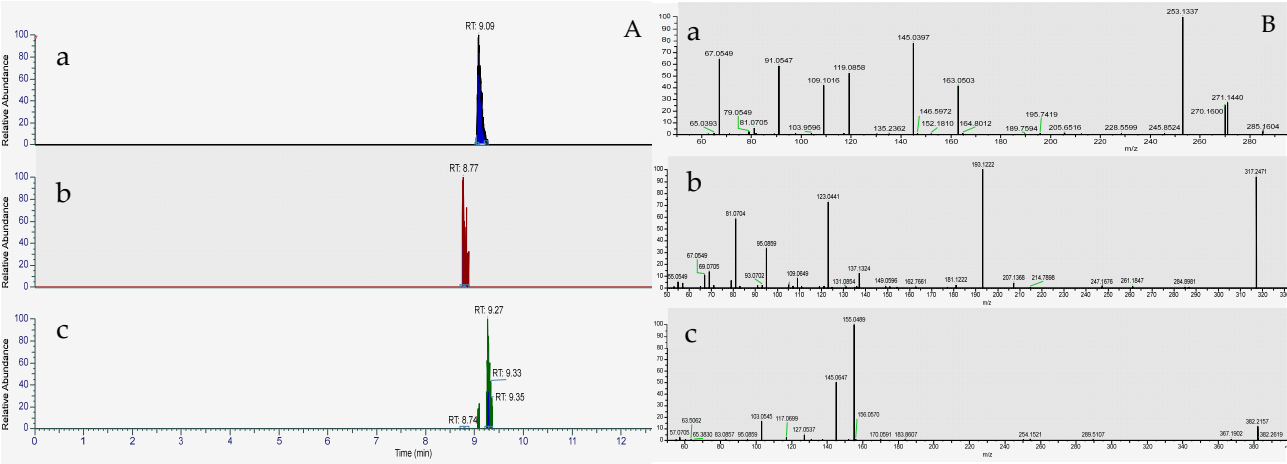


Table S1. Precursor ions, main identifying fragments and retention times of the analyzed standards.

Name	Class	Formula	RT	[M+ H] m/z	m/z fragments
1- Naphyrone	Synthetic cathinones	C19H23NO	6.07	282.1850	126.1278 141.0689 155.0491 169.0650 211.1116 282.1850
2C-B	Phenethylamines	C10H14BrNO2	4.94	260.0276	91.6768 212.9546 227.9780 243.0014
2'-F. o-F(±)-cis-3-methylfentanyl	Synthetic opioids	C23H28F2N2O	6.26	387.2237	69.0705 103.0545 123.0606 152.0807 220.1495 331.1978

					387.2237
2-FDCK	Arylcyclohexylamines	C13H16FNO	4.35	222.1288	67.0549 109.0450 147.0640 163.0917 191.0866 204.1183
2-methyl AP-237	Synthetic opioids	C18H26N2O	5.20	287.2115	115.0544 117.0700
2-methyl- α -PPP	Synthetic cathinones	C14H19NO	4.64	218.1538	98.0968 119.0857 129.0700 147.0803 218.1538
3-CMC	Synthetic cathinones	C10H12ClNO	4.34	198.068	103.0543 139.0305 144.0804 145.0883 165.0337 180.0571
3-MMC	Synthetic cathinones	C11H15NO	4.22	178.1222	119.0855 144.0805 145.0883 160.1118
3-methoxy-PCE	Arylcyclohexylamines	C15H23NO	5.55	234.1846	81.0702 91.0545 121.0647 166.0258 189.1269 220.5380
3,4-Pr-PipVP	Synthetic cathinones	C19H27NO	6.41	286.2158	98.0966

					115.0544
					131.0853
					140.1431
					145.0647
					201.1269
					243.1615
3-F- α -PVP	Synthetic cathinones	C15H20FNO	5.04	250.16	70.0657
					84.0812
					109.0449
					126.1277
					179.0864
					207.1051
3-HO-PCP	Arylcyclohexylamines	C17H25NO	4.95	260.2002	86.0968
					107.0493
					133.0642
					175.1113
4-BMC	Synthetic cathinones	C10H12BrNO	4.62	242.0172	104.0623
					132.0569
					144.0806
					145.0884
					182.9805
4-CMC	Synthetic cathinones	C10H12ClNO	4.34	198.068	103.0545
					139.0308
					144.0806
					145.0884
					165.0342
					180.0572
4-EEC	Synthetic cathinones	C13H19NO	5.08	206.15394	105.07
					117.0697
					132.0806
					144.0804

