

Supplemental Table 1. List of substances with corresponding elemental composition, exact mass, retention time (RT), minimum screening sensitivity, extraction recovery and the shifts of mass and retention time from three-day validation analysis.							
Substances	Elemental Composition	[M+H] ⁺ Exact mass	Mass Shift (ppm)	RT (min)	RT shift (s)	Minimum Screening Sensitivity (ng/mL)	Extraction Recovery
1,3-Benzodioxolyl-N-methylbutanamine	C12H17NO2	208.1332	0.1	3.13	0.8	0.50	96.6%
15β-Hydroxytestosterone	C19H28O3	305.2111	-1.1	3.50	-0.3	0.10	87.5%
16β-Hydroxytestosterone	C19H28O3	305.2111	-1.1	3.97	0.1	0.25	94.8%
2-(1-Hydroxyethyl) promazine sulfoxide	C19H24N2O2S	345.1631	-1.3	3.13	0.5	1.00	41.1%
2-(1-Hydroxypropyl)promazine sulfoxide	C20H26N2O2S	359.1788	-1.1	3.35	0.9	2.00	38.5%
2-Aminoheptane	C7H17N	116.1434	0.0	2.98	0.1	ND ¹	89.1%
2α-Hydroxymethylethisterone	C22H30O3	343.2268	-1.8	4.35	-0.2	0.25	96.8%
3,4-Methylenedioxyamphetamine	C10H13NO2	180.1019	0.1	2.78	0.0	0.50	73.8%
3,4-Methylenedioxypropylamphetamine	C13H19NO2	222.1489	-0.9	3.14	0.3	0.10	113.1%
3-Hydroxymepivacaine	C15H22N2O2	263.1754	-0.3	2.52	-0.6	0.20	89.2%
3-Hydroxypromazine	C17H20N2OS	301.1369	-0.7	3.60	-2.0	0.10	77.9%
3-OH Lidocaine	C14H22N2O2	251.1754	1.1	2.42	0.5	0.06	92.4%
4-Chloroamphetamine	C9H12ClN	170.0731	0.1	3.27	0.2	ND	91.8%
4-Hydroxypropranolol	C16H21NO3	276.1594	-0.7	3.17	2.7	0.20	83.7%
4-Methoxymethamphetamine	C11H17NO	180.1383	-0.4	2.96	0.0	0.05	72.7%
5,6-Methylenedioxy-2-aminoindane	C10H11NO2	178.0863	0.0	2.56	0.8	0.10	64.2%
6-Dehydroandrostenedione	C19H24O2	285.1849	-1.0	4.53	0.8	0.10	96.0%
6-Dehydronandrolone	C18H24O2	273.1849	-0.8	4.31	0.1	0.25	98.2%
6-Dehydrotestosterone	C19H26O2	287.2006	-1.3	4.49	0.1	0.10	87.3%
7-Aminoclonazepam	C15H12ClN3O	286.0742	-1.1	3.23	0.6	0.50	91.5%
7-Aminoflunitrazepam	C16H14FN3O	284.1194	-1.2	3.46	0.3	0.10	92.3%
7-Hydroxy Fluphenazine	C22H26F3N3O2S	454.1771	0.0	4.11	0.1	2.00	79.0%
7-Hydroxychlorpromazine	C17H19ClN2OS	335.0979	-0.8	3.90	0.6	0.20	79.4%
9-Dehydroandrostenedione	C19H24O2	285.1849	-1.1	4.68	-0.4	0.10	95.3%
9-Dehydromethyl-testosterone	C20H28O2	301.2162	-1.3	4.72	-0.2	0.25	93.3%
9-Dehydrotestosterone	C19H26O2	287.2006	-1.3	4.52	-1.7	0.10	87.3%
A-796,260	C22H30N2O2	355.2380	-1.3	5.31	-1.6	0.10	87.1%
AB Pinaca	C18H26N4O2	331.2129	-0.5	4.97	-1.8	0.25	93.0%
AB-Fubinaca	C20H21FN4O2	369.1721	-1.1	4.65	-1.6	0.10	95.2%
Acebutolol	C18H28N2O4	337.2122	-1.6	3.15	1.2	0.25	46.7%
Acetaminophen	C8H9NO2	152.0706	-0.1	2.22	-0.8	1.00	67.1%
Acetophenazine	C23H29N3O2S	412.2053	-1.6	3.92	1.7	0.25	89.0%
Adrenosterone	C19H24O3	301.1798	-1.1	4.11	0.4	0.10	96.1%
AH-7921	C16H22Cl2N2O	329.1182	-1.4	3.80	2.0	0.25	101.7%
Albuterol	C13H21NO3	240.1594	0.5	2.20	-0.7	1.00	7.0%
Alfentanil	C21H32N6O3	417.2609	-0.6	3.85	2.7	0.20	96.8%
Alprazolam	C17H13ClN4	309.0902	-0.5	4.43	1.8	0.25	90.7%
Alprenolol	C15H23NO2	250.1802	-0.9	3.66	0.2	0.10	92.1%
Altrenogest	C21H26O2	311.2006	-1.0	4.99	-0.2	0.10	90.6%
AM 2233	C22H23IN2O	459.0928	-0.3	4.00	0.1	0.10	86.6%
AM-2201	C24H22FNO	360.1758	-0.6	5.71	-2.8	0.10	107.5%
AM-2201 Benzimidazole analog	C23H21FN2O	361.1711	-0.6	5.89	-1.3	0.25	105.3%
AM-2201 N-(4-hydroxypentyl) Metabolite	C24H22FNO2	376.1707	-0.9	5.02	-2.4	0.10	88.0%
AM-630	C23H25IN2O3	505.0983	0.1	5.38	-1.7	0.25	75.8%
Ambroxol	C13H18N2OBr2	376.9859	-1.5	3.26	0.4	ND	96.0%
Amiloride	C6H8ClN7O	230.0552	-0.8	2.11	-0.1	1.00	2.5%
Aminopentamide	C19H24N2O	297.1961	-0.6	3.66	0.0	0.10	86.8%
Aminorex	C9H10N2O	163.0866	-0.6	2.54	0.1	0.10	82.4%
Amiphenazole (Diamino-5-phenylthiazole)	C9H9N3S	192.0590	-0.4	2.33	0.5	1.00	94.5%
Amoxapine	C17H16ClN3O	314.1055	-1.0	4.00	1.7	0.25	96.1%
Amphetamine	C9H13N	136.1121	-0.1	2.76	0.2	NA	74.6%
Anastrozole	C17H19N5	294.1713	-1.1	4.08	-0.4	0.50	106.4%
Androstatriendione	C19H22O2	283.1693	-1.1	4.47	-0.1	0.50	93.5%
Androstenedione	C19H26O2	287.2006	-1.1	4.80	0.6	1.00	94.0%
Antipyrine	C11H12N2O	189.1022	0.3	3.05	-0.7	0.25	38.2%
Apomorphine	C17H17NO2	268.1332	-0.2	2.88	1.3	1.00	84.7%
Aprindine	C22H30N2	323.2482	-1.2	4.60	1.7	0.10	96.4%
Aripiprazole	C23H27Cl2N3O2	448.1553	-1.0	4.21	0.1	1.00	78.2%
Asimilobine	C17H17NO2	268.1332	0.0	3.11	0.4	0.10	99.0%
Astemizole	C28H31FN4O	459.2555	-1.3	3.94	0.1	1.00	81.2%

