

Forensic Library

Forensic LC/MS/MS Library Version 1.0 for Cliquid® Software

The following description outlines the 1250 forensic compounds available in the MRM Catalogue and Library. This library and MRM catalogue, created under stringent quality control conditions using certified reference materials, can be used stand-alone to create custom screening and/or quantification methods or in conjunction with the iMethod™ Test for Drugs of Abuse Screening. The iMethod™ Test provides a pre-configured method for the screening of 700 drugs of abuse in a single run, via an MRM triggered EPI workflow on a QTRAP® series instrument. This library is verified for use on AB SCIEX 3200 QTRAP®, 4000 QTRAP® and AB SCIEX QTRAP® 5500 LC/MS/MS systems.

The MRM Catalog and Spectral Library both contain information on over 1250 drugs of abuse, metabolites, and other compounds of forensic interest. The MRM Catalog contains up to six MRM transitions and the Library contains up to 8 full scan EPI spectra for each compound. Each compound in the library has individual spectra acquired using three distinct collision energies (20 eV, 35 eV, or 50 eV), as well as a single spectrum that is a sum of the three energies. If it is possible to ionize the compound in both polarities, spectra for both are also included, bringing the potential total number of spectra present per compound to eight.



The MRM catalogue can be used to build methods without the need to re-infuse standards to determine and optimize MRM transitions. Screening methods can be created using either the MRM triggered EPI workflow on a QTRAP® type instrument, or for traditional quantification/confirmation, using two or more transitions per compounds and determining the ratio between the two transitions. This traditional MRM ratio approach can be used on either a triple quadrupole or QTRAP® instrument. Users select the analytes from the MRM catalog, the number of transitions per compound to use, and whether an MRM-EPI or MRM ratio method should be built. Cliquid® Software automatically creates the acquisition and processing methods.

The following is a list of the 1250 compounds currently present in the library. Please note that this library is continually being expanded to include additional compounds.

Compound	Formula	MW	CAS	# of spectra
(-)-Trans-delta-9-THC carboxylic acid A	C22H30O4	358,2144		4
17-alpha-Methyltestosterone	C20H30O2	302,2245	58-18-4	4
17alpha-Hydroxyprogesterone	C21H30O3	330,2194	68-96-2	8
2-Amino-5-chlorobenzophenone	C13H10ClNO	231,045	719-59-5	4
2-Amino-5-nitrobenzophenone	C13H10N2O3	242,0691	1775-95-7	8
2-Benzyltetronic acid	C11H10O3	190,0629	3734-22-3	4
2-Hydroxyethylflurazepam	C17H14ClFN2O2	332,0727	20971-53-3	4
3-Hydroxybromazepam	C14H10BrN3O2	330,9956	13132-73-5	4
3-Methylfentanyl	C23H30N2O	350,2358		4
3,4-Dimethoxyphenethylamine	C10H15NO2	181,1102	120-20-7	4
3,4-Methylenedioxyamphetamine	C10H13NO2	179,0946	13673-99-9	4
3,4-Methylenedioxyethylamphetamine	C12H17NO2	207,1259	82801-81-8	4
3,4-Methylenedioxymethamphetamine	C11H15NO2	193,1102	42542-10-9	4
3,5-Diiodotyrosine	C9H9I2NO3	432,8671	04/02/1966	4
4-Benzamidosalicylic acid	C14H11NO4	257,0688	13898-58-3	8
4-Methylumbelliferyl acetate	C12H10O4	218,0579	09/05/2747	4
5-(p-Methylphenyl)-phenylhydantoin	C16H14N2O2	266,1055	51169-17-6	4
5-Aminosalicylic acid	C7H7NO3	153,0425	89-57-6	4
6-Chlorothymolsulfonic acid	C10H13ClO4S	264,0222	83732-70-1	4
6-Mercaptourine	C5H4N4S	152,0156	50-44-2	8
6-O-Monoacetylmorphine	C19H21NO4	327,147	2784-73-8	4
7-Aminoclonazepam	C15H12ClN3O	285,0668	4959-17-5	4
7-Aminodesmethylflunitrazepam	C15H12FN3O	269,0964	894-76-8	4
7-Aminoflunitrazepam	C16H14FN3O	283,112	34084-50-9	4
7-Aminonitrazepam	C15H13N3O	251,1058	03/02/4928	4
8-Chlorotheophylline	C7H7ClN4O2	214,0257	85-18-7	8
8-Hydroxyquinoline	C9H7NO	145,0526	148-24-3	4
9-Hydroxyrisperidone	C23H27FN4O3	426,2067		4
Acebutolol	C18H28N2O4	336,2049	37517-30-9	4
Acecarbromal	C9H15BrN2O3	278,0266	77-66-7	8
Aceclidine	C9H15NO2	169,1102	827-61-2	4
Aceclofenac	C16H13Cl2NO4	353,0221	89796-99-6	8
Acemetacin	C21H18ClNO6	415,0822	53164-05-9	4
Acenocoumarol	C19H15NO6	353,0899	152-72-7	8

Compound	Formula	MW	CAS	# of spectra
Acepromazine	C19H22O2S	298,1391	61-00-7	4
Aceprometazine	C19H22N2O2S	326,1452	13461-01-3	4
Acetaminodantrolene	C16H14N4O4	326,1015	41515-09-7	4
Acetazolamide	C4H6N4O3S2	221,9881	59-66-5	4
Acetiamin	C16H22N4O4S	366,1361	28008-04-0	4
Acetylamino-nitroprophoxybenzene	C11H14N2O4	238,0953	553-20-8	8
Acetylsalicylamid	C9H9NO3	179,0582	487-48-9	8
Acetylsalicylic Acid	C9H8O4	180,0422	50-78-2	4
Aciclovir	C8H11N5O3	225,0861	59277-89-3	8
Acipimox	C6H6N2O3	154,0378	51037-30-0	4
Acrivastine	C22H24N2O2	348,1837	87848-99-5	4
Actinoquinol	C11H11NO4S	253,0408	15301-40-3	8
Adefovir	C8H12N5O4P	273,0626	106941-25-7	4
Adenine	C5H5N5	135,0544	73-24-5	8
Adenosine	C10H13N5O4	267,0967	58-61-7	8
Adrenalone	C9H11NO3	181,0738	99-45-6	8
Ajmaline	C20H26N2O2	326,1994	07/12/4360	4
Alachlor	C14H20ClNO2	269,1182	15972-60-8	4
Alclometasone-17,21-dipropionate	C28H37ClO7	520,2227	66734-13-2	4
Alcuronium	C44H50N4O2	666,3933	23214-96-2	4
Alfuzosine	C19H27N5O4	389,2063	81403-80-7	8
Alimemazine	C18H22N2S	298,1503	84-96-8	4
Alizapride	C16H21N5O2	315,1695	59338-93-1	8
Allopurinol	C5H4N4O	136,0385	315-30-0	8
Almitrine	C26H29F2N7	477,2452	27469-53-0	4
alpha-Hydroxyalprazolam	C17H13ClN4O	324,0777	37115-43-8	4
alpha-Hydroxymidazolam	C18H13ClFN3O	341,0731	59468-90-5	4
alpha-Hydroxytriazolam	C17H12Cl2N4O	358,0388	37115-45-0	4
Alprazolam	C17H13ClN4	308,0828	28981-97-7	4
Alprenolol	C15H23NO2	249,1728	13655-52-2	4
Alprostadil	C20H34O5	354,2406	745-65-3	4
Altretamine	C9H18N6	210,1592	645-05-6	4
Alypin	C16H26N2O2	278,1994	963-07-5	4
Amantadine	C10H17N	151,136	768-94-5	4

Compound	Formula	MW	CAS	# of spectra
Amibenonium	C28H42Cl2N4O2	536,2684	115-79-7	4
Ambroxol	C13H18Br2N2O	375,9785	18683-91-5	4
Ambucetamide	C17H28N2O2	292,215	519-88-0	4
Amcinonide	C28H35FO7	502,2366	51022-69-6	4
Ametryn	C9H17N5S	227,1204	834-12-8	4
Amezinium	C11H12N3O	202,098	30578-37-1	4
Amidopyrin	C13H17N3O	231,1371	58-15-1	4
Amidotrizoic Acid	C11H9I3N2O4	613,7696	117-96-4	4
Amiloride	C6H8ClN7O	229,0478	2609-46-3	4
Aminodantrolene	C14H12N4O3	284,0908	14663-28-6	4
Aminoglutethimide	C13H16N2O2	232,1211	125-84-8	4
Aminophenazone	C13H17N3O	231,1371	58-15-1	4
Aminopromazine	C19H25N3S	327,1769	58-37-7	4
Aminoquinuride	C21H20N6O	372,1698	3811-56-1	4
Aminorex	C9H10N2O	162,0793	2207-50-3	4
Amiodarone	C25H29I2NO3	645,0236	1951-25-3	4
Amiphenazole	C9H9N3S	191,0517	490-55-1	4
Amisulpride	C17H27N3O4S	369,1722	71675-85-9	4
Amitriptylin	C20H23N	277,183	50-48-6	4
Amitriptylinoxide	C20H23NO	293,1779	4317-14-0	4
Amitrole	C2H4N4	84,0435	61-82-5	4
Amlodipine	C20H25ClN2O5	408,1451	88150-42-9	4
Ammoidin	C12H8O4	216,0422	298-81-7	4
Amobarbital	C11H18N2O3	226,1317	57-43-2	4
Amorolfine	C21H35NO	317,2718	78613-35-1	4
Amoxapine	C17H16ClN3O	313,0981	14028-44-5	4
Amoxicillin	C16H19N3O5S	365,1045	26787-78-0	8
Amphetamine	C9H13N	135,1047	300-62-9	4
Amphotericin B	C47H73NO17	923,4878	1397-89-3	4
Ampicillin	C16H19N3O4S	349,1096	69-53-4	8
Amprolium	C14H19ClN4	278,1298	121-25-5	4
Amrinone	C10H9N3O	187,0745	60719-84-8	4
Anilazine	C9H5Cl3N4	273,9579	101-05-3	4
Antazoline	C17H19N3	265,1578	91-75-8	4

Compound	Formula	MW	CAS	# of spectra
Apalcillin	C25H23N5O6S	521,1369	63469-19-2	8
Apomorphine	C17H17NO2	267,1259	58-00-4	4
Apophedrin	C8H11NO	137,084	7568-93-6	4
Apraclonidin	C9H10Cl2N4	244,0282	66711-21-5	4
Aprinidine	C22H30N2	322,2408	37640-71-4	4
Arecoline	C8H13NO2	155,0946	63-75-2	4
Astemizole	C28H31FN4O	458,2481	68844-77-9	4
Asulam	C8H10N2O4S	230,0361	3337-71-1	4
Atenolol	C14H22N2O2	250,1681	29122-68-7	4
Atorvastatin	C33H35FN2O5	558,253	134523-00-5	8
Atraton	C9H17N5O	211,1433	1610-17-9	4
Atrazine	C8H14ClN5	215,0937	1912-24-9	4
Atrazine-desethyl	C6H10ClN5	187,0624	6190-65-4	4
Atropin-N-octylbromide	C25H40NO3	402,3008	5843-82-3	4
Atropine	C17H23NO3	289,1677	51-55-8	4
Atropinmethylbromid	C18H26NO3	304,1912	2870-71-5	4
Axeen	C10H14N1O4	212,0922	2537-29-3	4
Azapropazone	C16H20N4O2	300,1586	13539-59-8	8
Azatadine	C20H22N2	290,1782	3964-81-6	4
Azathioprine	C9H7N7O2S	277,0381	446-86-6	8
Azelaic Acid	C9H16O4	188,1048	123-99-9	4
Azelastine	C22H24ClN3O	381,1607	58581-89-8	4
Azidamphenicol	C11H13N5O5	295,0916	13838-08-9	4
Azidocillin	C16H17N5O4S	375,1001	17243-38-8	8
Azinhos methyl	C10H12N3O3PS2	317,0057	86-50-0	4
Azintamid	C10H14ClN3OS	259,0546	1830-32-6	4
Aziprotryne	C7H11N7S	225,0796	4658-28-0	4
Azithromycin	C38H72N2O12	748,5085	83905-01-5	4
Azoluron	C12H14N4O	230,1167	4058-90-6	4
Azosemide	C12H11ClN6O2S2	370,0073	27589-33-9	4
Aztreonam	C13H17N5O8S2	435,0518	78110-38-0	8
Bacampicillin	C21H27N3O7S	465,1569	50972-17-3	4
Baclofen	C10H12ClNO2	213,0556	1134-47-0	4
Bambuterol	C18H29N3O5	367,2106	81732-65-2	4

