

Supporting Materials

Investigation of New Psychoactive Substances (NPS), Other Illicit Drugs, and Drug-Related Compounds in a Taiwanese Wastewater Sample Using High-Resolution Mass-Spectrometry-Based Targeted and Suspect Screening

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Table S1. 92 identified substances based on suspect screening.

Compound name	Molecular formula	Theoretical m/z ($[M+H]^+$)	Measured m/z ($[M-H]^+$)	Mass error (ppm)	MS/MS similarity scores	Database
Paracetamol	C ₈ H ₉ NO ₂	152.0706	152.0703	-2.0	0.97	mzCloud
Ephedrine	C ₁₀ H ₁₅ NO	166.1226	166.1225	-0.8	0.93	mzCloud
11-ketotestosterone	C ₁₉ H ₂₆ O ₃	303.1955	303.1949	-1.9	0.88	mzCloud
Dextrorphan	C ₁₇ H ₂₃ NO	258.1852	258.1849	-1.3	0.88	mzCloud
1,4-Androstadiene-3,17-dione	C ₁₉ H ₂₄ O ₂	285.1849	285.1845	-1.4	0.87	mzCloud
Tramadol	C ₁₆ H ₂₅ NO ₂	264.1958	264.1956	-0.8	0.86	mzCloud
Levorphanol	C ₁₇ H ₂₃ NO	258.1852	258.1848	-1.7	0.86	mzCloud
Testosterone propionate	C ₂₂ H ₃₂ O ₃	345.2424	345.2420	-1.2	0.85	mzCloud
Hydromorphone	C ₁₇ H ₁₉ NO ₃	286.1438	286.1433	-1.6	0.83	mzCloud
Phenethylamine	C ₈ H ₁₁ N	122.0964	122.0965	0.6	0.82	mzCloud
Anthranilic acid	C ₇ H ₇ NO ₂	138.0550	138.0549	-0.4	0.82	mzCloud
N-Methyl-2-phenylpropan-1-amine	C ₁₀ H ₁₅ N	150.1277	150.1278	0.5	0.82	mzCloud
5alpha-Androstan-3,6,17-trione	C ₁₉ H ₂₆ O ₃	303.1955	303.1949	-1.9	0.81	mzCloud
6beta-Hydromorphol	C ₁₇ H ₂₁ NO ₃	288.1594	288.1590	-1.5	0.81	mzCloud
1,3-Dimethylbutylamine	C ₆ H ₁₅ N	102.1277	102.1277	-0.3	0.80	mzCloud
Diphenhydramine	C ₁₇ H ₂₁ NO	256.1696	256.1692	-1.5	0.80	mzCloud
N-Methyl-2-Al	C ₁₀ H ₁₃ N	148.1121	148.1120	-0.5	0.78	mzCloud
Formestane	C ₁₉ H ₂₆ O ₃	303.1955	303.1949	-1.9	0.78	mzCloud
Dihydromorphone	C ₁₇ H ₂₁ NO ₃	288.1594	288.1590	-1.5	0.78	mzCloud
Tapentadol	C ₁₄ H ₂₃ NO	222.1852	222.1847	-2.4	0.76	mzCloud
4-Methyl-N,N-dimethylcathinone	C ₁₂ H ₁₇ NO	192.1383	192.1381	-1.0	0.75	mzCloud
Testosterone cypionate	C ₂₇ H ₄₀ O ₃	413.3050	413.3042	-2.0	0.74	mzCloud
Methenolone	C ₂₀ H ₃₀ O ₂	303.2319	303.2314	-1.5	0.74	mzCloud
MDPV	C ₁₆ H ₂₁ NO ₃	276.1594	276.1591	-1.2	0.74	mzCloud
(-)-Caryophyllene oxide	C ₁₅ H ₂₄ O	221.1900	221.1899	-0.4	0.73	mzCloud
MEAI	C ₁₀ H ₁₃ NO	164.1070	164.1068	-1.2	0.72	mzCloud
Bufotenin	C ₁₂ H ₁₆ N ₂ O	205.1335	205.1335	-0.2	0.70	mzCloud
5-AEDB	C ₁₀ H ₁₃ NO	164.1070	164.1068	-1.2	0.70	mzCloud
Nicotine	C ₁₀ H ₁₄ N ₂	163.1230	163.1227	-0.7	0.97	MoNA
Cyclohexylamine	C ₆ H ₁₃ N	100.1121	100.1120	0.1	0.96	MoNA
Cimetidine	C ₁₀ H ₁₆ N ₆ S	253.1230	253.1224	-1.3	0.95	MoNA
Phenylacetaldehyde	C ₈ H ₈ O	121.0648	121.0649	1.8	0.95	MoNA
4-Methyl-5-thiazoleethanol	C ₆ H ₉ NOS	144.0478	144.0475	-0.9	0.94	MoNA
Carbamazepine	C ₁₅ H ₁₂ N ₂ O	237.1023	237.1020	0.0	0.94	MoNA
Atenolol	C ₁₄ H ₂₂ N ₂ O ₃	267.1703	267.1700	-0.2	0.94	MoNA
Trimethoprim	C ₁₄ H ₁₈ N ₄ O ₃	291.1452	291.1446	-0.9	0.94	MoNA
Sulfapyridine	C ₁₁ H ₁₁ N ₃ O ₂ S	250.0645	250.0643	0.3	0.94	MoNA
Progesterone	C ₂₁ H ₃₀ O ₂	315.2319	315.2314	-0.4	0.94	MoNA
Amantadine	C ₁₀ H ₁₇ N	152.1434	152.1432	-0.2	0.93	MoNA
Salicylamide	C ₇ H ₇ NO ₂	138.0550	138.0548	-0.2	0.93	MoNA
Bisoprolol	C ₁₈ H ₃₁ NO ₄	326.2326	326.2320	-0.8	0.93	MoNA
Caffeine	C ₈ H ₁₀ N ₄ O ₂	195.0877	195.0873	-0.8	0.93	MoNA
4-Androstene-3,17-dione	C ₁₉ H ₂₆ O ₂	287.2006	287.2002	-0.2	0.93	MoNA
Methocarbamol	C ₁₁ H ₁₅ NO ₅	242.1023	242.1021	0.2	0.92	MoNA
Levetiracetam	C ₈ H ₁₄ N ₂ O ₂	171.1128	171.1125	-0.8	0.92	MoNA
Pilocarpine	C ₁₁ H ₁₆ N ₂ O ₂	209.1285	209.1284	0.7	0.92	MoNA