Atenolol	C14H22N2O3	267.1703	-1.1	0.82	0.1	ND	0.8%
Atropine	C17H23NO3	290.1751	-1.0	2.99	1.7	0.10	60.0%
Azaperone	C19H22FN3O	328.1820	-1.1	3.60	1.3	0.25	80.9%
Azelastine	C22H24ClN3O	382.1681	-1.6	4.15	0.6	0.25	95.2%
Bambuterol	C18H29N3O5	368.2180	-1.5	3.41	1.2	0.50	46.4%
Benactyzine	C20H25NO3	328.1907	-1.2	3.75	1.6	0.10	95.5%
Benazepril	C24H28N2O5	425.2071	-0.3	4.53	0.4	ND	2.6%
Benzoyllecgonine	C16H19NO4	290.1387	-0.4	2.96	-1.4	20.0	0.3%
Benzphetamine	C17H21N	240.1747	-0.6	3.83	-0.7	0.05	109.9%
Betaxolol	C18H29NO3	308.2220	-1.3	3.75	1.4	0.10	96.3%
Biperiden	C21H29NO	312.2322	-1.3	4.15	1.7	0.25	90.6%
Bisoprolol	C18H31NO4	326.2326	-1.3	3.64	1.3	0.10	89.2%
Bolasterone	C21H32O2	317.2475	-1.9	4.95	0.3	0.10	89.0%
Boldenone	C19H26O2	287.2006	0.2	4.51	1.3	0.05	103.9%
Boldenone Acetate	C21H28O3	329.2111	-2.6	5.44	1.2	0.10	96.7%
Boldine	C19H21NO4	328.1543	-1.3	2.84	1.8	0.25	101.3%
Boldione	C19H24O2	285.1849	-1.0	4.53	0.6	0.10	96.0%
Bromazepam	C14H10BrN3O	316.0080	-1.1	3.99	1.6	0.25	94.0%
Brombuterol	C12H18Br2N2O	364.9859	-1.3	3.45	-1.0	ND	98.2%
Bromhexine	C14H20Br2N2	375.0066	-1.2	4.78	-1.0	ND	39.1%
Bromocriptine	C32H40BrN5O5	654.2286	-0.4	4.55	1.7	1.00	78.9%
Brompheniramine	C16H19BrN2	319.0804	-1.0	3.78	1.0	0.25	92.4%
Brotizolam	C15H10BrClN4S	392.9571	-1.4	4.58	1.3	ND	95.4%
Budesonide	C25H34O6	431.2428	-1.3	4.63	-0.4	1.00	104.4%
Buflomedil	C17H25NO4	308.1856	-1.1	3.36	0.9	0.10	87.2%
Bumetanide	C17H20N2O5S	365.1166	-1.7	4.58	0.4	20.0	5.5%
Buphedrone	C11H15NO	178.1226	-0.2	2.89	-0.3	0.05	122.3%
Bupivacaine	C18H28N2O	289.2274	-0.5	3.74	0.9	0.10	99.7%
Buprenorphine	C29H41NO4	468.3108	-0.4	4.06	1.0	ND	81.6%
Bupropion	C13H18ClNO	240.1150	-0.7	3.59	1.1	0.25	120.7%
Buspirone	C21H31N5O2	386.2551	-0.8	3.69	-2.0	0.20	97.6%
Butorphanol	C21H29NO2	328.2271	-0.1	3.54	-0.2	0.20	95.6%
Butylone	C12H15NO3	222.1125	-1.1	2.93	0.1	0.25	100.0%
Caffeine	C8H10N4O2	195.0877	0.3	2.72	-0.1	1.00	40.6%
Calusterone	C21H32O2	317.2475	-2.2	5.05	0.3	0.25	85.5%
Canrenone	C22H28O3	341.2111	-2.3	4.82	0.3	0.25	106.7%
Capsaicin	C18H27NO3	306.2064	-1.0	5.06	0.9	0.10	92.4%
Carazolol	C18H22N2O2	299.1754	-1.3	3.39	1.4	0.10	95.1%
Carbamazepine	C15H12N2O	237.1022	-0.9	4.14	0.6	0.10	93.0%
Carbinoxamine	C16H19ClN2O	291.1259	0.1	3.66	1.1	0.50	88.5%
Carfentanil	C24H30N2O3	395.2329	-0.5	4.08	-0.8	0.20	97.7%
Carisoprodol	C12H24N2O4	261.1809	-0.7	4.27	0.9	0.10	88.6%
Carteolol	C16H24N2O3	293.1860	-1.3	2.60	0.1	1.00	25.4%
Carvedilol	C24H26N2O4	407.1965	-1.7	4.04	0.7	0.25	92.0%
Cathinone	C9H11NO	150.0913	0.1	2.47	-1.1	ND	94.4%
Celecoxib	C17H14F3N3O2S	382.0832	-1.6	5.17	0.9	1.00	82.5%
Celiprolol	C20H33N3O4	380.2544	-1.3	3.41	0.8	0.25	30.4%
Cetirizine	C21H25ClN2O3	389.1627	-1.5	4.20	2.0	NA	2.7%
Chlordiazepoxide	C16H14ClN3O	300.0898	-0.8	4.22	1.0	0.10	98.6%
Chlorprothixene	C18H18ClNS	316.0921	-1.3	4.46	1.3	0.50	78.5%
Chlorthalidone	C14H11ClN2O4S	339.0201	-0.7	3.26	1.0	ND	77.5%
Cimaterol	C12H17N3O	220.1444	-2.7	2.17	-0.5	0.50	52.3%
Cimetidine	C10H16N6S	253.1230	-1.8	2.17	-1.9	ND	13.8%
Cinnarizine	C26H28N2	369.2325	-0.2	4.86	1.4	1.00	34.1%
Cisapride	C23H29ClFN3O4	466.1903	-1.1	3.98	0.5	0.25	93.7%
Citalopram	C20H21FN2O	325.1711	-1.1	3.90	1.5	1.00	97.7%
Clenbuterol	C12H18Cl2N2O	277.0869	0.3	3.30	0.4	0.04	94.6%
Clobazam	C16H13ClN2O2	301.0738	-1.1	4.65	1.0	0.25	98.9%
Clomipramine	C19H23ClN2	315.1623	-1.0	4.49	1.2	0.50	81.9%
Clonazepam	C15H10ClN3O3	316.0484	-1.1	4.36	0.7	1.00	94.8%
Clonidine	C9H9Cl2N3	230.0246	-1.1	2.63	1.8	0.25	94.8%
Clopamide	C14H20ClN3O3S	346.0987	-1.2	3.64	0.6	0.25	97.5%
Clostebol	C19H27ClO2	323.1772	-2.0	5.00	0.5	ND	95.9%
Clozapine	C18H19ClN4	327.1371	-1.2	3.88	1.2	ND	107.4%
Cocaethylene	C18H23NO4	318.1700	-1.1	3.67	1.2	0.10	98.1%
Cocaine	C17H21NO4	304.1543	-1.1	3.45	-0.3	0.10	98.1%

Cotinine	C10H12N2O	177.1022	0.0	2.02	0.0	0.10	10.4%
Cyclobenzaprine	C20H21N	276.1747	-0.3	4.20	1.3	0.25	91.3%
Danazol	C22H27NO2	338.2115	-1.8	5.37	0.6	0.10	76.9%
Dembrexine	C13H17Br2NO2	377.9699	-1.6	3.17	-0.1	ND	94.8%
Deoxycorticosterone	C21H30O3	331.2268	-1.1	4.65	-0.7	1.00	101.8%
Deracoxib	C17H14F3N3O3S	398.0781	-1.0	4.78	1.1	2.00	83.6%
Desalkylflurazepam	C15H10ClFN2O	289.0539	-0.2	4.55	0.5	1.00	100.5%
Deserpidine	C32H38N2O8	579.2701	-0.1	4.41	0.9	1.00	82.1%
Desipramine	C18H22N2	267.1856	-0.3	4.17	-0.1	0.20	91.2%
Desmethylmetoprolol	C14H23NO3	254.1751	-1.0	2.66	-0.4	2.00	27.0%
Desonide	C24H32O6	417.2272	-1.5	4.17	0.0	0.10	97.6%
Desoximetasone	C22H29O4F	377.2123	-1.7	4.30	-0.2	0.25	105.1%
Despropionylfentanyl	C19H24N2	281.2012	0.7	3.91	1.8	0.10	95.1%
Detomidine	C12H14N2	187.1230	1.1	3.42	0.4	0.20	91.2%
Dexamethasone	C22H29FO5	393.2072	-0.1	4.18	1.0	ND	90.5%
Dextromethorphan	C18H25NO	272.2009	-0.8	3.74	-2.3	0.10	98.0%
Dextropropan	C17H23NO	258.1852	-0.5	3.14	0.6	0.10	100.3%
Dezocine	C16H23NO	246.1852	-0.3	3.21	0.4	0.20	98.7%
Dibucaine	C20H29N3O2	344.2333	-1.0	4.34	0.4	0.25	92.4%
Dichlorisone acetate	C23H28Cl2O5	455.1387	-1.0	4.97	0.6	1.00	98.0%
Diclofenac	C14H11Cl2NO2	296.0240	0.1	5.16	0.2	ND	26.0%
Dicyclomine	C19H35NO2	310.2741	-0.8	4.88	1.2	0.25	66.5%
Diethylpropion	C13H19NO	206.1539	-0.4	2.95	0.0	ND	139.4%
Dihydrocapsaicin	C18H29NO3	308.2220	-1.2	5.17	0.3	0.10	81.2%
Dihydrocodeine	C18H23NO3	302.1751	-1.2	2.55	0.1	0.10	71.1%
Dihydromorphine	C17H21NO3	288.1594	-1.0	1.40	-0.1	0.25	30.7%
Diphenhydramine	C17H21NO	256.1696	-0.9	3.77	0.7	0.10	104.9%
Dobutamine	C18H23NO3	302.1751	-1.1	2.96	0.8	0.25	226.0%
Domperidone	C22H24ClN5O2	426.1691	-0.7	3.55	0.6	0.50	92.6%
Doxepin	C19H21NO	280.1696	-0.3	3.97	1.4	0.50	97.5%
Droperidol	C22H22FN3O2	380.1769	-1.0	3.67	1.1	0.25	94.8%
Ecgonine methyl ester	C10H17NO3	200.1281	-0.1	0.93	0.7	1.00	21.7%
Embutramide	C17H27NO3	294.2064	-0.1	4.28	0.5	0.10	102.8%
Ephedrine	C10H15NO	166.1226	-0.1	2.56	0.5	0.10	45.0%
Epiboldenone	C19H26O2	287.2006	-1.3	4.50	-0.5	0.10	87.3%
Epinandrolone	C18H26O2	275.2006	-1.2	4.68	-0.4	0.25	96.7%
Estazolam	C16H11ClN4	295.0745	-0.5	4.34	0.4	0.50	94.5%
Ethinyltestosterone	C21H28O2	313.2162	-1.2	4.79	-0.2	0.25	94.1%
Ethopropazine	C19H24N2S	313.1733	-0.8	4.32	0.6	0.25	216.6%
Ethylmorphine	C19H23NO3	314.1751	-1.2	2.79	-0.1	ND	86.3%
Ethylone	C12H15NO3	222.1125	-1.3	2.81	-0.2	0.05	100.9%
Etilamfetamine	C11H17N	164.1434	-0.3	3.06	-0.5	0.10	93.7%
Etilefrine	C10H15NO2	182.1176	-0.1	1.43	-0.4	1.00	21.8%
Etodolac	C17H21NO3	288.1594	0.1	5.09	0.4	ND	25.0%
Etorphine	C25H33NO4	412.2482	0.1	3.38	-1.1	ND	100.7%
Exemestane	C20H24O2	297.1849	-1.4	4.80	-0.3	0.50	110.0%
Famprofazone	C24H31N3O	378.2540	-1.0	5.69	0.8	0.50	101.6%
Felbamate	C11H14N2O4	239.1026	-0.8	3.33	0.7	1.00	92.7%
Fenfluramine	C12H16F3N	232.1308	-0.6	3.73	0.7	0.10	104.9%
Fenoterol	C17H21NO4	304.1543	-1.4	2.55	0.5	0.25	66.1%
Fentanyl	C22H28N2O	337.2274	-1.0	3.85	0.6	0.10	98.4%
Feprazone	C20H20N2O2	321.1598	-0.7	5.31	1.1	ND	32.3%
Firocoxib	C17H20O5S	337.1104	-0.2	4.74	-0.2	10.0	105.5%
Fludrocortisone Acetate	C23H31O6F	423.2177	-0.5	4.29	0.6	0.25	99.3%
Flufenamic Acid	C14H10F3NO2	282.0736	0.1	5.38	-0.1	50.0	49.0%
Flumethasone	C22H28F2O5	411.1978	-1.0	4.01	-0.3	1.00	93.6%
Flunisolide	C24H31FO6	435.2177	-1.3	4.21	-0.5	0.25	94.6%
Flunitrazepam	C16H12FN3O3	314.0936	-0.8	4.53	1.4	0.25	99.3%
Flunixin	C14H11F3N2O2	297.0845	-0.5	4.80	-0.2	2.00	19.6%
Fluocinolone Acetonide	C24H30F2O6	453.2083	-1.3	4.24	-0.8	ND	94.5%
Fluocinonide	C26H32O7F2	495.2189	-0.5	4.86	-0.3	0.10	109.0%
Fluocortolone	C22H29FO4	377.2123	-0.7	4.26	1.2	0.25	99.0%
Fluorometholone	C22H29FO4	377.2123	-1.7	4.30	-0.2	0.25	105.1%
Fluoxetine	C17H18F3NO	310.1413	-0.2	4.38	0.2	ND	90.6%
Fluoxymesterone	C20H29FO3	337.2174	-1.7	4.15	0.1	0.10	94.4%
Flupentixol	C23H25F3N2OS	435.1713	-1.5	4.58	-0.2	ND	56.2%