Compound	Formula	MW	CAS	# of spectra
Bamethan	C12H19NO2	209,1415	3703-79-5	4
Bamifylline	C20H27N5O3	385,2113	2016-63-9	4
Bamipin	C19H24N2	280,1939	4945-47-5	4
Barbital	C8H12N2O3	184,0847	57-44-3	4
Barverin	C29H43N5O3	509,3365	1639-79-8	4
Beclamide	C10H12ClNO	197,0607	501-68-8	4
Beclometasone dipropionate	C28H37ClO7	520,2227	08/09/5534	4
Befunolol	C16H21NO4	291,147	39552-01-7	4
Bemetizide	C15H16ClN3O4S2	401,027	1824-52-8	4
Benactyzine	C20H25NO3	327,1834	302-40-9	4
Benazolin-ethyl	C11H10ClNO3S	271,0068	25059-80-7	4
Bendamustine	C16H21Cl2N3O2	357,101	16506-27-7	4
Bendiacarb	C11H13NO4	223,0844	22781-23-3	4
Bendroflumethiazide	C15H14F3N3O4S2	421,0377	73-48-3	4
Benfluorex	C19H20F3NO2	351,1446	23602-78-0	4
Benfotiamin	C19H23N4O6PS	466,1075	22457-89-2	8
Benodanil	C13H10INO	322,9807	15310-01-7	4
Benorilate	C17H15NO5	313,095	5003-48-5	4
Benperidole	C22H24FN3O2	381,1852	2062-84-2	4
Benproperine	C21H27NO	309,2092	2156-27-6	4
Benserazid	C10H15N3O5	257,1011	322-35-0	8
Bensultap	C17H21NO4S4	431,0353	17606-31-4	4
Bentriomide	C23H20N2O5	404,1372	37106-97-1	8
Benzatropine	C21H25NO	307,1936	86-13-5	4
Benzethonium	C27H42NO2	412,3215	121-54-0	4
Benzocaine	C9H11NO2	165,0789	07/09/1994	4
Benzoctamine	C18H19N	249,1517	17243-39-9	4
Benzododecinium	C21H38N	304,3004	139-07-1	4
Benzoxonium	C23H42NO2	364,3215	19379-90-9	4
Benzoyllecgonine	C16H19NO4	289,1314	519-09-5	4
Benzquinamide	C22H32N2O5	404,2311	07/12/1963	4
Benzthiazide	C15H14ClN3O4S3	430,9834	91-33-8	8
Benzthiazuron	C9H9N3OS	207,0466	1929-88-0	4
Benzylamine	C19H23N3O	309,1841	642-72-8	4

Compound	Formula	MW	CAS	# of spectra
Benzyllectronic acid	C11H10O3	190,0629	3734-22-3	8
Berberine	C20H18NO4	336,1235	2086-83-1	4
Betaine	C5H11NO2	117,0789	107-43-7	4
Betamethasone-17-benzoate	C29H33FO6	496,2261	22298-29-9	4
Betamethasone 17-valerate	C27H37FO6	476,2574	2152-44-5	4
Betamethasone 21-phosphate	C22H30FO8P	472,1662	360-63-4	8
Betaxolol	C18H29NO3	307,2147	63659-18-7	4
Bethanidine	C10H15N3	177,1265	55-73-2	4
Bevonium	C22H28NO3	354,2069	5205-82-3	4
Bezafibrate	C19H20ClNO4	361,108	41859-67-0	8
Bezitramide	C31H32HN4O2	493,2603	15301-48-1	4
Bicalutamide	C18H14F4N2O4S	430,061	90357-06-5	4
Bidesmethylycitalopram	C18H17N2OF	296,1324		4
Bietamiverine	C19H30N2O2	318,2307	479-81-2	4
Bifonazole	C22H18N2	310,1469	60628-96-8	4
Biotin	C10H16N2O3S	244,0881	58-85-5	4
Biperiden	C21H29NO	311,2249	514-65-8	4
Bisacodyl	C22H19NO4	361,1314	603-50-9	4
Bisoprolol	C18H31NO4	325,2253	66722-44-9	4
Bitertanol	C20H23N3O2	337,1789	55179-31-2	4
Bopindolol	C23H28N2O	348,2201	62658-63-3	4
Bornaprine	C21H31NO2	329,2354	20448-86-6	4
Bosentan	C27H29N5O6S	551,1838	147536-97-8	8
Brallobarbital	C10H11BrN2O3	285,9953	561-86-4	4
Brimonidine	C11H10BrN5	291,0119	59803-98-4	4
Brivudine	C11H13BrN2O5	332,0007	69304-47-8	4
Brodifacoum	C31H23BrO	490,0932	56073-10-0	8
Bromacil	C9H13BrN2O2	260,016	314-40-9	8
Bromazepam	C14H10BrN3O	315,0007	1812-30-2	4
Bromazine	C17H20BrNO	333,0727	118-23-0	4
Bromchlorophen	C13H8Br2Cl2O2	423,8268	15435-29-7	4
Bromhexine	C14H20Br2N2	373,9993	3572-43-8	4
Bromocriptine	C32H40BrN5O5	653,2212	25614-03-3	4
Bromopride	C14H22BrN3O2	343,0895	4093-35-0	4

Compound	Formula	MW	CAS	# of spectra
Bromperidol	C21H23BrFNO2	419,0896	10457-90-6	4
Brompheniramine	C16H19BrN2	318,0731	86-22-6	4
Bromural	C6H11BrN2O2	222,0003	496-67-3	4
Bromurone	C9H11BrN2O	242,0054	3408-97-7	4
Brotizolam	C15H10BrCIN4S	391,9498	57801-81-7	4
Brucine	C23H26N2O4	394,1892	357-57-3	4
Bucetin	C12H17NO3	223,1208	1083-57-4	4
Buclosamide	C11H14CINO2	227,0713	575-74-6	4
Buclosamide	C11H14CINO2	227,0713	575-74-6	4
Budesonid	C25H34O6	430,2355	51333-22-3	4
Budipine	C21H27N	293,2143	57982-78-2	4
Bufexamac	C12H17NO3	223,1208	2438-72-4	8
Buflomedil	C17H25NO4	307,1783	55837-25-7	4
Bulbocapnin	C19H19NO4	325,1314	298-45-3	4
Bumadizone	C19H22N2O3	326,163	3583-64-0	4
Bumetanide	C17H20N2O5S	364,1092	28395-03-1	4
Bunazosin	C19H27N5O3	373,2113	80755-51-7	4
Bunitrolol	C14H20N2O2	248,1524	34915-68-9	4
Buphenine	C19H25NO2	299,1884	447-41-6	4
Bupivacaine	C18H28N2O	288,2201	2180-92-9	4
Bupranolol	C14H22CINO2	271,1339	14556-46-8	4
Buprenorphine	C29H51NO4	477,3818	52485-79-7	4
Buprenorphine-D4	C29H37D4NO4	471	136781-89-0	4
Buprofezin	C16H23N3OS	305,1561	69327-76-0	4
Buspirone	C21H31N5O2	385,2477	36505-84-7	4
Butalamine	C18H28N4O	316,2263	22131-35-7	4
Butalbital	C11H16N2O3	224,116	77-26-9	4
Butallylonal	C11H15BrN2O3	302,0266	1142-70-7	4
Butamirate	C18H29NO3	307,2147	18109-80-3	4
Butanilicain	C13H19CIN2O	254,1185	3785-21-5	4
Butaperazine	C24H31N3OS	409,2187	653-03-2	4
Butetamate	C16H25NO2	263,1884	14007-64-8	4
Butinoline	C20H21NO	291,1623	968-63-8	4
Butizide	C11H16CIN3O4S2	353,027	2043-38-1	4

Compound	Formula	MW	CAS	# of spectra
Butoxycaine	C17H27NO3	293,199	3772-43-8	4
Butoxycarboxim	C7H14N2O2S	190,0774	34681-10-2	4
Cabaryl	C13H14N2O	214,1106	63-25-2	4
Cabergoline	C26H37N5O2	451,2947	81409-90-7	4
Cabral	C13H14N2O	214,1106	553-69-5	4
Cafaminol	C11H17N5O3	267,1331	30924-31-3	4
Caffeine	C8H10N4O2	194,0803	02/08/1958	4
Calteridol	C17H32N4O7	404,227	121915-83-1	4
Camylofine	C19H32N2O2	320,2463	54-30-8	4
Candesartan	C24H20N6O3	440,1596	139481-59-7	4
Canrenoic Acid	C22H30O4	358,2144	4138-96-9	8
Capecitabine	C15H22FN3O6	359,1492	154361-50-9	8
Caproylesorcinol	C12H16O3	208,1099	70807-24-8	8
Captodiamine	C21H29NS2	359,1741	486-17-9	4
Captopril	C9H15NO3S	217,0772	62571-86-2	8
Carazolol	C18H22N2O2	298,1681	57775-29-8	4
Carbachol	C6H15N2O2	147,1133	51-83-2	4
Carbamazepine	C15H12N2O	236,0949	298-46-4	4
Carbamazepine 10,11-epoxide	C15H10N2O2	250,0742	36507-30-9	4
Carbaril	C12H11NO2	201,0789	63-25-2	4
Carbazochrom	C10H12N4O3	236,0909	69-81-8	4
Carbendazim	C9H9N3O2	191,0694	10605-21-7	4
Carbenoxolone	C34H50O7	570,3556	5697-56-3	8
Carbimazole	C7H10N2O2S	186,0462	22232-54-8	4
Carbinoxamine	C16H19CIN2O	290,1185	486-16-8	4
Carboxin	C12H13NO2S	235,0667	5234-68-4	4
Carbutamide	C11H17N3O3S	271,099	339-43-5	8
Carbuterol	C13H21N3O3	267,1582	34866-47-2	4
Carisoprodol	C12H24N2O4	260,1736	78-44-4	4
Carprofen	C15H12CINO2	273,0556	53716-49-7	8
Carteolol	C16H24N2O3	292,1786	51781-06-7	4
Carticain	C12H20N2O3S	272,1194	23964-58-1	4
Carvedilol	C24H26N2O4	406,1892	72956-09-3	4
Cefaclor	C15H14CIN3O4S	367,0393	70356-03-5	4

Compound	Formula	MW	CAS	# of spectra
Cefadroxil	C16H17N3O5S	363,0888	53994-73-3	4
Cefalexin	C16H17N3O4S	347,0939	15686-71-2	4
Cefamandole	C18H18N6O5S2	462,078	34444-01-4	4
Cefapirin	C17H17N3O6S2	423,0558	21593-23-7	4
Cefazedone	C18H15Cl2N5O5S3	546,9612	56187-47-4	4
Cefepime	C19H24N6O5S2	480,1249	88040-23-7	4
Cefetamet	C14H15N5O5S2	397,0514	65052-63-3	4
Cefixime	C16H15N5O7S2	453,0412	79350-37-1	4
Cefmenoxime	C16H17N9O5S3	511,0514	65085-01-0	8
Cefodizime	C20H20N6O7S4	584,0276	69739-16-8	4
Cefotaxime	C16H17N5O7S2	455,0569	63527-52-6	4
Cefotiam	C18H23N9O4S3	525,1035	61622-34-2	4
Cefpirome	C22H22N6O5S2	514,1093	84957-29-9	4
Ceftazidime	C22H22N6O7S2	546,0991	72558-82-8	4
Ceftizoxime	C13H13N5O5S2	383,0358	68401-81-0	4
Ceftriaxone	C18H18N8O7S3	554,046	73384-59-5	4
Cefuroxime	C16H16N4O8S	424,0688	55268-75-2	4
Celiprolol	C20H33N3O4	379,2471	56980-93-6	4
Cerivastatin	C26H34FNO5	459,2421	145599-86-6	4
Cetirizine	C21H25ClN2O3	388,1553	83881-52-1	4
Cetobemidone	C15H21NO2	247,1572	469-79-4	8
Chinine	C20H24N2O2	324,1837	130-95-0	4
Chlorambucil	C14H19Cl2NO2	303,0792	305-03-3	4
Chloramphenicol	C11H12Cl2N2O5	322,0123	56-75-7	4
Chlorazanol	C9H8ClN5	221,0468	500-42-5	4
Chlorbenzoxamine	C27H31ClN2O	434,2124	522-18-9	4
Chlorcyclizine	C18H21ClN2	300,1393	82-93-9	4
Chlordiazepoxide	C16H14ClN3O	299,0825	58-25-3	4
Chlordimeform	C10H13ClN2	196,0766	6164-98-3	4
Chlorfluazuron	C20H9Cl3F5N3O3	538,9629	71422-67-8	4
Chloridazon	C10H8ClN3O	221,0355	1698-60-8	8
Chlormadinone Acetate	C23H29ClO4	404,1754	302-22-7	4
Chlormequat	C5H13ClN	122,0736	999-81-5	4
Chlorphacinon	C23H15ClO3	374,0709	3691-35-8	4