Theobromine	C ₇ H ₈ N ₄ O ₂	181.0720	181.0717	-0.7	0.91	MoNA
THEOPHYLLINE	C ₇ H ₈ N ₄ O ₂	181.0720	181.0717	-0.7	0.91	MoNA
Ethambutol	C ₁₀ H ₂₄ N ₂ O ₂	205.1911	205.1909	0.2	0.91	MoNA
Dextromethorphan	C ₁₈ H ₂₅ NO	272.2009	272.2005	-0.4	0.91	MoNA
Lidocaine	C ₁₄ H ₂₂ N ₂ O	235.1805	235.1802	-0.2	0.91	MoNA
N-Methylephedrine	C ₁₁ H ₁₇ NO	180.1383	180.1382	0.5	0.90	MoNA
Celecoxib	C ₁₇ H ₁₄ F ₃ N ₃ O ₂ S	382.0832	382.0826	-0.4	0.90	MoNA
Piperine	C ₁₇ H ₁₉ NO ₃	286.1438	286.1433	-0.6	0.90	MoNA
Androsta-1,4-Dien-3,17-Dione	C ₁₉ H ₂₄ O ₂	285.1849	285.1844	-0.7	0.90	MoNA
Phenylalanine	C ₉ H ₁₁ NO ₂	166.0863	166.0861	0.0	0.90	MoNA
Adenine	C ₅ H ₅ N ₅	136.0618	136.0618	1.1	0.90	MoNA
Flecainide	C ₁₇ H ₂₀ F ₆ N ₂ O ₃	415.1451	415.1442	-1.1	0.89	MoNA
Fexofenadine	C ₃₂ H ₃₉ NO ₄	502.2952	502.2941	-1.1	0.88	MoNA
Propranolol	C ₁₆ H ₂₁ NO ₂	260.1645	260.1642	-0.2	0.88	MoNA
Diethyl-phthalate	C ₁₂ H ₁₄ O ₄	223.0965	223.0961	-0.7	0.88	MoNA
Acetaminophen	C ₈ H ₉ NO ₂	152.0706	152.0705	0.3	0.88	MoNA
Citalopram	C ₂₀ H ₂₁ FN ₂ O	325.1711	325.1707	-0.1	0.87	MoNA
Hexylamine	C ₆ H ₁₅ N	102.1277	102.1277	0.6	0.85	MoNA
Metronidazole	C ₆ H ₉ N ₃ O ₃	172.0717	172.0716	0.6	0.85	MoNA
Hordenine	C ₁₀ H ₁₅ NO	166.1227	166.1226	0.7	0.85	MoNA
3'-Aminoacetophenone	C ₈ H ₉ NO	136.0757	136.0757	1.0	0.84	MoNA
Fluconazole	C ₁₃ H ₁₂ F ₂ N ₆ O	307.1114	307.1111	0.2	0.84	MoNA
Cyclophosphamide	C ₇ H ₁₅ Cl ₂ N ₂ O ₂ P	261.0321	261.0320	0.7	0.83	MoNA
Phenylethanolamine	C ₈ H ₁₁ NO	138.0914	138.0913	0.6	0.82	MoNA
N-Methyl-2-pyrrolidone	C ₅ H ₉ NO	100.0757	100.0756	0.0	0.82	MoNA
Meperidine	C ₁₅ H ₂₁ NO ₂	248.1645	248.1642	-0.2	0.82	MoNA
Harmol	C ₁₂ H ₁₀ N ₂ O	199.0866	199.0865	0.5	0.81	MoNA
Tryptamine	C ₁₀ H ₁₂ N ₂	161.1073	161.1075	2.1	0.81	MoNA
Nalidixic acid	C ₁₂ H ₁₂ N ₂ O ₃	233.0921	233.0919	0.3	0.81	MoNA
Terbutaline	C ₁₂ H ₁₉ NO ₃	226.1438	226.1434	-0.6	0.79	MoNA
Venlafaxine	C ₁₇ H ₂₇ NO ₂	278.2115	278.2112	0.1	0.79	MoNA
Alpha-pyrrolidinovalerophenone	C ₁₅ H ₂₁ NO	232.1696	232.1692	-0.7	0.78	MoNA
(R)-(-)-Phenylephrine	C ₉ H ₁₃ NO ₂	168.1019	168.1019	0.9	0.76	MoNA
Indole	C ₈ H ₇ N	118.0651	118.0651	0.7	0.76	MoNA
Canrenone	C ₂₂ H ₂₈ O ₃	341.2111	341.2106	-0.5	0.74	MoNA
Thymol	C ₁₀ H ₁₄ O	151.1118	151.1117	0.7	0.73	MoNA
Norgestrel	C ₂₁ H ₂₈ O ₂	313.2162	313.2157	-0.6	0.73	MoNA
Linoleic acid	C ₁₈ H ₃₂ O ₂	281.2475	281.2472	-0.1	0.72	MoNA
Phenelzine	C ₈ H ₁₂ N ₂	137.1073	137.1073	0.8	0.72	MoNA
Betaxolol	C ₁₈ H ₂₉ NO ₃	308.2220	308.2216	-0.3	0.71	MoNA
Phenacetin	C ₁₀ H ₁₃ NO ₂	180.1019	180.1018	0.4	0.71	MoNA
Thymidine	C ₁₀ H ₁₄ N ₂ O ₅	243.0976	243.0973	0.0	0.70	MoNA
Benzoic acid	C ₇ H ₆ O ₂	121.0281	121.0284	-2.5	0.90	MoNA
4-Chlorophenol	C ₆ H ₅ ClO	126.9943	126.9945	-1.7	0.90	MoNA
Salicylic acid	C ₇ H ₆ O ₃	137.0232	137.0233	-0.9	0.80	MoNA
Acetaminophen	C ₈ H ₉ NO ₂	150.0546	150.0550	-2.4	0.92	MoNA