Fluphenazine	C22H26N3OSF3	438.1821	-1.1	4.48	0.7	0.10	104.3%
Fluphenazine sulfoxide	C22H26F3N3O2S	454.1771	-0.2	3.73	0.5	ND	63.4%
Flurazepam	C21H23ClFN3O	388.1586	-1.8	3.80	-0.6	0.10	95.7%
Fluticasone Propionate	C25H31F3O5S	501.1917	-0.5	5.23	0.9	0.25	83.9%
Fluvoxamine	C15H21F3N2O2	319.1628	-1.1	4.23	0.2	0.25	99.0%
Formoterol	C19H24N2O4	345.1809	-1.3	3.22	-0.6	0.10	65.9%
Gestodene	C21H26O2	311.2006	-1.4	4.76	-1.2	0.10	94.1%
Gestrinone	C21H24O2	309.1849	-1.4	4.71	0.2	0.10	90.1%
Glafenine	C19H17ClN2O4	373.0950	-1.1	3.27	0.3	0.25	95.4%
Glaucine	C21H25NO4	356.1856	-1.2	3.52	0.6	0.10	99.2%
Gliclazide	C15H21N3O3S	324.1376	-1.1	4.87	0.8	1.00	12.8%
Griseofulvin	C17H17O6Cl	353.0786	-1.7	4.38	0.8	1.00	101.6%
Guaifenesin	C10H14O4	199.0965	0.7	3.27	0.4	2.40	3.5%
Guanabenz	C8H8Cl2N4	231.0199	-0.7	3.39	0.4	0.10	92.9%
Halazepam	C17H12ClF3N2O	353.0663	-1.8	5.27	1.2	0.10	83.8%
Hydrocodone	C18H21NO3	300.1594	-1.0	2.81	0.5	0.10	91.5%
Hydromorphone	C17H19NO3	286.1438	-0.7	2.12	-0.6	2.00	52.5%
Hydroxymetoprolol	C15H25NO4	284.1856	-1.2	2.62	-0.2	0.20	14.0%
Hydroxyzine	C21H27ClN2O2	375.1834	-1.2	4.23	0.5	1.00	94.9%
Ibogaine	C20H26N2O	311.2118	0.1	3.62	1.2	0.10	198.0%
Imipramine	C19H24N2	281.2012	-0.6	4.21	1.4	0.10	96.0%
Indapamide	C16H16N3O3SCl	366.0674	-1.6	4.09	-0.1	1.00	104.6%
Indomethacin	C19H16ClNO4	358.0841	-1.0	5.14	0.2	5.00	17.1%
Indoprofen	C17H15NO3	282.1125	-0.3	4.30	-1.7	50.0	1.7%
Isoetharine	C13H21NO3	240.1594	-1.3	2.15	2.2	0.10	100.3%
Isofluprednone	C21H27FO5	379.1915	1.1	3.66	0.4	ND	86.4%
Isometheptene	C9H19N	142.1590	0.2	3.13	0.1	0.25	132.5%
Isoproterenol	C11H17NO3	212.1281	1.9	1.16	1.4	ND	11.9%
JWH 018 N-(5-hydroxypentyl) Metabolite	C24H23NO2	358.1802	-1.2	5.04	-1.7	0.10	88.4%
JWH 073 4-Hydroxybutyl Metabolite	C23H21NO2	344.1645	-0.9	4.89	-1.6	0.25	87.6%
JWH 122 N-(5-hydroxypentyl) Metabolite	C25H25NO2	372.1958	-0.9	5.23	-2.0	0.10	84.6%
JWH 250 N-(5-hydroxypentyl) Metabolite	C22H25NO3	352.1907	-0.9	4.78	-2.0	0.50	94.1%
JWH-015	C23H21NO	328.1696	-0.5	5.83	-1.8	0.50	112.7%
JWH-018	C24H23NO	342.1852	-0.5	6.15	-1.7	1.00	108.1%
JWH-030	C20H21NO	292.1696	0.3	5.80	-2.1	0.25	107.3%
JWH-073	C23H21NO	328.1696	-0.5	5.83	-1.8	0.50	112.7%
JWH-081	C25H25NO2	372.1958	-0.9	5.23	-2.0	0.10	84.6%
JWH-200	C25H24N2O2	385.1911	-1.3	5.00	-1.6	1.00	87.8%
JWH-203	C21H22ClNO	340.1463	-0.5	6.07	-3.0	ND	114.4%
JWH-210	C26H27NO	370.2165	-0.8	6.46	-0.1	ND	53.2%
JWH-250	C22H25NO2	336.1958	-0.7	5.90	-2.3	0.50	108.3%
Ketamine	C13H16ClNO	238.0993	-0.7	3.08	0.5	0.10	101.8%
Ketoprofen	C16H14O3	255.1016	0.1	4.63	0.3	6.00	5.3%
Ketorolac	C15H13NO3	256.0968	-0.3	4.11	2.7	50.0	1.1%
Labetalol	C19H24N2O3	329.1860	-1.3	3.38	0.6	0.10	97.6%
Lamotrigine	C9H7Cl2N5	256.0151	-0.4	3.20	0.7	0.25	88.6%
Letrozole	C17H11N5	286.1087	0.0	4.07	0.5	0.50	98.3%
Levorphanol	C17H23NO	258.1852	-0.4	3.12	1.3	0.02	92.3%
Liriodenine	C17H9NO3	276.0655	-0.7	4.16	1.6	0.25	96.2%
Lobelanidine	C22H29NO2	340.2271	-1.8	3.84	0.6	0.10	104.3%
Lobeline	C22H27NO2	338.2115	-1.1	3.99	1.3	0.50	100.5%
Loperamide	C29H33ClN2O2	477.2303	-1.1	4.63	1.5	0.25	91.4%
Loratadine	C22H23N2O2Cl	383.1521	-2.0	5.44	-0.4	0.50	103.6%
Lorazepam	C15H10Cl2N2O2	321.0192	-1.3	4.21	1.1	ND	95.3%
Lormetazepam	C16H12Cl2N2O2	335.0349	-1.6	4.57	1.0	0.25	96.1%
Mabuterol	C13H18ClF3N2O	311.1133	-0.6	3.55	0.8	0.25	100.2%
MAM-2201	C25H24FNO	374.1915	-0.6	5.87	-2.7	0.50	104.3%
Mapenterol	C14H20ClF3N2O	325.1289	-0.7	3.76	1.0	0.10	104.0%
Maprotiline	C20H23N	278.1903	-0.5	4.25	0.9	0.50	86.3%
Mebendazole	C16H13N3O3	296.1030	-0.8	4.20	0.5	0.50	95.1%
Meclofenamic Acid	C25H27ClN2	296.0240	-0.6	5.45	1.6	50.0	68.3%
Medetomidine	C13H16N2	201.1386	-0.2	3.58	1.6	0.10	99.5%
Mefenamic Acid	C15H15NO2	242.1176	-0.6	5.49	0.0	10.0	60.4%
Mefruside	C13H19ClN2O5S2	383.0497	-0.7	4.21	0.2	1.00	102.0%
Melengestrol	C23H30O3	355.2268	-2.0	4.96	-0.3	0.10	98.6%
Meperidine	C15H21NO2	248.1645	-0.9	3.48	-0.3	0.01	100.7%