Compound	Formula	MW	CAS	# of spectra
Chloropyramine	C16H20ClN3	289,1345	59-32-5	4
Chloroquine	C18H26ClN3	319,1815	07/05/1954	4
Chlorothiazide	C7H6ClN3O4S2	294,9488	58-94-6	4
Chlorphencyclan	C18H28ClNO	309,1859	5632-52-0	4
Chlorphenethiazine	C16H17N2SCl	304,08	2095-24-1	4
Chlorpheniramine	C16H19ClN2	274,1236	132-22-9	4
Chlorphenoxamine	C18H22ClNO	303,1389	77-38-3	4
Chlorpromazin-D3	C17H16ClD3N2S	321	136765-28-1	4
Chlorpromazine	C17H19ClN2S	318,0957	50-53-3	4
Chlorpromazine Sulfoxide	C17H19ClN2OS	334,0906	969-99-3	4
Chlorprothixene	C18H18ClNS	315,0847	113-59-7	4
Chlorthenoxazine	C10H10ClNO2	211,04	132-89-8	4
Chlorzoxazone	C7H4ClNO2	168,993	95-25-0	4
Ciclacillin	C15H23N3O4S	341,1409	3485-14-1	8
Cicletanine	C14H12ClNO2	261,0556	89943-82-8	5
Ciclonium Bromide	C22H34NO	328,264	29546-59-6	4
Cilastatin	C16H26N2O5S	358,1562	82009-34-5	8
Cilazapril	C22H33N3O6	435,2369	88768-40-5	8
Cimetidine	C10H16N6S	252,1157	51481-61-9	8
Cinchocaine	C20H29N3O2	343,2259	85-79-0	4
Cinchonidine	C19H22N2O	294,1732	485-71-2	8
Cinchonine	C19H22N2O	294,1732	118-10-5	8
Cinnarizine	C26H28N2	368,2251	298-57-7	4
Cinoxacin	C12H10N2O5	262,0589	28657-80-9	4
Ciprofloxacin	C17H18FN3O3	331,1332	85721-33-1	4
Cisapride	C23H29ClFN3O4	465,183	81098-60-4	4
Citalopram	C20H21FN2O	324,1637	59729-33-8	4
Cititolone	C6H9NO2S	159,0354	1195-16-0	4
Clarithromycin	C38H69NO13	747,4768	81103-11-9	4
Clemastine	C21H26ClNO	343,1702	15686-51-8	4
Clemizole	C19H20ClN3	325,1345	442-52-4	4
Clenbuterol	C12H18Cl2N2O	276,0796	37148-27-9	4
Clibucaine	C15H20Cl2N2O	314,0952	15302-10-0	4
Climbazole	C15H17ClN2O2	292,0978	38083-17-9	4

Compound	Formula	MW	CAS	# of spectra
Clindamycin	C ₁₈ H ₃₃ CIN ₂ O ₅ S	424,1798	18323-44-9	4
Clobazam	C ₁₆ H ₁₃ CIN ₂ O ₂	300,0665	22316-47-8	4
Clobenzepam	C ₁₇ H ₁₈ CIN ₃ O	315,1138	1159-93-9	4
Clobetasol-17-propionate	C ₂₅ H ₃₂ CIFO ₅	466,1922	25122-46-7	4
Clobetason-butyrate	C ₂₆ H ₃₂ CIFO ₅	478,1922	25122-57-0	4
Clobutinol	C ₁₄ H ₂₂ CINO	255,1389	14860-49-2	4
Clofedanol	C ₁₇ H ₂₀ CINO	289,1233	791-35-5	4
Clofenamide	C ₆ H ₇ CIN ₂ O ₄ S ₂	269,9535	511-46-6	4
Clofexamide	C ₁₄ H ₂₁ CIN ₂ O ₂	284,1291	1223-36-5	4
Clomethiazole	C ₆ H ₈ CINS	161,0065	533-45-9	4
Clomiphene	C ₂₆ H ₂₈ CINO	405,1859	911-45-5	4
Clomipramine	C ₁₉ H ₂₃ CIN ₂	314,1549	303-49-1	4
Clonazepam	C ₁₅ H ₁₀ CIN ₃ O ₃	315,041	1622-61-3	4
Clonidine	C ₉ H ₉ CI ₂ N ₃	229,0173	4205-90-7	4
Cloпамide	C ₁₄ H ₂₀ CIN ₃ O ₃ S	345,0913	636-54-4	8
Cloпenthixol	C ₂₂ H ₂₅ CIN ₂ OS	400,1376	982-24-1	4
Clopidogrel	C ₁₆ H ₁₆ CINO ₂ S	321,059	113665-84-2	4
Cloprednol	C ₂₁ H ₂₅ ClO ₅	392,139	5251-34-3	8
Clorindione	C ₁₅ H ₉ ClO ₂	256,0291	1146-99-2	4
Clotiapiпe	C ₁₈ H ₁₈ CIN ₃ S	343,0909	2058-52-8	4
Clotiazepam	C ₁₆ H ₁₅ CIN ₂ OS	318,0593	33671-46-4	4
Clotrimazol	C ₂₂ H ₁₇ CIN ₂	344,108	23593-75-1	4
Cloxiquine	C ₉ H ₆ CINO	179,0137	130-16-5	4
Clozapine	C ₁₈ H ₁₉ CIN ₄	326,1298	5786-21-0	4
Cocaine	C ₁₇ H ₂₁ NO ₄	303,147	50-36-2	4
Codeine	C ₁₈ H ₂₁ NO ₃	299,1521	76-57-3	4
Colchicine	C ₂₂ H ₂₅ NO ₆	399,1681	64-86-8	4
Coniine	C ₈ H ₁₇ N	127,136	458-88-8	4
Corticosterone	C ₂₁ H ₃₀ O ₄	346,2144	50-22-6	4
Cortisone	C ₂₁ H ₂₈ O ₅	360,1936	05/06/1953	8
Cotinine	C ₁₀ H ₁₂ N ₂ O	176,0949	486-56-6	4
Coumatetraalyl	C ₁₉ H ₁₆ O ₃	292,1099	5836-29-3	4
Croconazole	C ₁₈ H ₁₅ CIN ₂ O	310,0872	77175-51-0	4
Cromoglicic acid	C ₂₃ H ₁₆ O ₁₁	468,0692	16110-51-3	8

Compound	Formula	MW	CAS	# of spectra
Crotetamide	C12H22N2O2	226,1681	6168-76-9	4
Cyamemazine	C19H21N3S	323,1456	3546-03-0	4
Cyanazine	C9H13CIN6	240,089	21725-46-2	4
Cyclamic acid	C6H13NO3S	179,0616	100-88-9	4
Cyclicine	C18H22N2	266,1782	82-92-8	4
Cyclobenzaprine	C20H21N	275,1673	303-53-7	4
Cyclodrine	C19H29NO3	319,2147	52109-93-0	4
Cyclopentamine	C9H19N	141,1517	102-45-4	4
Cyclopentobarbital	C12H14N2O3	234,1004	76-68-6	4
Cyclopentolate	C17H25NO3	291,1834	512-15-2	4
Cyclophosphamide	C7H15Cl2N2O2P	260,0248	50-18-0	4
Cyclovalone	C22H22O5	366,1467	579-23-7	4
Cyproheptadine	C21H21N	287,1673	129-03-3	4
Cytarabine	C9H13N3O5	243,0855	147-94-4	4
D-Norpseudoephedrine	C9H13NO	151,0997	492-39-7	4
D10-Psilocin	C12H6D10N2O	214		4
D3-Atropin	C17H20D3NO3	292		4
D3-Benzoylcegonine	C16H16D3NO4	292	115732-68-8	4
D3-Cocaine	C17H18D3NO4	306	65266-73-1	4
D3-Codeine	C18H18D3NO3	302	70420-71-2	4
D3-Doxepine	C19H18NOD3	282		4
D3-Ecgonine methyl ester	C10H14D3NO3	202	136765-34-9	4
D3-LSD	C20H22D3N3O	326	136765-38-3	4
D3-Methadon	C21H24D3NO	312	60263-63-0	4
D3-Morphine-3-beta-glucuronide	C23H24D3NO9	464		4
D3-Morphine	C17H16D3NO3	288	67293-88-3	4
D5-Amphetamin	C9H8D5N	140	65538-33-2	4
D5-Diazepam	C16H8CIN2OD5	289		4
D5-Fentanyl	C22H23D5N2O	341	118357-29-2	4
D5-MBDB	C12H12D5NO2	212		4
D5-MDA	C10H8D5NO2	184	136765-42-9	4
D5-MDEA	C12H12D5NO2	212	160227-43-0	4
D5-MDMA	C11H10D5NO2	198	136765-43-0	4
D5-Metamphetamine	C10H10D5N	154	60124-88-1	4

Compound	Formula	MW	CAS	# of spectra
D7-7-Aminoflunitrazepam	C16H7D7FN3O	290		4
D7-Flunitrazepam	C16H5D7FN3O3	320		4
D9-Methadone	C21H18D9NO	318		4
Dacarbazin	C6H10N6O	182,0916	04/03/4342	4
Danazol	C22H27NO2	337,2041	17230-88-5	4
Dapiprazole	C19H27N5	325,2266	72822-12-9	4
Dapsone	C12H12N2O2S	248,0619	80-08-0	4
Daunorubicin	C27H29NO10	527,1791	20830-81-3	4
Debrisoquine	C10H13N3	175,1108	1131-64-2	4
Deflazacort	C25H31NO6	441,2151	14484-47-0	4
Dehydrocholic acid	C24H34O5	402,2406	81-32-2	4
Delorazepam	C15H10Cl2N2O	304,017	2894-67-9	4
Demecarium	C32H52N4O4	556,3988	56-94-0	4
Demeclocycline	C21H21ClN2O8	464,0986	127-33-3	4
Demeton-O	C8H19O3PS2	258,0513	298-03-3	4
Demeton-O-methyl	C6H15O3PS2	230,02	867-27-6	4
Demeton-S-methylsulfone	C6H15O5PS2	262,0098	17040-19-6	4
Demoxepam	C15H11N2O2Cl	286,0509	963-39-3	4
Denaverine	C24H33NO3	383,246	3579-62-2	4
Desallylflurazepam	C15H10N2OFCl	288,0465		4
Desipramine	C18H22N2	266,1782	50-47-5	4
Desmedipham	C16H16N2O4	300,111	13684-56-5	4
Desmethylcitalopram	C19H19N2OF	310,1481		4
Desmethylclobazam	C15H11ClN2O2	286,0509	22316-55-8	8
Desmethylclomipramine	C18H21ClN2	300,1393	303-48-0	4
Desoximethasone	C22H29FO4	376,2049	382-67-2	4
Desoxycortone 21-(3-phenylpropionate)	C30H38O4	462,277	14007-50-2	4
Desoxycortone enantate	C28H42O4	442,3083		4
Detajmium	C27H42N3O3	456,3226	33774-52-6	4
Dexamethasone	C22H29FO5	392,1999	02/02/1950	4
Dexamethasone 21-Acetate	C24H31FO6	434,2104	1177-87-3	8
Dexamethasone 21-isonicotinate	C28H32FNO6	497,2213	2265-64-7	4
Dexfenfluramine	C12H16F3N	231,1234	3239-44-9	4
Dextromethorphan	C18H25NO	271,1936	125-71-3	4

Compound	Formula	MW	CAS	# of spectra
Dextromoramide	C25H32N2O2	392,2463	357-56-2	4
Dextropropoxyphene	C22H29NO2	339,2198	469-62-5	4
Diaveridine	C13H16N4O2	260,1273	5355-16-8	4
Diazepam	C16H13ClN2O	284,0716	439-14-5	4
Diazoxide	C8H7ClN2O2S	229,9916	364-98-7	8
Dibenzepin	C18H21N3O	295,1684	4498-32-2	4
Dibutyl adipate	C14H26O4	258,1831	105-99-7	4
Dichlorophen	C13H10Cl2O2	268,0057	97-23-4	4
Diclofenac	C14H11Cl2NO2	295,0166	15307-86-5	8
Dicycloverine	C19H35NO2	309,2667	77-19-0	4
Didanosine	C10H12N4O3	236,0909	69655-05-6	8
Dienestrol	C18H18O2	266,1306	84-17-3	4
Dienogest	C20H25NO2	311,1884	65928-58-7	4
Diethazine	C18H22N2S	298,1503	60-91-3	4
Diethylcarbamazine	C10H21N3O	199,1684	90-89-1	4
Difenoconazole	C19H17Cl2N3O3	405,0646	119446-68-3	4
Difenoxuron	C16H18N2O3	286,1317	14214-32-5	4
Difenzoquat	C17H17N2	249,1391	43222-48-6	4
Diflorasone diacetate	C26H32F2O7	494,2116	33564-31-7	4
Diflucortolone	C22H28F2O4	394,1955	09/06/2607	4
Dihydralazine	C8H10N6	190,0966	484-23-1	4
Dihydrocodeine	C18H23NO3	301,1677	125-28-0	4
Dihydroergocristin	C35H41N5O5	611,3107	17479-19-5	4
Dihydroergokryptine	C32H43N5O5	577,3264	25447-66-9	8
Dihydroergotamine	C33H37N5O5	583,2794	511-12-6	4
Dihyprylone	C9H15NO2	169,1102	02/03/1977	4
Dilazep	C31H44N2O10	604,2995	35898-87-4	4
Diltiazem	C22H26N2O4S	414,1613	42399-41-7	4
Dimefuron	C15H19ClN4O3	338,1145	34205-21-5	8
Dimephenopam	C11H17N	163,136	17279-39-9	4
Dimetacrine	C20H26N2	294,2095	4757-55-5	4
Dimethachlor	C13H18ClNO2	255,1026	50563-36-5	4
Dimethomorph	C21H22ClNO4	387,1237	110488-70-5	4
Dimetindene	C20H24N2	292,1939	5636-83-9	4