					159.1039
					188.143
4-Cl- α -PVP	Synthetic cathinones	C15H20ClNO	5.56	266.1299	84.0811
					125.0151
					126.1276
					138.9943
					195.0568
4-F- α -PHP	Synthetic cathinones	C16H22FNO	5.47	264.1753	84.0811
					109.0448
					123.0240
					140.1430
					193.1020
4-F-MDMB-BUTINACA	Synthetic cannabinoids	C19H26FN3O3	8.00	364.202	145.0393
					163.0499
					219.0923
					237.1030
					304.1811
4-F-MDMB-BUTICA	Synthetic cannabinoids	C20H27FN2O3	7.82	363.2067	116.0494
					144.0440
					218.097
4-MEC metabolite	Synthetic cathinones	C12H19NO	3.34	194.1536	91.0545
					105.0700
					116.0621
					129.0698
					131.0853
					146.0960
					147.1040
					161.1196
					176.1430
MPHP	Synthetic cathinones	C17H25NO	5.88	260.2007	84.0812
					105.0701

					119.0492
					133.0646
					140.1432
					189.1274
5-Cl-THJ 018	Synthetic cannabinoids	C23H21ClN2O	9.06	377.141	145.0395
					163.0501
					213.1019
					249.0786
					267.0891
5C-MDA-19	Synthetic cannabinoids	C20H21N3O2	8.64	336.1701	53.0393
					95.0495
					105.0338
5-F-NNEI 2'-naphthyl isomer	Synthetic cannabinoids	C24H23FN2O	8.44	375.1861	116.0496
					144.0442
					232.1128
5-F-APP-PICA	Synthetic cannabinoids	C23H26FN3O2	7.45	396.2077	116.0496
					144.0442
					232.1129
5-F-CUMYL Pegaclone	Synthetic cannabinoids	C25H27FN2O	8.49	391.2175	91.0546
					119.0857
					185.0708
					197.0708
					253.1333
					273.1394
5-fluoro-CUMYL-P7AICA	Synthetic cannabinoids	C22H26FN3O	7.64	368.2126	91.0546
					119.0605
					131.0604
					145.0395
					162.0660
					174.0661
					187.1230

					207.1288
					233.1084
					250.1348
5-F-CUMYL-PICA	Synthetic cannabinoids	C23H27FN2O	8.17	367.2176	91.0546
					118.0653
					119.0857
					132.0807
					144.0443
					206.1337
					232.1131
					249.1396
5-F-CUMYL-PINACA	Synthetic cannabinoids	C22H26FN3O	8.42	368.2125	69.0705
					91.0546
					119.0857
					145.0395
					163.0501
					177.0458
					213.1020
					233.1084
					251.1189
5-F-MDMB-7-PAICA	Synthetic cannabinoids	C20H28FN3O3	7.45	378.2181	119.0604
					131.0603
					145.0394
					159.0552
					233.1083
					242.1282
					298.1907
					318.1971
5-methoxy AMT	Synthetic tryptamines	C12H16N2O	4.16	205.1335	130.0650
					132.0444
					145.0885

					147.0677
					160.0755
					173.0834
					188.1068
5-methoxy DALT	Synthetic tryptamines	C17H22N2O	5.28	271.1804	79.0544
					81.0701
					110.0966
					117.9913
					131.0730
					143.0724
					159.0674
					174.0913
					210.2690
5-methoxy MiPT	Synthetic tryptamines	C15H22N2O	4.69	247.1801	86.0968
					131.0728
					143.0727
					159.0676
					174.0910
6-MAPB	Phenethylamines	C12H15NO	4.65	190.1223	84.9601
					91.0546
					129.0698
					131.0490
					131.0853
					159.0802
9-HHC	Synthetic cannabinoids	C21H32O2	8.79	317.2647	81.0703
					95.0858
					109.0649
					123.0440
					137.0595
					193.1219
					207.1383

					317.2467
Acetyl fentanyl	Synthetic opioids	C21H26N2O	5.50	323.2111	103.0543 105.0700 132.0805 188.1429 202.1222 323.2111
ADB-4en-PINACA	Synthetic cannabinoids	C19H26N4O2	7.54	343.212	131.0605 145.0394 163.0500 171.0553 213.1018 231.1123 240.2318 298.1906
ADB-BUTINACA	Synthetic cannabinoids	C18H26N4O2	7.45	331.2125	98.9845 117.0448 145.0395 163.0501 177.0656 201.1021 219.1126 233.1279 286.1910 314.1856
AM2233	Synthetic cannabinoids	C22H23IN2O	6.39	459.0924	70.0658 94.0417 98.0968 112.1123 230.9294 362.0037