Mephedrone	C11H15NO	178.1226	-0.1	3.01	0.7	0.05	108.1%
Mephentermine	C11H17N	164.1434	0.4	3.06	0.6	0.10	77.5%
Mepivacaine	C15H22N2O	247.1805	0.2	3.02	2.4	0.03	94.5%
Meprobamate	C9H18N2O4	219.1339	-0.9	3.57	0.1	2.00	92.9%
Mescaline	C11H17NO3	212.1281	1.3	2.70	0.3	0.50	9.2%
Metaproterenol	C11H17NO3	212.1281	1.2	1.30	-0.4	ND	7.7%
Metaraminol	C9H13NO2	168.1019	0.1	1.15	2.1	1.00	17.1%
Metaxalone	C12H15NO3	222.1125	-0.6	4.38	0.4	0.25	99.0%
Methadone	C21H27NO	310.2165	-0.6	4.35	1.5	0.50	99.7%
Methamphetamine	C10H15N	150.1277	-0.1	2.97	-0.2	ND	84.8%
Methandrostenedione	C20H28O2	301.2162	-1.0	4.68	0.9	0.05	87.3%
Methapyrilene	C14H19N3S	262.1372	0.0	3.64	0.3	0.10	89.9%
Methaqualone	C16H14N2O	251.1179	-0.2	4.38	1.1	0.10	88.2%
Methcathinone	C10H13NO	164.1070	0.0	2.54	1.9	0.05	114.3%
Methenolone	C20H30O2	303.2319	-1.5	4.84	-0.6	0.10	92.5%
Methocarbamol	C11H15NO5	242.1023	0.1	3.40	-2.0	0.10	80.9%
Methoxamine	C11H17NO3	212.1281	-0.1	2.83	-0.2	1.00	37.3%
Methyl-1-testosterone	C20H30O2	303.2319	-1.0	5.11	0.1	0.10	97.0%
Methylboldenone	C20H28O2	301.2162	-1.4	4.54	-0.2	0.10	91.3%
Methylclostebol	C20H29ClO2	337.1929	-1.3	5.20	-0.4	ND	90.4%
Methyldienolone	C19H26O2	287.2006	-1.3	4.49	0.1	0.10	87.3%
Methylenedioxyethylamphetamine	C12H17NO2	208.1332	-0.1	3.05	-1.0	0.05	88.4%
Methylenedioxypyrovalerone	C16H21NO3	276.1594	-0.6	3.44	0.3	0.05	95.3%
Methylhexanamine	C7H17N	116.1434	0.0	2.84	1.8	ND	61.1%
Methylnortestosterone	C19H28O2	289.2162	-1.1	4.67	-2.5	0.10	91.6%
Methylone	C11H13NO3	208.0968	0.5	2.65	0.1	0.05	94.8%
Methylphenidate	C14H19NO2	234.1489	-1.1	3.16	0.0	0.50	115.4%
Methylprednisolone	C22H30O5	375.2166	-1.1	4.12	2.0	ND	88.4%
Methyltestosterone	C20H30O2	303.2319	-1.5	4.84	-0.6	0.10	92.5%
Metolazone	C16H16N3O3SCl	366.0674	-1.1	3.88	0.6	1.00	101.0%
Metoprolol	C15H25NO3	268.1907	-0.7	3.27	-0.1	0.25	88.3%
Mianserin	C18H20N2	265.1699	-0.4	3.79	1.5	0.10	94.5%
Mibolerone	C20H30O2	303.2319	-1.3	4.91	-0.6	0.03	91.7%
Midazolam	C18H13ClFN3	326.0855	-1.5	4.09	1.5	0.10	95.7%
Mitragynine	C23H30N2O4	399.2278	-1.2	3.97	0.6	0.10	97.9%
Morphine	C17H19NO3	286.1438	-0.6	1.46	-0.1	0.20	43.5%
N,N-Didesmethyl Trimebutine	C20H25NO5	360.1806	-2.0	2.69	-0.1	0.50	90.0%
Nadolol	C17H27NO4	310.2013	-1.3	2.79	-0.2	0.50	6.6%
Nalbuphine	C21H27NO4	358.2013	-1.2	2.93	-0.2	0.20	79.7%
Nalorphine	C19H21NO3	312.1594	-0.9	2.49	1.8	2.00	88.4%
Naloxone	C19H21NO4	328.1543	-1.8	2.55	-0.3	0.10	98.0%
Naltrexone	C20H23NO4	342.1700	-0.6	2.71	-0.4	0.10	97.7%
Nandrolone	C18H26O2	275.2006	0.3	4.60	1.2	0.10	104.9%
Nandrolone Acetate	C20H28O3	317.2111	-1.4	5.71	0.4	ND	101.0%
Naphyrone	C19H23NO	282.1852	-0.4	4.10	-0.1	ND	92.1%
N-Desmethylselegiline	C12H15N	174.1277	0.5	2.98	1.1	0.10	93.5%
N-Desmethyltrimipramine	C19H24N2	281.2012	-0.7	4.17	2.0	0.10	91.4%
Nebivolol	C22H25F2NO4	406.1824	-1.6	4.24	0.2	0.50	78.9%
Nefopam	C17H19NO	254.1539	-0.6	3.64	-0.5	0.10	103.2%
Nikethamide	C10H14N2O	179.1179	0.0	3.19	0.4	0.25	132.0%
Nitrazepam	C15H11N3O3	282.0873	-0.6	4.30	-0.1	0.25	100.6%
Nomifensine	C16H18N2	239.1543	-0.7	3.33	1.0	0.10	100.3%
Norbolethone	C21H32O2	317.2475	-1.6	5.48	0.3	0.10	62.2%
Norchlordiazepoxide	C15H12ClN3O	286.0742	-1.0	3.77	1.1	0.50	89.6%
Norclostebol	C18H25ClO2	309.1616	-1.4	4.87	-0.1	1.00	91.8%
Norcodeine	C17H19NO3	286.1438	-1.1	2.38	1.8	0.25	10.9%
Nordiazepam	C15H11ClN2O	271.0633	0.1	4.66	-0.7	0.20	89.2%
Norethandrolone	C20H30O2	303.2319	-1.0	5.12	-0.5	0.10	97.0%
Norfentanyl	C14H20N2O	233.1648	-1.1	3.09	-0.4	0.10	21.9%
Norfluoxetine	C16H16F3NO	296.1257	-0.6	4.30	0.0	ND	123.4%
Norgestrel	C21H28O2	313.2162	-1.4	4.98	-0.6	0.10	98.0%
Norketamine	C12H14ClNO	224.0837	-1.3	3.04	-0.2	0.10	103.7%
Norlutin	C20H26O2	299.2006	-1.4	4.63	-0.3	0.10	92.4%
Normeperidine	C14H19NO2	234.1489	-1.4	3.41	1.9	0.01	81.9%
Normorphine	C16H17NO3	272.1281	-0.9	1.18	2.2	ND	2.5%
Nortriptyline	C19H21N	264.1747	0.1	4.25	0.0	0.20	92.1%