Compound	Formula	MW	CAS	# of spectra
Dimetotiazine	C19H25N3O2S2	391,1388	7456-24-8	4
Dimetridazole	C5H7N3O2	141,0538	551-92-8	4
Dinoprost	C20H34O5	354,2406	551-11-1	4
Dioxethedrin	C11H17NO3	211,1208	497-75-6	8
Diphenamid	C16H17NO	239,131	957-51-7	4
Diphenhydramine	C17H21NO	255,1623	58-73-1	4
Diphenidol	C21H27NO	309,2092	972-02-1	4
Diphenylpyraline	C19H23NO	281,1779	147-20-6	4
Dipiproverine	C20H30N2O2	330,2307	117-30-6	4
Diponium	C20H38NO2	324,2902	58875-33-5	4
Diprophylline	C10H14N4O4	254,1015	479-18-5	4
Dipyridamole	C24H40N8O4	504,3172	58-32-2	4
Disopyramide	C21H29N3O	339,231	05/09/3737	4
Distigmin	C22H32N4O4	416,2423	15876-67-2	4
Disulfiram	C10H20N2S4	296,0509	97-77-8	4
Dixyrazine	C24H33N3O2S	427,2293	2470-73-7	4
Dobutamine	C18H23NO3	301,1677	34368-04-2	8
Dolasetron	C19H20N2O3	324,1473	115956-12-2	8
Domperidone	C22H24ClN5O2	425,1618	57808-66-9	8
Dopamin	C8H11NO2	153,0789	51-61-6	8
Dopexamine	C22H32N2O2	356,2463	86197-47-9	4
Dormovit	C12H14N2O4	250,0953	1146-21-0	4
Dorzolamide	C10H16N2O4S3	324,0272	120279-96-1	8
Dosulepin	C19H21NS	295,1394	113-53-1	4
Doxapram	C24H30N2O2	378,2307	309-29-5	4
Doxazosin	C23H25N5O5	451,1855	74191-85-8	4
Doxepin	C19H21NO	279,1623	1668-19-5	4
Doxorubicin	C27H29NO11	543,174	23214-92-8	4
Doxylamine	C17H22N2O	270,1732	469-21-6	4
Drazoloxon	C10H8ClN3O2	237,0305	5707-69-7	4
Drofenine	C20H31NO2	317,2354	1679-76-1	4
Dropropizine	C13H20N2O2	236,1524	17692-31-8	4
Drospirenone	C24H30O3	366,2194	67392-87-4	4
Ecgonin-D3	C9H12D3NO3	188		8

Compound	Formula	MW	CAS	# of spectra
Ecgoninemethylester	C10H17NO3	199,1208	01/09/7143	4
EDDP	C20H24N	278,1908	66729-78-0	4
EDDP-D3	C20H21D3N	280	136765-23-6	4
Eldoral	C11H17N3O3	239,1269	509-87-5	4
Embutramide	C17H27NO3	293,199	15687-14-6	4
Emepronium	C20H28N	282,2221	3614-30-0	4
Emetine	C29H40N2O4	480,2988	483-18-1	4
Emodin	C15H10O5	270,0528	518-82-1	4
Enalapril	C20H28N2O5	376,1998	75847-73-3	4
Endomide	C17H28N2O2	292,215	4582-18-7	4
Enoximone	C12H12N2O2S	248,0619	77671-31-9	4
Ephedrine	C10H15NO	165,1153	299-42-3	4
Epinephrine	C9H13NO3	183,0895	51-43-4	8
Eprazinone	C24H32N2O2	380,2463	10402-90-1	4
Eprosartan	C23H24N2O4S	424,1456	133040-01-4	4
Erythromycin	C37H67NO13	733,4612	114-07-8	4
Esculin	C15H16O9	340,0794	531-75-9	8
Esmolol	C16H25NO4	295,1783	103598-03-4	4
Estazolam	C16H11ClN4	294,0672	29975-16-4	4
Etafedrine	C12H19NO	193,1466	48141-64-6	4
Etafenone	C21H27NO2	325,2041	90-54-0	4
Etamiphyllin	C13H21N5O2	279,1695	314-35-2	4
Etamivan	C12H17NO3	223,1208	304-84-7	4
Ethacridine	C15H15N3O	253,1215	442-16-0	4
Ethacrynic Acid	C13H12Cl2O4	302,0112	58-54-8	8
Ethambutol	C10H24N2O2	204,1836	74-55-5	4
Ethaverine	C24H29NO4	395,2096	486-47-5	4
Ethenzamide	C9H11NO2	165,0789	938-73-8	4
Ethionamide	C8H10N2S	166,0564	536-33-4	8
Ethyl glucuronide	C8H14O7	222,0739		4
Ethyl glucuronide-D5	C8H9D5O7	227		4
Ethyl sulfate	C2H6O4S	125,9986		4
Ethyl sulfate-D5	C2HD5O4S	131		4
Ethylbenzhydramine	C19H25NO	283,1936	642-58-0	4

Compound	Formula	MW	CAS	# of spectra
Ethylparathion	C10H14NO5PS	291,033	56-38-2	4
Etidocaine	C17H28N2O	276,2201	36637-18-0	4
Etifelmin	C17H19N	237,1517	341-00-4	4
Etilamfetamine	C11H17N	163,136	457-87-4	4
Etilefrine	C10H15NO2	181,1102	709-55-7	4
Etiroxate	C18H17I4NO4	818,7336	17365-01-4	8
Etodolac	C17H21NO3	287,1521	41340-25-4	8
Etodroxizine	C23H31ClN2O3	418,2023	17692-34-1	4
Etofenamate	C18H18F3NO4	369,1187	30544-47-9	4
Etofibrate	C18H18ClNO5	363,0873	31637-97-5	4
Etofyllinclofibrate	C19H21ClN4O5	420,12	54504-70-0	4
Etofylline	C9H12N4O3	224,0909	519-37-9	4
Etoloxamine	C19H25NO	283,1936	1157-87-5	4
Etomidate	C14H16N2O2	244,1211	33125-97-2	4
Etophylline	C9H12N4O3	224,0909	519-37-9	4
Etoposide	C29H32O13	588,1842	33419-42-0	8
Etryptamine	C12H16N2	188,1313	2235-90-7	4
Eucatropine	C17H25NO3	291,1834	100-91-4	4
Exemestane	C20H24O2	296,1776	107868-30-4	4
Famciclovir	C14H19N5O4	321,1437	104227-87-4	4
Famotidine	C8H15N7O2S3	337,0449	76824-35-6	4
Famprofazone	C24H31N3O	377,2467	22881-35-2	4
Fedrilate	C20H29NO4	347,2096	23271-74-1	4
Felbamate	C11H14N2O4	238,0953	25451-15-4	4
Felodipine	C18H19Cl2NO4	383,0691	72509-76-3	8
Fenarimol	C17H12Cl2N2O	330,0326	60168-88-9	4
Fenbutrazate	C23H29NO3	367,2147	4378-36-3	4
Fendiline	C23H25N	315,1986	13042-18-7	4
Fenetylline	C18H23N5O2	341,1851	01/08/3736	4
Fenfluramine	C12H16F3N	231,1234	458-24-2	4
Fenfuram	C12H11NO2	201,0789	24691-80-3	4
Fenofibrate	C20H21ClO4	360	49562-28-9	4
Fenoprofen	C15H14O3	242,0942	31879-05-7	4
Fenoterol	C17H21NO4	303,147	13392-18-2	4

Compound	Formula	MW	CAS	# of spectra
Fenoxazoline	C13H18N2O	218,1419	4846-91-7	4
Fenpipramide	C21H26N2O	322,2045	77-01-0	4
Fenpiprane	C20H25N	279,1987	3329-14-4	4
Fenproporex	C12H16N2	188,1313	15686-61-0	4
Fentanyl	C22H28N2O	336,2201	437-38-7	4
Fenticonazole	C24H20Cl2N2OS	454,0673	72479-26-6	4
Fexofenadine	C32H39NO4	501,2879	83799-24-0	4
Finasteride	C23H36N2O2	372,2776	98319-26-7	4
Flavoxate	C24H25NO4	391,1783	15301-69-6	4
Flecainide	C17H20F6N2O3	414,1378	54143-55-4	4
Fleroxacin	C17H18F3N3O3	369,13	79660-72-3	4
Flocoumafen	C33H25F3O4	542,1704		8
Floctafenine	C20H17F3N2O4	406,1139	23779-99-9	4
Fluanisone	C21H25FN2O2	356,19	1480-19-9	4
Flucloxacillin	C19H17ClFN3O5S	453,0561	5250-39-5	8
Fluconazole	C13H12F2N6O	306,104	86386-73-4	4
Fludrocortisone	C21H29FO5	380,1999	514-36-3	4
Flufenamic Acid	C14H10F3NO2	281,0663	530-78-9	8
Flumazenil	C15H14FN3O3	303,1019	78755-81-4	4
Flunarizine	C26H26F2N2	404,2064	52468-60-7	4
Flunitrazepam	C16H12FN3O3	313,0862	1622-62-4	4
Fluocinolone Acetonide	C24H30F2O6	452,201	67-73-2	4
Fluocinonide	C26H32F2O7	494,2116	356-12-7	4
Fluocortin Butyl	C26H35FO5	446,2468	41767-29-7	8
Fluocortolone	C22H29FO4	376,2049	152-97-6	4
Fluorouracil	C4H3FN2O2	130,0178	51-21-8	4
Fluoxetine	C17H18NOF3	309,134	54910-89-3	4
Flupentixol	C23H25F3N2OS	434,1639	2709-56-0	4
Fluphenazine	C22H26F3N3OS	437,1748	69-23-8	4
Flupirtine	C15H17FN4O2	304,1335	56995-20-1	4
Flunarizine	C26H26F2N2	404,2064	52468-60-7	4
Flunitrazepam	C16H12FN3O3	313,0862	1622-62-4	4
Fluocinolone Acetonide	C24H30F2O6	452,201	67-73-2	4
Fluocinonide	C26H32F2O7	494,2116	356-12-7	4

Compound	Formula	MW	CAS	# of spectra
Fluocortin Butyl	C26H35FO5	446,2468	41767-29-7	8
Fluocortolone	C22H29FO4	376,2049	152-97-6	4
Fluorouracil	C4H3FN2O2	130,0178	51-21-8	4
Fluoxetine	C17H18NOF3	309,134	54910-89-3	4
Flupentixol	C23H25F3N2OS	434,1639	2709-56-0	4
Fluphenazine	C22H26F3N3OS	437,1748	69-23-8	4
Flupirtine	C15H17FN4O2	304,1335	56995-20-1	4
Fluprednylidene 21-Acetate	C24H29FO6	432,1948	1255-35-2	8
Flurazepam	C21H23CIFN3O	387,1513	17617-23-1	4
Flurbiprofen	C15H13FO2	244,0899	5104-49-4	4
Flurochloridone	C12H10Cl2F3NO	311,0091	61213-25-0	4
Fluspirilen	C29H31F2N3O	475,2435	1841-19-6	8
Flutamide	C11H11F3N2O3	276,0721	13311-84-7	4
Fluticasone Propionate	C25H31F3O5S	500,1844	80474-14-2	4
Fluvastadine	C24H26FNO4	411,1845	93957-54-1	8
Fluvoxamine	C15H21F3N2O2	318,1555	54739-18-3	4
Fominoben	C21H24CIN3O3	401,1506	18053-31-1	4
Fomocain	C20H25NO2	311,1885	17692-39-6	4
Formetanate	C11H15N3O2	221,1164	22259-30-9	4
Formylsulfamethine	C13H14N4O3S	306,0786	795-13-1	8
Fosinopril	C30H46NO7P	563,3011	98048-97-6	8
Fuberidazole	C11H8N2O	184,0636	3878-19-1	8
Furalaxyl	C17H19NO4	301,1314	57646-30-7	4
Furaltadone	C13H16N4O6	324,1069	139-91-3	4
Furazolidone	C8H7N3O5	225,0385	67-45-8	4
Furosemid	C12H11CIN2O5S	330,0077	54-31-9	4
Gabapentin	C9H17NO2	171,1259	60142-96-3	4
Galantamine	C17H21NO3	287,1521	357-70-0	4
Gallopamil	C28H40N2O5	484,2937	16662-47-8	4
gamma-Hydroxybutyric acid	C4H8O3	104,0473	502-85-2 (sodium salt)	4
gamma-Hydroxybutyric acid-D6	C4H2D6O3	110		4
Gemcitabine	C9H11F2N3O4	263,0717	95058-81-4	4
Gemfibrozil	C15H22O3	250,1568	25812-30-0	4
Gepefrine	C9H13NO	151,0997	18840-47-6	4