AP-237	Synthetic opioids	C17H24N2O	5.13	273.1957	91.0546 115.0543 117.0699
AP-238	Synthetic opioids	C18H26N2O	5.28	287.2214	91.0546 115.0544 117.0700
APP FUBINACA	Synthetic cannabinoids	C24H21FN4O2	7.74	417.1721	109.045 225.0823 253.0767 271.0875 372.1494
Brorphine	Synthetic opioids	C20H22BrN3O	5.95	400.1013	84.0812 104.0623 135.0552 173.0708 182.9802 218.1285
Butonitazene	Synthetic opioids	C24H32N4O3	6.72	425.2542	72.0814 100.1124 107.0494 282.0996
Butyryl fentanyl	Synthetic opioids	C23H30N2O	6.16	351.2425	103.0545 105.0701 132.0807 146.0961 188.1432 230.1538 351.2425
Butyryl norfentanyl	Synthetic opioids	C15H22N2O	4.89	247.1804	84.0813 94.0655 94.0665

					164.1062
					177.1387
					247.1804
BZO-4en-POXIZID	Synthetic cannabinoids	C20H19N3O2	8.46	334.1543	95.0495
					105.0337
					105.0440
Cis 3-methyl norfentanyl	Synthetic opioids	C15H22N2O	4.72	247.1803	69.0705
					94.0655
					98.0968
					150.0915
CUMYL-CH-MeGACLONE	Synthetic cannabinoids	C27H30N2O	9.11	399.2429	91.0547
					119.0858
					185.0710
					281.1648
CUMYL-NBMINACA	Synthetic cannabinoids	C25H29N3O	9.11	388.238	67.0549
					91.0547
					109.1016
					119.0858
					145.0397
					163.0503
					253.1337
					270.1600
					271.1440
					285.0160
Cyclopropyl fentanyl	Synthetic opioids	C23H28N2O	6.09	349.2272	69.0342
					103.0546
					105.0702
					132.0809
					146.0968
					188.1434
					238.1388

					349.2275
Deschloro-N-ethyl-ketamine	Arylcyclohexylamines	C14H19NO	4.65	218.1538	67.055 91.0548 107.0496 117.0701 129.0700 145.1013 173.0965 218.1544
EDMB-PINACA	Synthetic cannabinoids	C21H31N3O3	8.64	374.2436	145.0396 163.0502 215.1179 233.1286 300.2068
Ethyleneoxynitazene	Synthetic opioids	C22H26N4O3	5.68	395.2075	72.0814 100.1125 133.0648 395.2076
Etodesnitazene	Synthetic opioids	C22H29N3O	5.07	352.238	72.0814 100.1125
4-FMC metabolite	Synthetic cathinones	C10H14FNO	3.69	184.1132	70.0658 109.0451 115.0546 115.0546 133.0450 135.0605 151.0793 166.1028 184.1138
Fluetizolam	Benzodiazepine	C17H15FN4S	7.44	327.1073	138.0372 206.0742

					243.0519
					298.0682
					327.1073
Furanyl norfentanyl	Synthetic opioids	C16H18N2O2	4.76	271.1438	56.0502
					84.0812
					95.0131
					188.0705
					271.1438
Furanyl fentanyl	Synthetic opioids	C24H26N2O2	6.07	375.2065	95.0133
					103.0547
					105.0703
					188.1435
					375.2066
JWH-016	Synthetic cannabinoids	C24H23NO	8.90	342.1852	103.0545
					127.054
					145.0647
					155.0491
					158.0600
					214.1224
MDMB-4en-PICA	Synthetic cannabinoids	C21H28N2O3	8.11	357.2169	69.0705
					116.0497
					130.0653
					144.0444
					158.0602
					212.1069
MDMB-4en-PINACA metabolite	Synthetic cannabinoids	C17H25N3O3	7.79	344.1968	131.0604
					145.0397
					163.0503
					171.0554
					213.1022
					298.1911

					344.1968
MDMB-BUTINACA	Synthetic cannabinoids	C19H27N3O3	8.29	346.2122	57.0707 117.0450 145.0397 163.0503 201.1023 219.1128 286.1914
Methoxyacetyl fentanyl	Synthetic opioids	C22H28N2O2	5.38	353.2221	103.0546 105.0702 117.0702 134.0966 188.1434 353.2222
Methoxyacetyl norfentanyl	Synthetic opioids	C14H20N2O2	3.86	249.1596	55.055 84.0813 106.0654 166.0861
Metodesnitazene	Synthetic opioids	C21H27N3O	4.63	338.2224	72.0815 100.1125 338.222
MMB2201	Synthetic cannabinoids	C20H27FN2O3	7.77	363.2078	69.0706 116.0497 144.0444 232.1133
N-cyclohexyl butylone	Synthetic cathinones	C17H23NO3	5.73	290.1747	83.086 105.0704 117.0577 132.0808 133.0647 143.0231