Norverapamil	C26H36N2O4	441.2748	-1.2	4.06	2.0	0.10	96.2%
Nylidrin	C19H25NO2	300.1958	-1.1	3.63	0.2	0.25	97.9%
O-Desmethylpyrilamine	C16H21N3O	272.1757	-1.1	3.17	0.6	0.10	112.5%
O-Desmethyltramadol	C15H23NO2	250.1802	-0.3	2.82	-0.9	0.02	80.2%
Omeprazole Sulfide	C17H19N3O2S	330.1271	-0.1	4.24	1.9	0.20	87.4%
Orphenadrine	C18H23NO	270.1852	-0.7	3.98	0.4	0.10	107.3%
Oxandrolone	C19H30O3	307.2268	-1.7	4.52	0.6	1.00	86.3%
Oxazepam	C15H11ClN2O2	287.0582	0.1	4.28	0.2	0.20	89.8%
Oxilofrine	C10H15NO2	182.1176	0.4	1.03	2.4	ND	10.0%
Oxprenolol	C15H23NO3	266.1751	-0.2	3.54	-0.6	0.10	97.0%
Oxycodone	C18H21NO4	316.1543	-1.4	2.73	-0.1	0.10	101.8%
Oxymetazoline	C16H24N2O	261.1961	-0.6	3.86	0.3	0.25	56.3%
Oxymorphone	C17H19NO4	302.1387	-0.7	1.68	0.1	0.20	59.8%
Oxyphencyclimine	C20H28N2O3	345.2173	-1.6	4.25	-0.2	1.00	32.7%
Oxyphenylbutazone	C19H20N2O3	325.1547	-1.0	4.61	2.8	5.00	12.3%
Papaverine	C20H21NO4	340.1543	-1.9	3.44	0.0	0.10	101.1%
Paroxetine	C19H20FNO3	330.1500	-1.4	4.09	-0.4	0.25	86.6%
PB-22	C23H22N2O2	359.1754	-0.2	5.92	-2.6	1.00	110.2%
Penbutolol	C18H29NO2	292.2271	-0.7	4.40	-0.6	0.10	101.3%
Pentazocine	C19H27NO	286.2165	-0.1	3.60	2.2	0.01	96.0%
Perphenazine	C21H26ClN3OS	404.1558	-1.4	4.32	2.3	0.25	83.3%
Pheniramine	C16H20N2	241.1699	-1.2	3.31	-0.4	0.10	89.3%
Phentermine	C10H15N	150.1277	-0.1	2.87	0.4	0.05	82.6%
Phenylbutazone	C19H20N2O2	309.1598	-0.7	5.34	0.5	5.00	14.8%
Phenylpropanolamine	C9H13NO	152.1070	-0.2	2.41	-0.8	2.00	36.8%
p-hydroxy Benzphetamine	C17H21NO	256.1696	-0.8	3.26	-0.2	0.25	99.0%
Pimobendan	C19H18N4O2	335.1503	-0.6	3.57	0.9	0.25	95.7%
Pimozide	C28H29F2N3O	462.2352	-0.4	4.53	-0.2	ND	70.1%
Pindolol	C14H20N2O2	249.1598	-0.9	2.88	-0.1	0.10	93.9%
Piperidolate	C21H25NO2	324.1958	-1.5	4.18	-0.5	0.50	56.0%
Piretanide	C17H18N2O5S	363.1009	-0.7	4.21	0.5	ND	2.2%
Pirlindole	C15H18N2	227.1543	-0.6	3.82	-0.2	0.10	89.8%
Piroxicam	C15H13N3O4S	332.0700	-0.6	4.33	0.0	5.00	7.4%
Prazepam	C19H17ClN2O	325.1102	-1.3	5.34	1.2	0.10	91.0%
Prednisolone	C21H28O5	361.2010	-0.5	3.89	0.1	0.10	99.4%
Prednisone	C21H26O5	359.1853	-0.9	3.84	0.0	2.00	86.5%
Prilocaine	C13H20N2O	221.1648	-1.2	2.97	1.1	0.10	122.2%
Probenecid	C13H19NO4S	286.1108	-0.5	4.66	-2.7	50.00	4.9%
Procainamide	C13H21N3O	236.1757	-1.2	1.85	-0.4	0.50	27.4%
Procaine	C13H20N2O2	237.1598	-1.3	2.54	0.0	0.20	64.8%
Procatenol	C16H22N2O3	291.1703	-1.2	2.28	1.7	0.25	17.6%
Procyclidine	C19H29NO	288.2322	-0.8	4.17	0.0	0.10	98.8%
Promazine	C17H20N2S	285.1420	-0.6	4.12	-0.2	0.10	115.7%
Pronethalol	C15H19NO	230.1539	-1.5	3.51	-0.4	0.10	99.9%
Propionylpromazine	C20H24N2OS	341.1682	-1.6	4.31	-0.7	0.10	110.6%
Propofol	C12H18O	179.1430	0.1	4.35	-0.6	1.00	102.0%
Propoxyphene	C22H29NO2	340.2271	-1.8	4.16	0.6	0.25	106.5%
Propranolol	C16H21NO2	260.1645	-0.4	3.76	-0.4	0.10	99.3%
propylamphetamine	C12H19N	178.1590	0.0	3.31	-0.3	0.05	104.0%
Protopine	C20H19NO5	354.1336	-1.1	3.30	0.7	0.10	99.4%
Protriptyline	C19H21N	264.1747	-0.4	4.17	-0.4	0.25	94.8%
Pseudoephedrine	C10H15NO	166.1226	-0.1	2.56	0.5	0.10	45.0%
Pyrilamine	C17H23N3O	286.1914	-0.5	3.81	-0.8	0.10	90.1%
Pyrovalerone	C16H23NO	246.1852	-0.4	3.77	-0.8	0.05	104.8%
Quetiapine	C21H25N3O2S	384.1740	-1.8	3.94	-0.3	0.25	91.2%
Quinapril	C25H30N2O5	439.2228	1.0	4.52	-0.3	ND	0.9%
Quinidine	C20H24N2O2	325.1911	-1.6	3.34	-0.1	0.10	91.6%
Ractopamine	C18H23NO3	302.1751	-1.0	2.96	0.4	0.50	77.8%
Raloxifene	C28H27NO4S	474.1734	-0.7	3.63	0.6	0.25	88.1%
Ramipril	C23H32N2O5	417.2384	-0.5	4.49	0.1	ND	2.0%
Ranitidine	C13H22N4O3S	315.1485	0.6	2.35	-0.5	15.0	6.0%
RCS-4	C21H23NO2	322.1802	-0.5	5.83	-2.3	0.10	108.5%
RCS-8	C25H29NO2	376.2271	-1.5	6.30	0.3	ND	99.1%
Rescinnamine	C35H42N2O9	635.2963	-1.5	4.32	0.4	1.00	119.0%
Risperidone	C23H27FN4O2	411.2191	-1.1	3.63	-0.5	0.25	91.3%
Ritodrine	C17H21NO3	288.1594	-1.0	2.68	-0.3	0.10	76.0%

Ropivacaine	C17H26N2O	275.2118	-1.0	3.49	-0.6	0.10	103.2%
Salmeterol	C25H37NO4	416.2795	-1.4	4.39	-0.1	0.25	84.3%
Selegiline	C13H17N	188.1434	-0.3	3.09	0.5	1.00	8.3%
Sertraline	C17H17Cl2N	306.0811	-1.1	4.29	0.1	0.10	78.3%
Sibutramine	C17H26ClN	280.1827	-0.9	4.41	1.5	0.10	70.0%
Sildenafil	C22H30N6O4S	475.2122	-0.5	3.86	2.0	ND	102.6%
Sotalol	C12H20N2O3S	273.1267	-1.3	2.11	0.2	1.00	13.4%
Sparteine	C15H26N2	235.2169	-1.5	3.18	-0.1	1.00	33.3%
Stanozolol	C21H32N2O	329.2587	0.3	5.15	-0.5	ND	81.1%
Strychnine	C21H22N2O2	335.1754	-1.5	2.78	1.2	0.10	88.7%
Sufentanil	C22H30N2O2S	387.2101	0.3	4.22	1.4	1.00	93.4%
Sulpiride	C15H23N3O4S	342.1482	-1.9	2.25	0.6	0.10	42.8%
Suxibuzone	C24H26N2O6	439.1864	-1.3	4.92	0.1	0.25	44.0%
Tadalafil	C22H19N3O4	390.1448	-1.6	4.22	0.2	0.50	90.0%
Tapentadol	C14H23NO	222.1852	-1.2	3.17	1.0	0.10	98.8%
Telmisartan	C33H30N4O2	515.2442	-0.8	4.94	-0.3	0.25	20.6%
Temazepam	C16H13ClN2O2	301.0738	-0.3	4.62	0.1	0.02	93.8%
Tenoxicam	C13H11N3O4S2	338.0264	-0.8	3.56	0.8	ND	0.7%
Terfenadine	C32H41NO2	472.3210	-0.5	4.76	1.7	0.25	66.6%
Testosterone	C19H28O2	289.2162	0.4	4.78	1.6	0.05	100.5%
Testosterone Acetate	C21H30O3	331.2268	-1.2	5.88	0.3	0.25	94.2%
Tetrahydrogestrinone (THG)	C21H28O2	313.2162	-0.7	5.36	-1.6	0.03	82.0%
Tetrahydrozoline	C13H16N2	201.1386	-0.1	2.88	1.1	0.10	12.1%
Theobromine	C7H8N4O2	181.0720	0.7	1.79	-1.8	ND	10.8%
Theophylline	C7H8N4O2	181.0720	0.2	2.39	0.0	2.00	32.6%
Thioridazine	C21H26N2S2	371.1610	-2.1	4.52	0.1	0.10	94.3%
THJ-2201	C23H21FN2O	361.1711	-0.9	5.73	-0.5	0.25	96.3%
Tianeptine	C21H25ClN2O4S	437.1296	-1.4	4.05	-1.0	ND	63.7%
Timolol	C13H24N4O3S	317.1642	-1.8	3.02	0.3	0.10	91.8%
Tiquizium	C19H24NS2	330.1345	-1.2	3.96	1.6	ND	0.3%
Tolbutamide	C12H18N2O3S	271.1111	-0.7	4.42	-0.7	0.50	19.0%
Tolmetin	C15H15NO3	258.1125	0.2	4.40	1.5	ND	1.5%
Torasemide	C16H20N4O3S	349.1329	-1.2	3.59	0.7	ND	2.9%
Trazodone	C19H22ClN5O	372.1586	-1.9	3.51	0.4	0.10	95.5%
Trenbolone	C18H22O2	271.1693	-0.3	4.41	0.5	0.25	87.7%
Trestolone	C19H28O2	289.2162	-1.1	4.62	0.5	0.10	91.6%
Triamcinolone	C21H27O6F	395.1864	-1.4	3.32	0.3	ND	88.7%
Triamcinolone acetonide	C24H31FO6	435.2177	0.5	4.30	1.5	ND	95.4%
Triazolam	C17H12Cl2N4	343.0512	-1.8	4.32	-0.1	0.10	88.1%
Trifluoperidol	C22H23F4NO2	410.1738	-2.1	4.10	0.1	0.10	88.2%
Trimipramine	C20H26N2	295.2169	-1.3	4.24	-0.1	0.10	86.0%
Tripelennamine	C16H21N3	256.1808	-1.0	3.63	0.5	0.10	99.6%
Tulobuterol	C12H18ClNO	228.1150	-1.3	3.14	0.1	0.25	96.3%
Turinabol	C20H27ClO2	335.1772	-1.8	4.98	-0.6	0.25	98.2%
UR-144	C21H29NO	312.2322	0.4	6.40	0.3	ND	82.7%
URB-597	C20H22N2O3	339.1703	-1.7	4.72	-1.6	1.00	89.3%
Vardenafil	C23H32N6O4S	489.2279	-0.9	3.63	0.4	0.10	81.9%
Venlafaxine	C17H27NO2	278.2115	-0.7	3.45	0.5	0.10	101.3%
W-18	C19H20ClN3O4S	422.0936	-0.4	5.08	0.8	0.25	101.2%
WIN 54,461	C23H25BrN2O3	457.1121	-0.3	5.24	-1.7	0.25	79.3%
WIN 55,212-2	C27H26N2O3	427.2016	-1.1	5.44	-2.3	0.50	78.2%
XLR-11 4-OH-Pentyl metabolite	C21H28FNO2	346.2177	-0.6	5.15	-2.4	0.10	90.9%
Xylazine	C12H16N2S	221.1107	-1.3	3.29	-0.9	0.02	99.3%
Yohimbine	C21H26N2O3	355.2016	-2.4	3.24	0.2	0.10	93.6%
Zaleplon	C17H15N5O	306.1349	-1.2	3.98	-0.1	0.10	91.8%
Zimeldine	C16H17BrN2	317.0648	-1.3	3.53	1.2	0.50	78.5%
Zinterol	C19H26N2O4S	379.1686	-1.7	3.32	-0.3	0.25	78.5%
Zolpidem	C19H21N3O	308.1757	-1.9	3.41	1.4	0.10	91.0%
Zomepirac	C15H14ClNO3	292.0735	-0.5	4.70	0.2	50.0	2.4%
Zopiclone	C17H17ClN6O3	389.1123	-1.5	3.04	1.0	0.10	97.4%
Δ1-Adrenosterone	C19H22O3	299.1642	-1.2	4.15	-0.1	0.10	94.9%