Compound	Formula	MW	CAS	# of spectra
Gestodene	C21H26O2	310,1932	60282-87-3	4
Gibberelic acid	C19H22O6	346,1416	05/06/1977	4
Gitoxigenin	C23H34O5	390,2406	545-26-6	4
Glafenin	C19H17CIN2O4	372,0876	3820-67-5	4
Glibenclamide	C23H28CIN3O5S	493,1438	10238-21-8	4
Glibornuride	C18H26N2O4S	366,1613	26944-48-9	4
Gliclazide	C15H21N3O3S	323,1303	21187-98-4	4
Glimepiride	C24H34N4O5S	490,2249	93479-97-1	8
Glipizide	C21H27N5O4S	445,1783	29094-61-9	4
Gliquidone	C27H33N3O6S	527,2089	33342-05-1	8
Glisoxepide	C20H27N5O5S	449,1732	25046-79-1	8
Glucosamine	C6H13NO5	179,0793	3416-24-8	4
Glymidine	C13H15N3O4S	309,0783	3459-20-9	4
Granisetron	C18H24N4O	312,195	109889-09-0	4
Grepafloxacin	C19H22FN3O3	359,1645	161967-81-3	4
Griseofulvin	C17H17ClO6	352,0713	126-07-8	4
Guafecainol	C16H27NO4	297,194	36199-78-7	4
Guaifenesin	C10H14O4	198,0892	93-14-1	4
Guanabenz	C8H8Cl2N4	230,0126	5051-62-7	4
Guanacline	C9H18N4	182,1531	1463-28-1	4
Guanethidine	C10H22N4	198,1844	55-65-2	4
Guanfacine	C9H9Cl2N3O	245,0122	29110-47-2	8
Gestodene	C21H26O2	310,1932	60282-87-3	4
Gibberelic acid	C19H22O6	346,1416	05/06/1977	4
Gitoxigenin	C23H34O5	390,2406	545-26-6	4
Glafenin	C19H17CIN2O4	372,0876	3820-67-5	4
Glibenclamide	C23H28CIN3O5S	493,1438	10238-21-8	4
Glibornuride	C18H26N2O4S	366,1613	26944-48-9	4
Gliclazide	C15H21N3O3S	323,1303	21187-98-4	4
Glimepiride	C24H34N4O5S	490,2249	93479-97-1	8
Glipizide	C21H27N5O4S	445,1783	29094-61-9	4
Gliquidone	C27H33N3O6S	527,2089	33342-05-1	8
Glisoxepide	C20H27N5O5S	449,1732	25046-79-1	8
Glucosamine	C6H13NO5	179,0793	3416-24-8	4

Compound	Formula	MW	CAS	# of spectra
Glymidine	C13H15N3O4S	309,0783	3459-20-9	4
Granisetron	C18H24N4O	312,195	109889-09-0	4
Grepaflloxacin	C19H22FN3O3	359,1645	161967-81-3	4
Griseofulvin	C17H17ClO6	352,0713	126-07-8	4
Guafecainol	C16H27NO4	297,194	36199-78-7	4
Guaifenesin	C10H14O4	198,0892	93-14-1	4
Guanabenz	C8H8Cl2N4	230,0126	5051-62-7	4
Guanacline	C9H18N4	182,1531	1463-28-1	4
Guanethidine	C10H22N4	198,1844	55-65-2	4
Guanfacine	C9H9Cl2N3O	245,0122	29110-47-2	8
Glymidine	C13H15N3O4S	309,0783	3459-20-9	4
Granisetron	C18H24N4O	312,195	109889-09-0	4
Grepaflloxacin	C19H22FN3O3	359,1645	161967-81-3	4
Griseofulvin	C17H17ClO6	352,0713	126-07-8	4
Guafecainol	C16H27NO4	297,194	36199-78-7	4
Guaifenesin	C10H14O4	198,0892	93-14-1	4
Guanabenz	C8H8Cl2N4	230,0126	5051-62-7	4
Guanacline	C9H18N4	182,1531	1463-28-1	4
Guanethidine	C10H22N4	198,1844	55-65-2	4
Guanfacine	C9H9Cl2N3O	245,0122	29110-47-2	8
Glymidine	C13H15N3O4S	309,0783	3459-20-9	4
Granisetron	C18H24N4O	312,195	109889-09-0	4
Grepaflloxacin	C19H22FN3O3	359,1645	161967-81-3	4
Griseofulvin	C17H17ClO6	352,0713	126-07-8	4
Guafecainol	C16H27NO4	297,194	36199-78-7	4
Guaifenesin	C10H14O4	198,0892	93-14-1	4
Guanabenz	C8H8Cl2N4	230,0126	5051-62-7	4
Guanacline	C9H18N4	182,1531	1463-28-1	4
Guanethidine	C10H22N4	198,1844	55-65-2	4
Guanfacine	C9H9Cl2N3O	245,0122	29110-47-2	8
Guanoxan	C10H13N3O2	207,1007	2165-19-7	4
Halcinonide	C24H32ClFO5	454,1922	3093-35-4	8
Halofantrine	C26H30Cl2F3NO	499,1656	69756-53-2	4
Halofuginone	C16H17BrClN3O3	413,0141	55837-20-2	8

Compound	Formula	MW	CAS	# of spectra
Halometasone	C22H27CIF2O5	444,1515	50629-82-8	4
Haloperidol	C21H23CIFNO2	375,1401	52-86-8	4
Haloperidol-D4	C21H19CID4FNO2	379	136765-35-0	4
Haloxyfop ethoxyethyl ester	C19H19CIF3NO5	433,0903	87237-48-7	4
Hapargosid	C24H30O11	494,1788		8
Heptaminol	C8H19NO	145,1466	372-66-7	4
Heroin	C21H23NO5	369,1576	561-27-3	4
Hesperidin	C28H34O15	610,1897	520-26-3	4
Hexacarbacholine	C18H40N4O4	376,3049	306-41-2	4
Hexachlorophene	C13H6Cl6O2	403,8498	70-30-4	4
Hexamethonium	C12H30N2	202,2408	60-26-4	4
Hexamidine	C20H26N4O2	354,2055	3811-75-4	4
Hexazinone	C12H20N4O2	252,1586	51235-04-2	4
Hexobendine	C30H44N2O10	592,2995	05/03/1954	4
Histamine	C5H9N3	111,0796	51-45-6	4
Histapyrrodine	C19H24N2	280,1939	493-80-1	4
Histidine	C6H9N3O2	155,0694	71-00-1	4
Homatropine	C16H21NO3	275,1521	87-00-3	4
Homofenazine	C23H28F3N3OS	451,1905	1256-01-5	4
Hordenine	C10H15NO	165,1153	539-15-1	4
Hydralazine	C8H8N4	160,0748	86-54-4	4
Hydrochlorothiazide	C7H8ClN3O4S2	296,9644	58-93-5	4
Hydrocodone	C18H21NO3	299,1521	125-29-1	4
Hydrocortisone	C21H30O5	362,2093	50-23-7	4
Hydrocortisone 21-acetate	C23H32O6	404,2198	03/03/1950	4
Hydrocortisone 21-hydrogen succinate	C25H33O8	461,2175	125-04-2	4
Hydrocortisone buteprate	C28H40O7	488,2774	72590-77-3	4
Hydroflumethiazide	C8H8F3N3O4S2	330,9908	135-09-1	4
Hydromorphone	C17H19NO3	285,1364	466-99-9	4
Hydroxychlorquine	C18H26ClN3O	335,1764	118-42-3	4
Hydroxymethylpyridine	C6H7NO	109,0527		4
Hydroxyzine	C21H27ClN2O2	374,1761	68-88-2	4
Hymecromone	C10H8O3	176,0473	90-33-5	8
Hyoscyamine	C17H23NO3	289,1677	101-31-5	4

Compound	Formula	MW	CAS	# of spectra
Ibogaine	C20H26N2O	310,2045	83-74-9	4
Idarubicin	C26H27NO9	497,1685	58957-92-9	4
Idoxuridine	C9H11N2O5	353,9712	54-42-2	4
Ifosfamide	C7H15Cl2N2O2P	260,0248	3778-73-2	4
Imiclopazine	C25H32ClN5OS	485,2016	7224-08-0	4
Imidapril	C20H27N3O6	405,1899	89371-37-9	4
Iminostilbene	C14H11N	193,0891	256-96-2	4
Imipramine	C19H24N2	280,1939	50-49-7	4
Imiquimod	C14H16N4	240,1374	99011-02-6	4
Imolamine	C14H20N4O	260,1637	318-23-0	4
Indanazoline	C12H15N3	201,1265	40507-78-6	4
Indapamine	C16H16ClN3O3S	365,06	26807-65-8	4
Indinavir	C36H47N5O4	613,3628	150378-17-9	4
Indomethacin	C19H16ClNO3	341,0818	53-86-1	4
Indoprofen	C17H15NO3	281,1051	31842-01-0	4
Indoramin	C22H25N3O	347,1997	26844-12-2	4
Inosine	C10H12N4O5	268,0807	58-63-9	8
lobitridol	C20H28I3N3O9	834,8959	136949-58-1	4
loglicic acid	C13H12I3N3O5	670,7911	49755-67-1	4
Iopodic acid	C12H13I3N2O2	597,8111	5587-89-3	4
Ipratropium	C20H30NO3	332,2225	22254-24-6	4
Iprazochrome	C12H16N4O3	264,1222	7248-21-7	8
Ibogaine	C20H26N2O	310,2045	83-74-9	4
Idarubicin	C26H27NO9	497,1685	58957-92-9	4
Idoxuridine	C9H11N2O5	353,9712	54-42-2	4
Ifosfamide	C7H15Cl2N2O2P	260,0248	3778-73-2	4
Imiclopazine	C25H32ClN5OS	485,2016	7224-08-0	4
Imidapril	C20H27N3O6	405,1899	89371-37-9	4
Iminostilbene	C14H11N	193,0891	256-96-2	4
Imipramine	C19H24N2	280,1939	50-49-7	4
Imiquimod	C14H16N4	240,1374	99011-02-6	4
Imolamine	C14H20N4O	260,1637	318-23-0	4
Indanazoline	C12H15N3	201,1265	40507-78-6	4
Indapamine	C16H16ClN3O3S	365,06	26807-65-8	4

Compound	Formula	MW	CAS	# of spectra
Indinavir	C36H47N5O4	613,3628	150378-17-9	4
Indomethacin	C19H16ClNO3	341,0818	53-86-1	4
Indoprofen	C17H15NO3	281,1051	31842-01-0	4
Indoramin	C22H25N3O	347,1997	26844-12-2	4
Inosine	C10H12N4O5	268,0807	58-63-9	8
lobitridol	C20H28I3N3O9	834,8959	136949-58-1	4
loglicic acid	C13H12I3N3O5	670,7911	49755-67-1	4
lopodic acid	C12H13I3N2O2	597,8111	5587-89-3	4
Ipratropium	C20H30NO3	332,2225	22254-24-6	4
Iprazochrome	C12H16N4O3	264,1222	7248-21-7	8
Iprindole	C19H28N2	284,2252	5560-72-5	4
Irbesartan	C25H28N6O	428,2324	138402-11-6	4
Isoaminile	C16H24N2	244,1939	77-51-0	4
Isocarboxazid	C12H13N3O2	231,1007	59-63-2	4
Isoconazole	C18H14Cl4N2O	413,986	24168-96-5	4
Isoniazide	C6H7N3O	137,0589	54-85-3	4
Isoprenaline	C11H17NO3	211,1208	7683-59-3	8
Isoproturon	C12H18N2O	206,1419	34123-59-6	4
Isothipendyl	C16H19N3S	285,1299	482-15-5	4
Isoxicam	C14H13N3O5S	335,0575	34552-84-6	8
Isoxsuprine	C18H23NO3	301,1677	395-28-8	4
Isradipine	C19H21N3O5	371,1481	75695-93-1	4
Kavain	C14H14O3	230,0942	500-64-1	4
Ketamine	C13H16ClNO	237,092	6740-88-1	4
Ketazolam	C20H17ClN2O3	368,0927	27223-35-4	4
Ketoconazole	C26H28Cl2N4O4	530,1487	65277-42-1	4
Ketoprofen	C16H14O3	254,0942	22071-15-4	4
Ketorolac	C15H13NO3	255,0895	74103-06-3	4
Ketotifen	C19H19NOS	309,1187	34580-13-7	4
Khellin	C14H12O5	260,0684	82-02-0	4
Labetalol	C19H24N2O3	328,1786	36894-69-6	4
Lacidipine	C26H33NO6	455,2307	103890-78-4	8
Lactitol	C12H24O11	344,1318	585-86-4	4
Lamivudine	C8H11N3O3S	229,0521	134678-17-4	4