					160.0757
					161.0597
					190.0862
					191.0698
					208.0968
N-ethyl heptedrone	Synthetic cathinones	C15H23NO	5.72	234.1853	91.0548
					105.0339
					107.0495
					117.0577
					118.0655
					130.0653
					145.0887
					146.0965
					158.0964
N-ethyl pentylone	Synthetic cathinones	C14H19NO3	5.00	250.1436	100.1125
					135.0441
					145.0887
					149.0235
					160.0759
					173.0835
					174.055
					189.0784
					202.1227
					232.1332
					250.1441
N-piperidiny l etonitazene	Synthetic opioids	C23H28N4O3	6.07	409.2232	69.0706
					84.0814
					107.0495
					112.1124
					135.0806
N-pyrrolidin etonitazene	Synthetic opioids	C22H26N4O3	5.90	395.2075	98.0967

					107.0493
					135.0805
p-F-furanyl fentanyl	Synthetic opioids	C ₂₄ H ₂₅ FN ₂ O ₂	6.10	393.1969	79.0548
					95.0132
					103.0546
					105.0702
					186.1287
					188.1434
					272.1091
					393.1971
Phenyl fentanyl	Synthetic opioids	C ₂₆ H ₂₈ N ₂ O	6.37	385.2271	105.0703
					146.0964
					188.1434
Pravadoline	Synthetic cannabinoids	C ₂₃ H ₂₆ N ₂ O ₃	6.40	379.2016	70.0658
					95.0496
					105.0452
					114.0917
					125.0599
					135.0442
Protonitazene	Synthetic opioids	C ₂₃ H ₃₀ N ₄ O ₃	6.38	411.239	72.0814
					100.1125
					107.0495
					282.0991
					411.2392
Trans 3-methyl norfentanyl	Synthetic opioids	C ₁₅ H ₂₂ N ₂ O	4.72	247.1805	69.0706
					96.0658
					98.0969
					150.0912
					247.1807
α-PiHP	Synthetic cathinones	C ₁₆ H ₂₃ NO	5.43	246.1853	84.0813
					91.0547

					105.0339
					119.0494
					133.0649
					140.1434
					189.1149
					246.1853
α -PHP	Synthetic cathinones	C16H23NO	5.43	246.1852	84.0813
					91.0548
					105.0339
					119.0494
					133.0647
					140.1434
					175.1120
					189.1100
					246.1854
α -PHP metabolite	Synthetic cathinones	C16H25NO	5.57	248.2009	72.0815
					79.0549
					91.0548
					104.0625
					107.0496
					117.0702
					173.1199
					230.1906
					248.2010
β -hydroxy fentanyl	Synthetic opioids	C22H28N2O2	5.55	353.2223	91.0547
					105.0703
					117.0702
					130.0653
					132.0809
					134.0965
					144.0809

					146.0966 174.1279 186.1278 204.1384 279.1855 335.2218
β -hydroxy thiofentanyl	Synthetic opioids	C20H26N2O2S	5.41	359.1786	97.0111 111.0267 123.0266 132.0809 146.0965 158.0968 192.0842 285.1418 341.1680 359.1785
β -Pentedrone	Synthetic cathinones	C12H17NO	4.54	192.1383	91.0548 105.0339 117.0577 128.0196 130.0654 131.0732 132.0810 145.0888 161.0960 174.1279
β -phenyl fentanyl	Synthetic opioids	C28H32N2O	6.92	413.2585	91.0547 105.0703 132.0808 188.1435
2-CMC	Synthetic cathinones	C10H12ClNO	4.43	198.0678	103.0544

					139.0308
					144.0806
					145.0885
					165.0339
					180.0573
					198.0679
2-MMC	Synthetic cathinones	C11H15NO	4.23	178.1225	91.0546
					119.0857
					130.0651
					144.0807
					145.0885
					160.1120
					178.1223
MDPiHP	Synthetic cathinones	C17H23NO3	5.55	290.1747	84.0813
					98.0968
					135.0440
					140.1433
					149.0233
					219.1014
1CP-LSD	Synthetic cannabinoids	C24H29N3O2	6.26	392.2329	69.0341
					74.097
					90.977
					128.1070
					180.0806
					192.0809
					207.0913
					208.0755
					223.1227
					291.1490
					392.2329
JWH-147	Synthetic cannabinoids	C27H27NO	9.29	382.2161	103.0545

					117.0699
					127.0537
					131.0488
					145.0647
					155.0489
					367.1902
ADB-5Br-INACA	Synthetic cannabinoids	C14H17BrN4O2	6.43	353.0603	86.0969
					116.0369
					194.9552
					222.9497
					240.9603
					308.0388
					336.0340