¹ ND: not determined

Supplement Table 2. List of substances with normalized collision energies (NCEs) and fragment ions

Substances	NCE	Fragment ions		
1,3-Benzodioxolyl-N-methylbutanamine	20	177.0910	147.0804	135.0440
15 β -Hydroxytestosterone	40	123.0806	109.0650	97.0650
16 β -Hydroxytestosterone	40	123.0806	109.0650	97.0650
2-(1-Hydroxyethyl) promazine sulfoxide	50	242.0633	86.0964	58.0654
2-(1-Hydroxypropyl)promazine sulfoxide	45	257.0867	86.0964	58.0654
2-Aminoheptane	10	105.0447	95.0492	53.0392
2 α -Hydroxymethylethisterone	40	139.0756	121.0651	109.0651
3,4-Methylenedioxyamphetamine	10	163.0753	135.0440	105.0699
3,4-Methylenedioxypropylamphetamine	30	163.0753	135.0440	86.0967
3-Hydroxymepivacaine	35	263.1755	99.0997	98.0964
3-Hydroxypromazine	35	228.0476	86.0964	58.0655
3-OH Lidocaine	35	251.1753	86.0963	87.0997
4-Chloroamphetamine	30	153.0465	126.0186	125.0152
4-Hydroxypropranolol	40	199.0754	173.0597	116.1070
4-Methoxymethamphetamine	30	149.0960	121.0647	150.0992
5,6-Methylenedioxy-2-aminoindane	40	161.0596	131.0491	103.0541
6-Dehydroandrostenedione	45	149.0960	107.0854	105.0698
6-Dehydronandrolone	40	151.1120	133.1014	105.0701
6-Dehydrotestosterone	40	133.1013	151.1119	105.0700
7-Aminoclonazepam	50	250.0976	222.1026	121.0761
7-Aminoflunitrazepam	50	256.1245	227.0978	135.0917
7-Hydroxy Fluphenazine	40	296.0350	171.1491	143.1179
7-Hydroxychlorpromazine	35	262.0087	86.0964	58.0655
9-Dehydroandrostenedione	45	252.1506	227.1428	147.0803
9-Dehydromethyl-testosterone	40	159.1171	147.0806	225.1641
9-Dehydrotestosterone	40	121.0650	145.1015	147.0807
A-796,260	30	295.2095	125.0964	114.0916
AB Pinaca	10	314.1873	286.1924	215.1181
AB-Fubinaca	10	352.1463	324.1515	253.0772
Acebutolol	30	260.1280	116.1069	98.0963
Acetaminophen	60	110.0600	93.0335	111.0439
Acetophenazine	35	254.0634	171.1492	143.1180
Adrenosterone	40	257.1542	121.0650	225.1279
AH-7921	30	284.0602	172.9557	95.0855
Albuterol	30	222.1486	166.0862	148.0756
Alfentanil	30	314.1859	268.1766	197.1284
Alprazolam	50	281.0710	274.1211	241.0524
Alprenolol	50	173.0960	116.1069	74.0604
Altrenogest	40	227.1434	251.1435	225.1279
AM 2233	25	362.0043	230.9307	112.1123
AM-2201	30	127.0544	155.0495	232.1140
AM-2201 Benzimidazole analog	30	251.1197	233.1091	213.1029
AM-2201 N-(4-hydroxypentyl) Metabolite	35	155.0493	248.1087	156.0526
AM-630	20	135.0443	114.0916	136.0476
Ambroxol	20	263.8839	261.8860	116.1069
Amiloride	30	189.0174	171.0068	60.0559
Aminopentamide	35	252.1381	207.1166	131.0854
Aminorex	30	120.0807	121.0840	93.0698
Amiphenazole (Diamino-5-phenylthiazole)	70	117.0574	106.0652	133.0762
Amoxapine	40	271.0629	245.0473	70.0651
Amphetamine	30	119.0856	91.0542	105.0334
Anastrozole	30	225.1383	226.1417	266.1650
Androstatrienedione	30	121.0650	147.0807	173.0966
Androstenedione	40	97.0650	109.0650	123.0807
Antipyrine	80	147.0916	130.0650	106.0651
Apomorphine	30	238.0941	237.0908	219.0803
Aprindine	20	250.1587	114.1276	86.0963
Aripiprazole	40	285.0916	176.0705	98.0963
Asimilobine	30	251.1067	219.0804	191.0856
Astemizole	30	308.1552	218.1536	135.0802
Atenolol	45	190.0861	145.0647	74.0604
Atropine	60	124.1120	93.0698	67.0544
Azaperone	30	165.0710	147.0916	121.0760

Azelastine	40	112.1120	81.0699	58.0655
Bambuterol	30	312.1551	294.1446	72.0444
Benactyzine	30	239.1064	118.1225	100.1120
Benazepril	30	351.1698	190.0862	117.0698
Benzoylcegonine	45	168.1019	150.0913	105.0335
Benzphetamine	30	122.0964	119.0855	91.0542
Betaxolol	45	161.0962	116.1070	98.0965
Biperiden	40	98.0963	143.0854	99.0996
Bisoprolol	30	116.1069	74.0601	147.0804
Bolasterone	35	203.1749	123.0804	97.0648
Boldenone	30	173.0961	135.1167	121.0647
Boldenone Acetate	25	269.1900	135.1168	121.0648
Boldine	30	297.1117	265.0857	237.0908
Boldione	45	121.0646	133.1010	151.1115
Bromazepam	40	273.0600	209.0946	182.0838
Brombuterol	25	346.9749	290.9126	211.9942
Bromhexine	25	261.8860	114.1276	
Bromocriptine	30	301.0331	346.0545	195.0991
Brompheniramine	40	274.0223	167.0727	275.0257
Brotizolam	35	184.0734	149.0232	93.0366
Budesonide	10	413.2315	341.1741	323.1637
Buflomedil	30	237.1118	140.1069	238.1152
Bumetanide	20	284.1279	240.1381	184.0757
Buphedrone	50	160.1119	131.0728	91.0541
Bupivacaine	40	140.1432	98.0963	150.0913
Buprenorphine	60	396.2167	187.0755	84.0808
Bupropion	30	184.0523	166.0418	131.0729
Buspirone	50	265.1910	222.1487	122.0712
Butorphanol	50	310.2162	242.1538	124.1120
Butylone	30	204.1017	174.0912	191.0702
Caffeine	70	138.0661	110.0713	83.0603
Calusterone	35	203.1794	123.0804	97.0648
Canrenone	45	283.1689	187.1115	107.0854
Capsaicin	20	182.1539	137.0596	170.1538
Carazolol	40	222.0913	184.0759	116.1070
Carbamazepine	40	194.0963	192.0808	220.0756
Carbinoxamine	30	202.0417	167.0729	72.0808
Carfentanil	30	335.2112	279.1852	246.1486
Carisoprodol	10	200.1647	176.1284	158.1177
Carteolol	30	237.1232	202.0862	74.0600
Carvedilol	30	283.1438	224.1277	100.0755
Cathinone	20	132.0807	117.0572	105.0698
Celecoxib	50	362.0762	332.0754	301.0945
Celiprolol	30	307.1651	251.1026	233.0919
Cetirizine	20	201.0463	202.0496	187.1076
Chlordiazepoxide	20	283.0867	241.0524	227.0492
Chlorprothixene	30	271.0342	231.0027	86.0963
Chlorthalidone	40	321.9933	243.0208	241.0051
Cimaterol	30	202.1339	160.0869	141.0004
Cimetidine	30	159.0698	117.0480	95.0603
Cinnarizine	10	167.0854	201.1384	
Cisapride	35	184.0158	234.1286	96.0807
Citalopram	40	262.1025	234.0711	109.0447
Clenbuterol	30	259.0763	203.0137	204.0173
Clobazam	40	259.0631	224.0943	
Clomipramine	30	271.0341	86.0963	58.0654
Clonazepam	50	302.0449	270.0553	241.0524
Clonidine	70	212.9978	186.9823	171.9714
Clopamide	50	250.0048	169.0164	121.1121
Clostebol	30	143.0261	131.0261	251.1799
Clozapine	40	270.0790	227.0368	84.0807
Cocaeethylene	40	196.1332	150.0913	82.0651
Cocaine	45	182.1175	150.0913	82.0651
Cotinine	70	146.0601	98.0601	80.0495
Cyclobenzaprine	40	216.0933	231.1168	205.1012
Danazol	40	310.2161	148.0756	120.0807