Compound	Formula	MW	CAS	# of spectra
Lamotrigine	C ₉ H ₇ Cl ₂ N ₅	255,0078	84057-84-1	4
Lauroguadine	C ₂₀ H ₃₆ N ₆ O	376,295	135-43-3	4
Leflunomide	C ₁₂ H ₉ F ₃ N ₂ O ₂	270,0616	75706-12-6	4
Lercanidipine	C ₃₆ H ₄₁ N ₃ O ₆	611,2995	100427-26-7	4
Levallorphan	C ₁₉ H ₂₅ NO	283,1936	152-02-3	4
Levobunolol	C ₁₇ H ₂₅ NO ₃	291,1834	47141-41-4	4
Levocabastine	C ₂₆ H ₂₉ FN ₂ O ₂	420,2213	79516-68-0	4
Levodopa	C ₉ H ₁₁ NO ₄	197,0688	59-92-7	8
Levomepromazine	C ₁₉ H ₂₄ N ₂ OS	328,1609	60-99-1	4
Levopropylhexedrin	C ₁₀ H ₂₁ N	155,1673	6192-97-8	4
Lidocaine	C ₁₄ H ₂₂ N ₂ O	234,1732	137-58-6	4
Lincomycin	C ₁₈ H ₃₄ N ₂ O ₆ S	406,2137	154-21-2	4
Liothyronine	C ₁₅ H ₁₂ I ₃ NO ₄	650,79	03/02/6893	8
Lisinopril	C ₂₁ H ₃₁ N ₃ O ₅	405,2263	76547-98-3	4
Lisurid	C ₂₀ H ₂₆ N ₄ O	338,2106	18016-80-3	4
Lobeline	C ₂₂ H ₂₇ NO ₂	337,2041	90-69-7	4
Lofepramine	C ₂₆ H ₂₇ CIN ₂ O	418,1811	23047-25-8	4
Lonazolac	C ₁₇ H ₁₃ CIN ₂ O ₂	312,0665	53808-88-1	4
Loperamide	C ₂₉ H ₃₃ CIN ₂ O ₂	476,223	53179-11-6	4
Loracarbef	C ₁₆ H ₁₆ CIN ₃ O ₄	349,0829	76470-66-1	4
Loratadine	C ₂₂ H ₂₃ CIN ₂ O ₂	382,1447	79794-75-5	4
Lorazepam	C ₁₅ H ₁₀ Cl ₂ N ₂ O ₂	320,0119	846-49-1	4
Lormetazepam	C ₁₆ H ₁₂ Cl ₂ N ₂ O ₂	334,0274	848-75-9	4
Lornoxicam	C ₁₃ H ₁₀ CIN ₃ O ₄ S ₂	370,9801	70374-39-9	8
Losartan	C ₂₂ H ₂₃ CIN ₆ O	422,1621	114798-39-9	4
Lovastatin	C ₂₄ H ₃₆ O ₅	404,2562	75330-75-5	4
Loxapine	C ₁₈ H ₁₈ CIN ₃ O	327,1138	02/10/1977	4
Lysergide	C ₂₀ H ₂₅ N ₃ O	323,1997	50-73-3	4
Mafenide	C ₇ H ₁₀ N ₂ O ₂ S	186,0462	138-39-6	4
Maprotiline	C ₂₀ H ₂₃ N	277,183	10262-69-8	4
Mazindol	C ₁₆ H ₁₃ CIN ₂ O	284,0716	22232-71-9	4
Mebendazole	C ₁₆ H ₁₃ N ₃ O ₃	295,0956	31431-39-7	4
Mebeverine	C ₂₅ H ₃₅ NO ₅	429,2515	07/06/3625	4
Meclizine	C ₂₅ H ₂₇ CIN ₂	390,1862	31884-77-2	4

Compound	Formula	MW	CAS	# of spectra
Meclofenamic acid	C14H11Cl2NO2	295,0166	644-62-2	8
Meclofenoxate	C12H16ClNO3	361,0174	51-68-3	4
Mecloxamine	C19H24ClNO	317,1546	04/06/5668	4
Meclozine	C25H27ClN2	390,1862	569-65-3	4
Medazepam	C16H15ClN2	270,0923	06/12/2898	4
Mefenamic acid	C15H15NO2	241,1102	61-68-7	8
Mefenorex	C12H18ClN	211,1127	17243-57-1	4
Mefexamide	C15H24N2O3	280,1786	1227-61-8	4
Mefloquine	C17H16F6N2O	378,1166	53230-10-7	4
Mefruside	C13H189ClN2O5S2	657,3082	7195-27-9	8
Melatonin	C13H16N2O2	232,1211	73-31-4	8
Melitracen	C21H25N	291,1987	5118-29-6	4
Meloxicam	C14H13N3O4S2	351,0347	71125-38-7	4
Melperone	C16H22FN2O	263,1685	3575-80-2	4
Melphalan	C13H18Cl2N2O2	304,0745	148-82-3	4
Mepacrine	C23H30ClN3O	399,2077	83-89-6	4
Meperidine-D4	C15H17D4NO2	251	53484-73-4	4
Mephentermine	C11H17N	163,136	100-92-5	4
Mepindolol	C15H22N2O2	262,1681	23694-81-7	4
Mepivacaine	C15H22N2O	246,1732	96-88-8	4
Meproamate	C9H18N2O4	218,1266	57-53-4	4
Meptazinol	C15H23NO	233,1779	54340-58-8	4
Mequitazine	C20H22N2S	322,1503	29216-28-2	4
Mescaline	C11H17NO3	211,1208	06/04/1954	4
Mesoridazine	C21H26N2OS2	386,1486	5588-33-0	4
Mesuximide	C12H13NO2	203,0946	77-41-8	4
Metaclazepam	C18H18BrClN2O	392,0291	65517-27-3	4
Metamfepramone	C11H15NO	177,1153	15351-09-4	4
Metamitron	C10H10N4O	202,0854	41394-05-2	8
Metamizol	C13H16N3O4S	310,0861	68-89-3	8
Metamphetamine	C10H15N	149,1204	537-46-2	4
Metazachlor	C14H16ClN3O	277,0981	67129-08-2	4
Metenolone acetate	C22H32O3	344,2351	434-05-9	4
Metformin	C4H11N5	129,1014	657-24-9	4

Compound	Formula	MW	CAS	# of spectra
Methabenzthiazuron	C10H11N3OS	221,0622	18691-97-9	4
Methadone	C21H27NO	309,2092	76-99-3	4
Methamphetamine-D11	C10H4D11N	160	152477-88-8	4
Methamphetamine-D8	C10H7D8N	157	136765-40-7	4
Methanthelinium	C21H26NO3	340,1912	53-46-3	4
Methaphenilene	C15H20N2S	260,1347	493-78-7	4
Methapyrilene	C14H19N3S	261,1299	91-80-5	4
Methaqualone	C16H14N2O	250,1106	72-44-6	4
Methazolamide	C5H8N4O3S2	236,0037	554-57-4	8
Methfuroxam	C14H15NO2	229,1102	28730-17-8	4
Methocarbamol	C11H15NO5	241,095	532-03-6	4
Methohexital	C14H18N2O3	262,1317	151-83-7	4
Methohexital-D5	C14H13D5N2O3	267	160227-45-2	4
Methoprotryne	C11H21N5OS	271,1466	841-06-5	4
Methotrexate	C20H22N8O5	454,1713	02/05/1959	4
Methyl nicotinate	C7H7NO2	137,0476	93-60-7	4
Methyl dopa	C10H13NO4	211,0844	555-30-6	8
Methylephedrine	C11H14NO	176,1075	552-79-4	4
Methylphenidate	C14H19NO2	233,1415	113-45-1	4
Methylprednisolone	C22H30O5	374,2093	83-43-2	8
Methylscopolamine	C18H23NO4	317,1627	155-41-9	4
Methylthiouracil	C5H6N2OS	142,02	02/04/1956	8
Methysergide	C21H27N3O2	353,2103	361-37-5	4
Metipranolol	C17H27NO4	309,194	22664-55-7	4
Metixene	C20H23NS	309,1551	02/02/4969	4
Metoclopramide	C14H22ClN3O2	299,14	364-62-5	4
Metofenazate	C31H36ClN3O5S	597,2064	388-51-2	4
Metoprolol	C15H25NO3	267,1834	37350-58-6	4
Metronidazole	C6H9N3O3	171,0643	443-48-1	4
Metsulfuron-methyl	C14H15N5O6S	381,0743	74223-64-6	8
Metyrapone	C14H14N2O	226,1106	54-36-4	4
Mexiletine	C11H17NO	179,131	31828-71-4	4
Mezlocillin	C21H25N5O8S2	539,1144	51481-65-3	4
Mianserin	C18H20N2	264,1626	24219-97-4	4

Compound	Formula	MW	CAS	# of spectra
Miconazole	C18H14Cl4N2O	413,986	22916-47-8	4
Midazolam	C18H13ClFN3	325,0782	59467-70-8	4
Midodrine	C12H18N2O4	254,1266	42794-76-3	4
Milrinone	C12H9N3O	211,0745	78415-72-2	8
Miltefosine	C21H46NO4P	407,3164	58066-85-6	4
Minocycline	C23H27N3O7	457,1849	10118-90-8	4
Minoxidil	C9H15N5O	209,1276	38304-91-5	4
Mirtazapine	C17H19N3	265,1578	61337-67-5	4
Mizolastine	C24H25FN6O	432,2073	108612-45-9	4
Moclobemide	C13H17ClN2O2	268,0978	71320-77-9	4
Modafinil	C15H15NO2S	273,0823	68693-11-8	4
Mofebutazone	C13H16N2O2	232,1211	68693-11-8	8
Molindone	C16H24N2O2	276,1837	7416-34-4	4
Molsidomine	C9H14N4O4	242,1015	25717-80-0	4
Monocrotophos	C7H14NO5P	223,0609	6923-22-4	4
Monolinuron	C9H11ClN2O2	214,0509	1746-81-2	4
Monuron	C9H11ClN2O	198,0559	150-68-5	4
Moperone	C22H26FNO2	355,1947	1050-79-7	4
Morantel	C12H16N2S	220,1034	20574-50-9	4
Morazone	C23H27N3O2	377,2103	6536-18-1	4
Morphin-3 β -D-glucuronide-D3	C23H24D3NO9	464		8
Morphine	C17H19NO3	285,1364	57-27-2	4
Morphine-3- β -D-glucuronide	C23H27NO9	461,1685	20290-09-9	4
Moxaverine	C20H21NO2	307,1572	10539-19-2	4
Moxisylyte	C16H25NO3	279,1834	54-32-0	4
Moxonidine	C9H12ClN5O	241,073	75438-57-2	4
N-Despropylpropafenone	C18H21NO3	299,1521		4
N-Isopropylsalicylamide	C10H13NO2	179,0946	551-35-9	8
N-Methyl-1-(1.3-benzodioxol-5-yl)-2-butanamine	C12H17NO2	207,1259	103818-46-8	4
N-Methylephedrine	C11H17NO	179,131	552-79-4	4
N,N-Diethyl-m-toluamide	C12H17NO	191,131	134-62-3	4
N2-Ethylguanin	C7H9N5O	179,0807		8
Nabumetone	C15H16O2	228,115	42924-53-8	4
Nadolol	C17H27NO4	309,194	42200-33-9	4