Table S2. Information of 18 standards for high confidence identification.

Compound name	Molecular formula	Theoretical m/z ([M+H] ⁺)	Type of drugs
Methamphetamine	C ₁₀ H ₁₅ N	150.1277	Traditional drugs
Amphetamine	C ₉ H ₁₃ N	136.1121	Traditional drugs
Ketamine	C ₁₃ H ₁₆ CINO	238.0993	Traditional drugs
Norketamine	C ₁₂ H ₁₄ CINO	224.0837	Traditional drugs
Morphine	C ₁₇ H ₁₉ NO ₃	286.1438	Traditional drugs
Codeine	C ₁₈ H ₂₁ NO ₃	300.1594	Traditional drugs
THC ¹	C ₂₁ H ₃₀ O ₂	315.2319	Traditional drugs
THC-COOH ¹	C ₂₁ H ₂₈ O ₄	345.2061	Traditional drugs
MDMA ¹	C ₁₁ H ₁₅ NO ₂	194.1176	Traditional drugs
Mephedrone	C ₁₁ H ₁₅ NO	178.1227	Traditional drugs
Flunitrazepam	C ₁₆ H ₁₂ FN ₃ O ₃	314.0936	Traditional drugs
7-Aminoflunitrazepam	C ₁₆ H ₁₄ FN ₃ O	284.1194	Traditional drugs
Nimetazepam	C ₁₆ H ₁₃ N ₃ O ₃	296.1030	Traditional drugs
7-Aminonimetazepam	C ₁₆ H ₁₅ N ₃ O	266.1288	Traditional drugs
Zopiclone	C ₁₇ H ₁₇ CIN ₆ O ₃	389.1124	Traditional drugs
4-Cl-α-PPP ¹	C ₁₃ H ₁₆ CINO	238.0993	NPS
4-F-α-PVP ¹	C ₁₅ H ₂₀ FNO	250.1602	NPS
JWH-249 ¹	C ₂₁ H ₂₂ BrNO	384.0958	NPS

1. Names are abbreviated, full names are in section 5.1