Dembrexine	30	281.8943	264.8678	81.0699
Deoxycorticosterone	40	123.0803	109.0647	97.0648
Deracoxib	50	378.0713	303.0736	283.0675
Desalkylflurazepam	55	226.0900	165.0214	140.0262
Deserpidine	35	367.2010	335.1750	195.0651
Desipramine	30	236.1433	208.1121	72.0808
Desmethylmetoprolol	40	177.0910	116.1070	72.0808
Desonide	10	399.2157	341.1740	323.1635
Desoximetasone	10	357.2054	339.1948	321.1844
Despropionylfentanyl	50	188.1433	134.0963	105.0698
Detomidine	70	99.0552	82.0479	81.0447
Dexamethasone	15	373.2003	355.1898	337.1794
Dextromethorphan	60	213.1273	171.0805	147.0804
Dextrorphan	70	199.1118	157.0648	133.0648
Dezocine	25	229.1585	147.0804	97.1011
Dibucaine	30	271.1443	215.0815	74.0965
Dichlorisone acetate	10	419.1618	359.1405	305.1536
Diclofenac	20	278.0137	250.0182	215.0492
Dicyclomine	40	237.1849	165.1639	109.1012
Diethylpropion	50	133.0647	105.0698	100.1119
Dihydrocapsaicin	10	184.1696	137.0597	172.1696
Dihydrocodeine	60	227.1070	199.0755	171.0806
Dihydromorphine	70	185.0599	211.0755	157.0650
Diphenhydramine	10	168.0888	167.0855	211.1229
Dobutamine	60	137.0598	107.0492	91.0543
Domperidone	30	175.0866	147.0552	176.0899
Doxepin	40	235.1118	117.0699	107.0491
Droperidol	20	194.0975	165.0710	195.1008
Ecgonine methyl ester	50	182.1176	150.0917	82.0651
Embutramide	30	121.0649	191.1432	208.1697
Ephedrine	40	148.1120	133.0885	117.0698
Epiboldenone	40	121.0651	135.1171	173.0966
Epinandrolone	45	109.0650	145.1014	83.0493
Estazolam	50	267.0559	241.0527	205.0760
Ethinyltestosterone	45	97.0650	109.0650	123.0807
Ethopropazine	25	240.0841	198.0372	114.1277
Ethylmorphine	60	183.0804	165.0698	58.0654
Ethylone	30	204.1017	174.0912	72.0808
Etilamfetamine	30	119.0855	91.0542	
Etilefrine	20	164.1071	165.1103	121.0648
Etodolac	30	270.1488	210.1277	172.1121
Etorphine	55	249.0909	87.0804	58.0655
Exemestane	35	149.0959	121.1010	93.0700
Famprofazone	40	217.1335	162.1278	119.0856
Felbamate	30	117.0699	178.0864	
Fenfluramine	30	187.0730	159.0416	160.0449
Fenoterol	20	286.1439	135.0805	152.0706
Fentanyl	40	216.1383	188.1434	105.0699
Feprazone	35	265.0973	253.0973	211.0660
Firocoxib	20	283.0633	265.0529	237.0579
Fludrocortisone Acetate	45	239.1432	181.1023	265.1590
Flufenamic Acid	60	244.0566	216.0618	195.0677
Flumethasone	10	371.1847	335.1637	253.1221
Flunisolide	20	397.2000	339.1581	321.1477
Flunitrazepam	50	300.0904	268.1007	239.0979
Flunixin	70	264.0503	259.0677	109.0448
Fluocinolone Acetonide	10	413.2655	317.1951	69.9157
Fluocinonide	20	337.1429	319.1323	291.1377
Fluocortolone	20	303.1743	171.0805	321.1847
Fluorometholone	10	357.2055	339.1949	279.1743
Fluoxetine	10	148.1119	310.1411	
Fluoxymesterone	40	131.0858	181.1026	241.1591
Flupentixol	40	390.1367	305.0603	100.0756
Fluphenazine	35	280.0400	171.1490	143.1178
Fluphenazine sulfoxide	50	280.0403	266.0247	143.1179
Flurazepam	30	315.0693	288.0585	100.1120

Fluticasone Propionate	15	313.1596	293.1535	205.0659
Fluvoxamine	20	258.1102	226.0837	71.0492
Formoterol	30	327.1697	149.0960	121.0647
Gestodene	40	109.0651	201.1281	159.0808
Gestrinone	50	199.1122	241.1590	262.1357
Glafenine	30	299.0579	281.0475	282.0508
Glaucine	20	325.1432	310.1199	294.1251
Gliclazide	30	153.1022	127.1229	110.0964
Griseofulvin	30	285.0525	215.0105	165.0547
Guaifenesin	20	163.0753	151.0753	125.0597
Guanabenz	50	213.9932	188.9981	171.9715
Halazepam	60	290.1024	241.0526	193.0888
Hydrocodone	60	241.0858	199.0753	171.0805
Hydromorphone	60	227.0701	199.0753	185.0596
Hydroxymetoprolol	45	116.0171	98.0965	74.0601
Hydroxyzine	20	201.0464	202.0497	173.1285
Ibogaine	60	188.1070	174.0914	122.0964
Imipramine	30	208.1121	86.0964	58.0655
Indapamide	10	132.0806	324.8934	234.9937
Indomethacin	20	174.0914	138.9945	339.2714
Indoprofen	50	236.1068	218.0963	181.0885
Isoetharine	30	222.1488	180.1020	60.0811
Isofluprednone	30	265.1587	237.1273	147.0804
Isometheptene	60	58.0657	55.0548	69.0703
Isoproterenol	20	194.1176	158.0271	141.0005
JWH 018 N-(5-hydroxypentyl) Metabolite	25	155.0494	230.1182	156.0527
JWH 073 4-Hydroxybutyl Metabolite	30	155.0495	216.1026	156.0528
JWH 122 N-(5-hydroxypentyl) Metabolite	30	169.0652	230.1183	170.0685
JWH 250 N-(5-hydroxypentyl) Metabolite	25	121.0651	186.1284	204.1391
JWH-015	35	200.1077	155.0495	156.0528
JWH-018	35	214.1225	155.0491	93.0367
JWH-030	25	155.0494	164.1074	156.0527
JWH-073	35	200.1077	155.0495	156.0527
JWH-081	30	230.1183	169.0653	170.0686
JWH-200	25	155.0493	114.0916	156.0526
JWH-203	35	188.1440	125.0155	93.0369
JWH-210	30	183.0805	161.1324	147.1168
JWH-250	25	200.1440	188.1440	121.0651
Ketamine	45	207.0572	179.0623	125.0153
Ketoprofen	30	209.0960	177.0546	105.0335
Ketorolac	30	105.0334	106.0367	210.0912
Labetalol	20	311.1751	294.1488	207.1126
Lamotrigine	60	210.9823	186.9825	166.0293
Letrozole	90	190.0652	215.0603	163.0543
Levorphanol	70	199.1117	157.0648	133.0647
Liriodenine	80	190.0652	218.0601	248.0707
Lobelanidine	40	218.1539	202.1589	98.0965
Lobeline	30	216.1383	200.1434	96.0807
Loperamide	50	266.1539	238.1225	210.1276
Loratadine	40	337.1096	294.1041	267.0808
Lorazepam	30	303.0084	275.0137	229.0527
Lormetazepam	25	317.0240	289.0292	291.0260
Mabuterol	30	237.0401	217.0339	293.1028
MAM-2201	35	293.1406	232.1138	169.0652
Mapenterol	20	237.0400	307.1182	71.0855
Maprotiline	40	250.1590	219.1167	169.1012
Mebendazole	40	264.0767	105.0335	
Meclofenamic Acid	45	278.0133	243.0444	242.0366
Medetomidine	35	95.0603	93.0367	68.0496
Mefenamic Acid	40	224.1069	209.0836	223.0992
Mefruside	20	129.1148	284.9765	99.0804
Melengestrol	35	279.1748	236.1564	237.1643
Meperidine	60	220.1331	174.1278	70.0652
Mephedrone	50	160.1120	145.0885	119.0855
Mephentermine	35	133.1012	105.0699	91.0542
Mepivacaine	80	99.0996	98.0964	70.0652