Compound	Formula	MW	CAS	# of spectra
Naftidrofuryl	C24H33NO3	383,246	31329-57-4	4
Naftifine	C21H21N	287,1673	65472-88-0	4
Nalidixic acid	C12H12N2O3	232,0847	389-08-2	4
Nalorphine	C19H21NO3	311,1521	62-67-9	4
Naloxone	C19H21NO4	327,147	465-65-6	4
Naltrexone	C20H23NO4	341,1626	16590-41-3	4
Nandrolone	C18H26O2	274,1932	434-22-0	4
Naphazoline	C14H14N2	210,1156	835-31-4	4
Napropamide	C17H21NO2	271,1572	15299-99-7	4
Naproxen	C14H14O3	230,0942	22204-53-1	4
Natamycin	C33H47NO13	665,3047	7681-93-8	4
Nebivolol	C22H25F2NO4	405,1751	99200-09-6	4
Nefazodone	C25H32CIN5O2	469,2244	83366-66-9	4
Nefopam	C17H19NO	253,1466	13669-70-0	4
Nicametate	C12H18N2O2	222,1368	3099-52-3	4
Nicardipine	C26H29N3O6	479,2056	5598-32-5	4
Nicergoline	C24H26BrN3O3	483,1157	27848-84-6	4
Nicotinamide	C6H6N2O	122,048	98-92-0	4
Nicotine	C10H14N2	162,1156	05/11/1954	4
Nifedipine	C17H18N2O6	346,1164	21829-25-4	4
Nifenazone	C17H16N4O2	308,1273	2139-47-1	4
Niflumic acid	C13H9F3N2O2	282,0616	4394-00-7	8
Nilvadipine	C19H19N3O6	385,1273	75530-68-6	4
Nimodipine	C21H26N2O7	418,174	66085-59-4	4
Nimorazole	C9H14N4O3	226,1065	6506-37-2	4
Nimustine	C9H13CIN6O2	272,0788	42471-28-3	4
Nisoldipine	C20H24N2O6	388,1634	63675-72-9	4
Nitrazepam	C15H11N3O3	281,08	146-22-5	4
Nitrendipine	C18H20N2O6	360,1321	39562-70-4	4
Nizatidine	C12H21N5O2S2	331,1136	76963-41-2	4
Nomifensine	C16H18N2	238,1469	24526-64-5	4
Nonivamide	C17H27NO3	293,199	2444-46-4	4
Norbuprenorphine	C25H35NO4	413,2566	78715-23-8	4
Norbuprenorphine-D3	C25H32D3NO4	417		4

Compound	Formula	MW	CAS	# of spectra
Nordiazepam	C15H11ClN2O	270,0559	1088-11-5	4
Nordiazepam-D5	C15H6ClD5N2O	275	65891-80-7	4
Norephedrine	C9H13NO	151,0997	14838-15-4	4
Norepinephrine	C8H11NO3	169,0738	51-41-2	4
Norethisterone	C20H26O2	298,1932	68-22-4	4
Norethisterone acetate	C22H28O3	340,2038	51-98-9	4
Norfenfrine	C8H11NO2	153,0789	536-21-0	4
Norfentanyl	C14H20N2O	232,1575		4
Norfloxacin	C16H18FN3O3	319,1332	70458-96-7	4
Normorphine	C16H17NO3	271,1207	466-97-7	4
Norpropoxyphene	C21H27NO2	325,2041	3376-94-1	4
Norpseudoephedrine	C9H13NO	151,0997	492-39-7	4
Nortriptyline	C19H21N	263,1673	72-69-5	4
Noscapine	C22H23NO7	413,1474	128-62-1	4
Nuarimol	C17H12ClFN2O	314,0622	63284-71-9	4
Obidoxime	C14H16N4O3	288,1222	7683-36-5	4
Octopamine	C8H11NO2	153,0789	104-14-3	4
Ofloxacin	C18H20FN3O4	361,1437	82419-36-1	4
Olanzapine	C17H20N4S	312,1408	132539-06-1	4
Olsalazine	C14H10N2O6	302,0538	15772-48-2	4
Omeprazole	C17H19N3O3S	345,1147	73590-58-6	4
Ondansetron	C18H19N3O	293,1528	99614-02-5	4
Opi Pramol	C23H29N3O	363,231	315-72-0	4
Orciprenaline	C11H17NO3	211,1208	586-06-1	4
Ornidazole	C7H10ClN3O3	219,041	16773-42-5	4
Orphenadrine	C18H23NO	269,1779	83-98-7	4
Oxadixyl	C14H18N2O4	278,1266	77732-09-3	4
Oxamyl	C7H13N3O3S	219,0677	23135-22-0	4
Oxatomide	C27H30N4O	426,2419	60607-34-3	4
Oxazepam	C15H11ClN2O2	286,0509	604-75-1	4
Oxcarbazepine	C15H12N2O2	252,0898	28721-07-5	4
Oxedrine	C9H13NO2	167,0946	05/07/1994	4
Oxeladin	C20H33NO3	335,246	468-61-1	4
Oxetacaine	C28H41N3O3	467,3147	126-27-2	4

Compound	Formula	MW	CAS	# of spectra
Oxiconazole	C18H13Cl4N3O	426,9812	64211-45-6	4
Oxilofrine	C10H15NO2	181,1102	365-26-4	4
Oxitriptan	C11H12N2O3	220,0847	08/09/4350	8
Oxitropium	C19H26NO4	332,1861	30286-75-0	4
Oxomemazine	C18H22N2O2S	330,1401	3689-50-7	4
Oxprenolol	C15H23NO3	265,1677	6452-71-7	4
Oxybuprocaine	C17H28N2O3	308,2099	99-43-4	4
Oxybutynin	C22H31NO3	357,2303	5633-20-5	4
Oxycodone	C18H21NO4	315,147	76-42-6	4
Oxyfedrine	C19H23NO3	313,1677	15687-41-9	4
Oxymetazoline	C16H24N2O	260,1888	1491-59-4	4
Oxymorphone C17H19NO4	301,1314	76-41-5		4
Oxiconazole	C18H13Cl4N3O	426,9812	64211-45-6	4
Oxilofrine	C10H15NO2	181,1102	365-26-4	4
Oxitriptan	C11H12N2O3	220,0847	08/09/4350	8
Oxitropium	C19H26NO4	332,1861	30286-75-0	4
Oxomemazine	C18H22N2O2S	330,1401	3689-50-7	4
Oxprenolol	C15H23NO3	265,1677	6452-71-7	4
Oxybuprocaine	C17H28N2O3	308,2099	99-43-4	4
Oxybutynin	C22H31NO3	357,2303	5633-20-5	4
Oxycodone	C18H21NO4	315,147	76-42-6	4
Oxyfedrine	C19H23NO3	313,1677	15687-41-9	4
Oxymetazoline	C16H24N2O	260,1888	1491-59-4	4
Oxymorphone	C17H19NO4	301,1314	76-41-5	4
Oxypendyl	C20H26N4OS	370,1827	17297-82-4	4
Oxypertine	C23H29N3O2	379,2259	153-87-7	4
Oxytetracycline	C22H24N2O9	460,1481	79-57-2	4
p-(Aminomethyl)benzoic acid	C8H9NO2	151,0633	56-91-7	4
Papaverine	C20H21NO4	339,147	58-74-2	4
Paracetamol	C8H9NO2	151,0633	103-90-2	4
Paraoxon	C10H14NO6P	275,0557	311-45-5	4
Paroxetine	C19H20FNO3	329,1427	61869-08-7	4
Penbutolol	C18H29NO2	291,2198	38363-40-5	4
Penfluridol	C28H27ClF5NO	523,1701	26864-56-2	4

Compound	Formula	MW	CAS	# of spectra
Pentamidine	C19H24N4O2	340,1899	100-33-4	4
Pentobarbital	C11H18N2O3	226,1317	76-74-4	4
Pentobarbital-D5	C11H13D5N2O3	231	52944-66-8	4
Pentoxifylline	C13H18N4O3	278,1378	06/05/6493	4
Pentoxyverine	C20H31NO3	333,2303	77-23-6	4
Perazine	C20H25N3S	339,1769	84-97-9	4
Pergolide	C19H26N2S	314,1816	66104-22-1	4
Periciazine	C21H23N3OS	365,1561	2622-26-6	4
Perindopril	C19H32N2O5	368,2311	82834-16-0	4
Perphenazine	C21H26CIN3OS	403,1485	58-39-9	4
Pethidine	C15H21NO2	247,1572	57-42-1	4
Phenacetin	C10H13NO2	179,0946	62-44-2	4
Phenazone	C12H8N2	180,0687	60-80-0	4
Phenazopyridine	C11H11N5	213,1014	94-78-0	4
Phencyclidine	C17H25N	243,1987	01/10/1977	4
Phenelzine	C8H12N2	136,1	51-71-8	4
Phenethylamin	C8H11N	121,0891	64-04-0	4
Phenindione	C15H10O2	222,068	05/12/1983	8
Pheniramine	C16H20N2	240,1626	86-21-5	4
Phenmedipham	C16H16N2O4	300,111	13684-63-4	4
Phenobarbital	C12H12N2O3	232,0847	06/06/1950	4
Phenobarbital-D5	C12H7D5N2O3	237	72793-46-5	4
Phenothiazine	C12H9NS	199,0455	92-84-2	4
Phenoxyethylpenicillin	C16H18N2O5S	350,0936	01/08/1987	8
Phenprobamate	C10H13NO2	179,0946	673-31-4	4
Phenprocoumon	C18H16O3	280,1099	435-97-2	4
Phentolamine	C17H19N3O	281,1528	50-60-2	4
Phenylbutazone	C19H20N2O2	308,1524	50-33-9	4
Phenylephrine	C9H13NO2	167,0946	59-42-7	4
Phenylpropanolamine	C9H13NO	151,0997	14838-15-4	4
Phenyltoloxamine	C17H21NO	255,1623	06/12/1992	4
Phenytoin	C15H12N2O2	252,0898	57-41-0	4
Pholedrine	C10H15NO	165,1153	370-14-9	4
Phthalylsulfathiazole	C17H13N3O5S2	403,0296	85-73-4	8

Compound	Formula	MW	CAS	# of spectra
Physostigmine	C15H21N3O2	275,1633	57-47-6	4
Pilocarpine	C11H16N2O2	208,1211	92-13-7	4
Pimozide	C28H29F2N3O	461,2278	2062-78-4	4
Pindolol	C14H20N2O2	248,1524	13523-86-9	4
Pioglitazone	C19H20N2O3S	356,1194	111025-46-8	4
Pipamperone	C21H30FN3O2	375,2322	1893-33-0	4
Pipemidic acid	C14H17N5O3	303,1331	51940-44-4	4
Piperacillin	C23H27N5O7S	517,1631	61477-96-1	4
Piprozolin	C14H22N2O3S	298,1351	17243-64-0	4
Piracetam	C6H10N2O2	142,0742	7491-74-9	4
Pirbuterol	C12H20N2O3	240,1473	38677-81-5	4
Pirenzepine	C19H21N5O2	351,1695	28797-61-7	4
Piretanide	C17H18N2O5S	362,0936	55837-27-9	8
Piritramide	C27H34N4O	430,2732	302-41-0	4
Piroxicam	C15H13N3O4S	331,0625	36322-90-4	4
Pizotifen	C19H21NS	295,1394	15574-96-6	4
Polythiazide	C11H13ClF3N3O4S3	438,9708	346-18-9	4
Practolol	C14H22N2O3	266,163	6673-35-4	4
Prajmalium	C23H33N2O2	369,2542	35080-11-6	4
Pramipexole	C10H17N3S	211,1143	104632-26-0	4
Prazepam	C19H17ClN2O	324,1029	2955-38-6	4
Prazosin	C19H21N5O4	383,1592	19216-56-9	4
Prednisolone	C21H28O5	360,1936	50-24-8	8
Prednisone	C21H26O5	358,178	02/03/1953	8
Prenylamine	C24H27N	329,2143	390-64-7	4
Prilocaine	C13H20N2O	220,1575	721-50-6	4
Primaquine	C15H21N3O	259,1684	90-34-6	4
Primidone	C12H14N2O2	218,1055	125-33-7	4
Procainamide	C13H21N3O	235,1684	09/06/1951	4
Procaine	C13H20N2O2	236,1524	59-46-1	4
Prochlorperazine	C20H24ClN3S	373,1379	58-38-8	4
Procyclidine	C19H29NO	287,2249	77-37-2	4
Profenamine	C19H24N2S	312,166	522-00-9	4
Progesterone	C21H30O2	314,2245	57-83-0	4