Meprobamate	10	97.1012	158.1177	141.0005
Mescaline	10	195.1015	180.0780	141.0004
Metaproterenol	30	194.1178	152.0707	141.0005
Metaraminol	10	150.0914	133.0648	84.9597
Metaxalone	15	161.0960	135.0803	123.0804
Methadone	30	265.1585	223.1115	105.0334
Methamphetamine	40	119.0854	91.0541	92.0575
Methandrostenolone	30	173.0962	149.1325	121.0648
Methapyrilene	30	217.0792	97.0106	119.0603
Methaqualone	70	161.0710	132.0808	91.0542
Methcathinone	40	146.0963	131.0728	105.0698
Methenolone	50	187.1487	83.0943	145.1015
Methocarbamol	25	163.0754	125.0597	118.0499
Methoxamine	25	194.1175	162.0912	141.0004
Methyl-1-testosterone	50	201.1643	145.1015	159.1172
Methylboldenone	40	173.0965	149.1327	121.0649
Methylclostebol	40	131.0261	143.0261	189.1642
Methyldienolone	40	135.0806	159.0807	161.0964
Methylenedioxyethylamphetamine	40	163.0753	135.0439	105.0698
Methylenedioxypropylvalerone	40	205.0857	175.0753	126.1276
Methylhexanamine	10	60.0447	116.1070	57.0702
Methylnortestosterone	40	231.1744	232.1775	271.2057
Methylone	30	190.0862	160.0757	58.0654
Methylphenidate	30	84.0810	85.0843	174.1275
Methylprednisolone	30	253.1587	161.0961	135.0804
Methyltestosterone	50	109.0650	97.0650	227.1800
Metolazone	60	258.9940	211.0031	151.0184
Metoprolol	40	116.1069	191.1066	159.0804
Mianserin	50	208.1121	176.1071	58.0655
Mibolerone	50	177.1273	121.1011	95.0854
Midazolam	50	291.1164	244.0323	209.0636
Mitragynine	40	174.0914	226.1436	238.1437
Morphine	70	201.0909	181.0647	165.0698
N,N-Didesmethyl Trimebutine	35	342.1694	324.1589	270.1123
Nadolol	30	254.1384	236.1279	201.0909
Nalbuphine	40	340.1902	296.1642	272.1280
Nalorphine	70	201.0785	181.0648	165.0699
Naloxone	40	310.1435	268.1332	253.1097
Naltrexone	40	324.1591	270.1125	267.1254
Nandrolone	45	239.1793	145.1011	109.0648
Nandrolone Acetate	40	257.1897	239.1791	109.0647
Naphyrone	40	211.1115	141.0697	126.1276
N-Desmethylselegiline	30	119.0856	91.0542	56.0499
N-Desmethyltrimipramine	25	250.1589	208.1120	86.0964
Nebivolol	40	151.0553	123.0604	58.0654
Nefopam	55	181.1011	166.0777	153.0698
Nikethamide	60	108.0443	72.0808	80.0495
Nitrazepam	50	268.0842	236.0943	207.0916
Nomifensine	50	196.1122	118.0651	91.0543
Norbolethone	35	109.0650	227.1799	245.1904
Norchlordiazepoxide	35	269.0712	241.0526	227.0496
Norclostebol	40	143.0261	213.1643	237.1045
Norcodeine	60	225.0910	181.0649	165.0700
Nordiazepam	60	208.0994	165.0214	140.0261
Norethandrolone	50	109.0651	135.0807	231.1748
Norfentanyl	40	177.1386	150.0913	84.0807
Norfluoxetine	50	134.0966	105.0704	91.0542
Norgestrel	45	109.0651	135.0807	245.1906
Norketamine	30	207.0571	179.0622	125.0152
Norlutin	35	231.1747	145.1014	109.0650
Normeperidine	50	160.1120	131.0855	56.0498
Normorphine	70	181.0650	165.0700	153.0700
Nortriptyline	40	233.1324	105.0699	91.0542
Norverapamil	30	165.0911	289.1909	150.0676
Nylidrin	30	282.1850	150.0913	91.0542
O-Desmethylpyrilamine	55	227.1174	121.0761	107.0491

O-Desmethyltramadol	20	250.1800	232.1695	58.0654
Omeprazole Sulfide	40	182.0634	149.0709	120.0807
Orphenadrine	10	181.1010	165.0688	103.0389
Oxandrolone	25	253.1956	229.1955	121.1014
Oxazepam	40	269.0475	241.0526	231.0683
Oxilofrine	50	164.1072	105.0336	149.0837
Oxprenolol	30	225.1358	116.1069	72.0808
Oxycodone	40	298.1435	256.1331	241.1096
Oxymetazoline	65	231.1491	205.1335	135.0804
Oxymorphone	40	284.1280	242.1174	227.0939
Oxyphencyclimine	35	129.1021	327.2063	189.1273
Oxyphenylbutazone	30	204.1018	160.1120	120.0443
Papaverine	50	324.1224	202.0862	171.0678
Paroxetine	40	192.1182	151.0389	70.0652
PB-22	20	214.1233	109.1015	95.0858
Penbutolol	40	236.1643	201.1273	133.0647
Pentazocine	50	218.1538	175.1118	69.0700
Perphenazine	35	246.0137	171.1492	143.1179
Pheniramine	20	196.1120	118.0646	
Phentermine	30	119.0855	91.0542	92.0575
Phenylbutazone	40	211.0864	160.1120	120.0443
Phenylpropanolamine	50	134.0963	117.0698	115.0542
p-hydroxy Benzphetamine	35	135.0804	107.0491	91.0542
Pimobendan	60	319.1187	292.1315	250.0970
Pimozide	40	328.1868	201.1022	147.0604
Pindolol	40	172.0757	146.0600	116.1069
Piperidolate	35	167.0855	130.1226	112.1120
Piretanide	40	282.1125	196.0758	236.1070
Pirlindole	50	210.1277	184.1122	198.1278
Piroxicam	30	164.0818	121.0396	95.0603
Prazepam	40	271.0632	140.0262	255.0683
Prednisolone	25	343.1900	307.1691	147.0804
Prednisone	20	341.1740	313.1794	147.0803
Prilocaine	10	163.0752	90.9768	86.0966
Probenecid	30	244.0637	202.0168	184.9904
Procainamide	30	163.0865	120.0443	100.1119
Procaine	30	164.0705	120.0443	100.1120
Procaterol	25	273.1597	231.1127	162.0550
Procyclidine	30	84.0807	270.2216	58.0654
Promazine	30	86.0964	85.0654	240.0840
Pronethalol	10	212.1432	170.0963	213.1465
Propionylpromazine	40	268.0790	86.0963	58.0654
Propofol	50	161.1323	119.0855	95.0855
Propoxyphene	10	323.1635	266.1902	58.0655
Propranolol	40	183.0804	157.0647	116.1069
propylamphetamine	40	119.0855	91.0541	60.0810
Protopine	50	189.0786	149.0598	188.0707
Protriptyline	40	233.1323	191.0854	155.0854
Pseudoephedrine	40	148.1120	133.0885	117.0698
Pyrilamine	20	241.1333	121.0647	
Pyrovalerone	40	175.1115	126.1275	105.0697
Quetiapine	30	279.0948	253.0792	158.1175
Quinapril	25	365.1856	234.1488	130.0862
Quinidine	50	253.1333	184.0757	160.0756
Ractopamine	30	284.1643	164.1070	121.0647
Raloxifene	40	269.0266	112.1120	84.0810
Ramipril	30	380.2579	343.2012	234.1487
Ranitidine	30	224.0976	176.0488	124.0757
RCS-4	35	135.0443	214.1233	136.0476
RCS-8	30	121.0650	228.1753	240.1753
Rescinnamine	25	474.2115	397.2112	221.0804
Risperidone	30	191.1178	55.0540	
Ritodrine	30	270.1487	150.0913	121.0647
Ropivacaine	30	126.1277	150.0914	
Salmeterol	20	398.2684	380.2579	232.1694
Selegiline	30	119.0855	91.0542	70.0652

Sertraline	10	275.0390	158.9759	129.0699
Sibutramine	25	153.0465	139.0309	125.0152
Sildenafil	40	311.1500	283.1188	100.0993
Sotalol	25	255.1161	213.0691	176.1307
Sparteine	80	129.0697	98.0965	84.0810
Stanozolol	90	107.0855	93.0699	81.0447
Strychnine	80	184.0758	156.0808	129.0698
Sufentanil	40	355.1833	238.1257	111.0262
Sulpiride	45	214.1067	112.1120	98.0964
Suxibuzone	25	309.1595	267.1128	160.1120
Tadalafil	20	268.1081	302.0808	135.0440
Tapentadol	50	135.0804	121.0648	107.0491
Telmisartan	45	497.2333	276.1367	211.0752
Temazepam	30	283.0630	255.0682	256.0715
Tenoxicam	25	164.0817	121.0395	95.0603
Terfenadine	30	454.3099	436.2994	262.1589
Testosterone	40	253.1951	109.0648	97.0648
Testosterone Acetate	30	253.1947	109.0647	97.0647
Tetrahydrogestrinone (THG)	45	266.1664	241.1584	159.0803
Tetrahydrozoline	85	131.0855	91.0542	71.0605
Theobromine	90	138.0663	122.0588	67.0293
Theophylline	70	124.0505	96.0556	69.0448
Thioridazine	30	258.0406	126.1277	98.0964
THJ-2201	30	273.1032	251.1198	155.0494
Tianeptine	10	292.0192	250.1770	210.1100
Timolol	30	261.1016	244.0750	188.0489
Tiquizium	60	217.0139	185.0422	135.0263
Tolbutamide	20	172.0428	155.0161	74.0965
Tolmetin	20	119.0490		
Torasemide	50	264.0801	183.0918	125.0168
Trazodone	40	176.0819	148.0505	237.1153
Trenbolone	60	253.1586	199.1118	72.0444
Trestolone	40	253.1948	159.1242	93.0699
Triamcinolone	10	357.1691	339.1585	225.1273
Triamcinolone acetonide	20	397.2005	339.1587	321.1482
Triazolam	50	315.0322	308.0823	138.0106
Trifluoperidol	30	392.1629	165.0711	123.0240
Trimipramine	30	208.1121	100.1120	58.0655
Tripelennamine	20	211.1227	212.1260	72.0811
Tulobuterol	30	172.0525	154.0419	57.0702
Turinabol	25	155.0260	149.1327	161.1328
UR-144	40	125.0963	279.1990	97.1015
URB-597	20	214.0868	197.0604	171.0809
Vardenafil	40	376.1070	344.1474	169.0971
Venlafaxine	25	260.2008	215.1428	58.0657
W-18	40	174.9615	111.0917	273.0460
WIN 54,461	20	135.0443	114.0917	136.0477
WIN 55,212-2	30	155.0494	100.0760	156.0527
XLR-11 4-OH-Pentyl metabolite	35	248.1089	249.1124	174.9532
Xylazine	70	164.0528	147.0917	90.0372
Yohimbine	40	224.1280	212.1280	144.0808
Zaleplon	50	264.1243	236.0929	219.0664
Zimeldine	10	272.0069	193.0887	274.0047
Zinterol	25	247.0746	229.0640	133.1011
Zolpidem	50	263.1179	235.1230	221.1076
Zomepirac	35	138.9945	95.0491	81.0699
Zopiclone	10	345.1221	263.0330	245.0224
Δ^1 -Adrenosterone	35	171.0809	223.1122	147.0807