Compound	Formula	MW	CAS	# of spectra
Promazine	C17H20N2S	284,1347	58-40-2	4
Promethazine	C17H20N2S	284,1347	60-87-7	4
Prometryn	C10H19N5S	241,1361	7287-19-6	4
Propafenone	C21H27NO3	341,199	54063-53-5	4
Propallylonal	C10H13BrN2O3	288,0109	545-93-7	4
Propham	C10H13NO2	179,0946	122-42-9	4
Propiconazole	C15H17Cl2N3O2	341,0697	60207-90-1	4
Propionylpromazine	C20H24N2OS	340,1609	3568-24-9	4
Propipocaine	C17H25NO2	275,1885	3670-68-6	4
Propiverine	C24H31NO2	365,2354	60569-19-9	4
Propranolol	C16H21NO2	259,1572	525-66-6	4
Propyphenazone	C14H18N2O	230,1419	479-92-5	4
Prothiopendyl	C16H19N3S	285,1299	303-69-5	4
Protionamide	C9H12N2S	180,0721	14222-60-7	8
Protriptyline	C19H21N	263,1673	438-60-8	4
Proximpham	C10H12N2O2	192,0898	2828-42-4	4
Pseudoephedrine	C10H15NO	165,1153	90-82-4	4
Psilocin	C12H16N2O	204,1262	520-53-6	4
Pyranocoumarin	C20H18O4	322	518-20-7	4
Pyribenzamine	C16H21N3	255,1735	91-81-6	4
Pyridoxine	C8H11NO3	169,0738	65-23-6	4
Pyrilamine	C17H23N3O	285,1841	91-84-9	4
Pyrimethamine	C12H13ClN4	248,0828	58-14-0	4
Pyritinol	C16H20N2O4S2	368,0864	1098-97-1	8
Pyrvinium	C26H28N3	382,2283	548-84-5	4
Quetiapine	C21H25N3O2S	383,1667	111974-72-2	4
Quinapril	C25H30N2O5	438,2154	85441-61-8	4
Quinaprilat	C23H26N2O5	410,1841	82768-85-2	8
Quinidine	C20H24N2O2	324,1837	56-54-2	4
Quinine	C20H24N2O2	324,1837	130-95-0	4
Ramifenazone	C14H19N3O	245,1528	3615-24-5	4
Ramipril	C23H32N2O5	416,2311	87333-19-5	4
Ranitidine	C13H22N4O3S	314,1412	66357-35-5	4
Raubasine	C21H24N2O3	352,1786	483-04-5	4

Compound	Formula	MW	CAS	# of spectra
Raupin	C19H22N2O2	310,1681	482-68-8	4
Reboxetine	C19H23NO3	313,1677	98769-81-4	4
Remoxipride	C16H23BrN2O3	370,0892	80125-14-0	4
Repaglinide	C27H36N2O4	452,2675	135062-02-1	4
Reproterol	C18H23N5O5	389,1699	540-63-54-6	4
Reserpin	C33H40N2O9	608,2732	50-55-5	4
Rifampicin	C43H58N4O12	822,4051	13292-46-1	4
Riluzole	C8H5F3N2OS	234,0074	1744-22-5	4
Risperidone	C23H27FN4O2	410,2118	106266-06-2	4
Ritodrine	C17H21NO3	287,1521	26652-09-5	4
Rizatriptan	C15H19N5	269,164	145202-66-0	4
Rocuronium	C32H53N2O4	529,4005	119302-91-9	4
Ropinirole	C16H24N2O	260,1888	91374-21-9	4
Ropivacaine	C17H26N2O	274,2045	84057-95-4	4
Rosiglitazon	C18H19N3O3S	357,1147	122320-73-4	4
Rosiglitazon	C18H19N3O3S	357,1147	122320-73-4	4
Salbutamol	C13H21NO3	239,1521	18559-94-9	4
Salicylamide	C7H7NO2	137,0476	65-45-2	8
Salmeterol	C25H37NO4	415,2722	89365-50-4	4
Salsalate	C14H10O5	258,0528	552-94-3	4
Scopolamine	C17H21NO4	303,147	51-34-3	4
Sebuthylazine	C9H16CIN5	229,1094	7286-69-3	4
Secbutabarbital	C10H16N2O3	212,116	125-40-6	4
Selegilin	C13H17N	187,136	14611-51-9	4
Serotonin	C10H12N2O	176,0949	50-67-9	4
Sertindole	C24H26CIFN4O	440,1779	106516-24-9	4
Sertraline	C17H17Cl2N	305,0738	79559-97-0	4
Sibutramin	C17H26CIN	279,1753	106650-56-0	4
Sildenafil	C22H30N6O4S	474,2049	139755-83-2	4
Simazine	C7H12CIN5	201,0781	122-34-9	4
Simvastatin	C25H38O5	418,2719	79902-63-9	4
Sotalol	C12H20N2O3S	272,1194	959-24-0	4
Spirapril	C22H30N2O5S2	466,1596	83647-97-6	8
Stanozolol	C21H32N2O	328,2514	10418-03-8	4

Compound	Formula	MW	CAS	# of spectra
Sulfabenzamide	C13H12N2O3S	276,0568	127-71-9	8
Sulfacetamide	C8H10N2O3S	214,0412	144-80-9	4
Sulfaclomide	C12H13ClN4O2S	312,0447	4015-18-3	8
Sulfadiazine	C10H10N4O2S	250,0524	68-35-9	4
Sulfadiazine	C11H14N2O3S	254,0725	115-68-4	8
Sulfadoxine	C12H14N4O4S	310,0735	2447-57-6	8
Sulfaethidole	C10H12N4O2S2	284,0401	94-19-9	8
Sulfaguanidine	C7H10N4O2S	214,0524	57-67-0	4
Sulfalene	C11H12N4O3S	280,063	152-47-6	4
Sulfamerazine	C11H12N4O2S	264,068	127-79-7	4
Sulfamethizole	C9H10N4O2S2	270,0245	144-82-1	8
Sulfamethoxazole	C10H11N3O3S	253,0521	723-46-6	8
Sulfamethoxypyridazine	C11H12N4O3S	280,063	80-35-3	4
Sulfanilic Acid	C6H7NO3S	173,0146	121-57-3	4
Sulfapyridine	C11H11N3O2S	249,0571	144-83-2	4
Sulfaquinoxaline	C14H12N4O2S	300,068	59-40-5	8
Sulfasalazine	C18H14N4O5S	398,0684	599-79-1	4
Sulfathiazole	C9H9N3O2S2	255,0136	42-14-0	8
Sulfinpyrazone	C23H20N2O3S	404,1194	57-96-5	4
Sulindac	C20H17FO3S	356,0881	38194-50-2	4
Sulpiride	C15H23N3O4S	341,1409	15676-16-1	4
Sultiam	C10H14N2O4S2	290,0395	61-56-3	8
Sumatriptan	C14H21N3O2S	295,1354	103628-46-2	4
Suxibuzone	C24H26N2O6	438,179	27470-51-5	8
Tacrine	C13H14N2	198,1156	321-64-2	4
Tadalafil	C22H19N3O	341,1528		4
Talinolol	C20H33N3O3	363,2521	57460-41-0	4
Tamoxifen	C26H29NO	371,2249	10540-29-1	4
Tebuconazole	C16H22ClN3O	307,1451	107534-96-3	4
Telmisartan	C33H30N4O2	514,2368	144701-48-4	4
Temazepam	C16H13ClN2O2	300,0665	846-50-4	4
Teniposide	C32H32O13S	656,1563	29767-20-2	4
Tenoxicam	C13H11N3O4S2	337,019	59804-37-4	4
Terazosine	C19H25N5O4	387,1906	63590-64-7	4

Compound	Formula	MW	CAS	# of spectra
Terbinafine	C ₂₁ H ₂₅ N	291,1986	91161-71-6	4
Terbumeton	C ₁₀ H ₁₉ N ₅ O	225,1589	33693-04-8	4
Terbutaline	C ₁₂ H ₁₉ NO ₃	225,1364	23031-25-6	4
Terbutylazine	C ₉ H ₁₆ CIN ₅	229,1094	5915-41-3	4
Terbutryn	C ₁₀ H ₁₉ N ₅ S	241,1361	886-50-0	4
Terconazole	C ₂₆ H ₃₁ Cl ₂ N ₅ O ₃	531,1803	67915-31-5	4
Terfenadine	C ₃₂ H ₄₁ NO ₂	471,3137	50679-08-8	4
Tertalolol	C ₁₆ H ₂₅ NO ₂ S	295,1606	34784-64-0	4
Testosterone	C ₁₉ H ₂₈ O ₂	288,2089	58-22-0	4
Testosterone benzoate	C ₂₁ H ₃₀ O ₃	330,2194	2088-71-3	4
Tetracaine	C ₁₅ H ₂₄ N ₂ O ₂	264,1837	94-24-6	4
Tetracycline	C ₂₂ H ₂₄ N ₂ O ₈	444,1532	60-54-8	4
Tetramethrin	C ₁₉ H ₂₅ NO ₄	331,1783	7696-12-0	4
Tetrazepam	C ₁₆ H ₁₇ CIN ₂ O	288,1029	10379-14-3	4
Tetroxoprim	C ₁₆ H ₂₂ N ₄ O ₄	334,1641	53808-87-0	4
Tetryzoline	C ₁₃ H ₁₆ N ₂	200,1313	84-22-0	4
THC	C ₂₁ H ₃₀ O ₂	314,2245	7683-36-5	4
THC-COOH	C ₂₁ H ₂₈ O ₄	344,1986	23978-85-0	8
THC-OH	C ₂₁ H ₃₀ O ₃	330,2194	366557-05-08	8
Thebacon	C ₂₀ H ₂₃ NO ₄	341,1626	466-90-0	4
Thenalidine	C ₁₇ H ₂₂ N ₂ S	286,1503	04/12/1986	4
Theobromine	C ₇ H ₈ N ₄ O ₂	180,0646	83-67-0	4
Theodrenaline	C ₁₇ H ₂₁ N ₅ O ₅	375,1542	13460-98-5	4
Theophylline	C ₇ H ₈ N ₄ O ₂	180,0646	58-55-9	4
Thiabendazole	C ₁₀ H ₇ N ₃ S	201,036	148-79-8	4
Thiamazole	C ₄ H ₆ N ₂ S	114,0251	60-56-0	4
Thiamine	C ₁₂ H ₁₇ N ₄ O ₅	265,1123	59-43-8	4
Thiazaflurone	C ₆ H ₇ F ₃ N ₄ O ₅	240,0292	25366-23-8	8
Thiazinamium	C ₁₈ H ₂₃ N ₂ S	299,1581	2338-21-8	4
Thiethylperazine	C ₂₂ H ₂₉ N ₃ S ₂	399,1802	1420-55-9	4
Thiobutabarbital	C ₁₀ H ₁₆ N ₀ O ₂ O ₂ S	228,0932	2095-57-0	4
Thiodicarb	C ₁₀ H ₁₈ N ₄ O ₄ S ₃	354,049	59669-26-0	4
Thiofanox	C ₉ H ₁₈ N ₂ O ₂ S	218,1088	39196-18-4	4
Thioguanine	C ₅ H ₅ N ₅ S	167,0265	154-42-7	4

Compound	Formula	MW	CAS	# of spectra
Thiopental	C11H17N2O2S	241,101	76-75-5	4
Thiopropazate	C23H28CIN3O2S	445,159	84-06-0	4
Thiopropazine	C22H30N4O2S2	446,181	316-81-4	4
Thioridazine	C21H26N2S2	370,1537	50-52-2	4
Thiothixene	C23H29N3O2S2	443,1701	5591-45-7	4
Thiram	C6H12N2S4	239,9883	137-26-8	4
Thonzylamine	C16H22N4O	286,1793	91-85-0	4
Thymopentin	C30H49N9O9	679,3653	69558-55-0	4
Tiagabine	C20H25NO2S2	375,1326	115103-54-3	4
Tiapride	C15H24N2O4S	328,1456	51012-32-9	4
Ticlopidine	C14H14CINS	263,0535	55142-85-3	4
Tiemonium	C18H24NO2S	318,1527	144-12-7	4
Tilidine	C17H23NO2	273,1728	20380-58-9	4
Timolol	C13H24N4O3S	316,1569	26839-75-8	4
Tinidazole	C8H13N3O4S	247,0626	19387-91-8	4
Tiocarlide	C23H32N2O2S	400,2184	910-86-1	8
Tiracizine	C21H25N3O3	367,1895	83275-56-3	4
Tizanidine	C9H8CIN5S	253,0188	51322-75-9	4
Tocainide	C11H16N2O	192,1262	41708-72-9	4
Tolazamide	C14H21N3O3S	311,1303	1156-19-0	8
Tolazoline	C10H12N2	160,1	59-98-3	4
Tolbutamide	C12H18N2O3S	270,1038	64-77-7	4
Toliprolol	C13H21NO2	223,1572	2933-94-0	4
Tolmetin	C15H15NO3	257,1051	26171-23-3	4
Tolnaftate	C19H17NOS	307,103	2398-96-1	4
Tolpropamine	C18H23N	253,183	5632-44-0	4
Tolycaine	C15H22N2O3	278,163	3686-58-6	4
Topotecan	C23H23N3O5	421,1637	123948-87-8	4
Torasemide	C16H20N4O3S	348,1256	56211-40-6	8
Tramadol	C16H25NO2	263,1884	27203-92-5	4
Tranexamic acid	C8H15NO2	157,1102	1197-18-8	4
Tranlycypromine	C9H11N	133,0891	155-09-9	4
Trapidil	C10H15N5	205,1327	15421-84-8	4
Trazodone	C19H22CIN5O	371,1512	19794-93-5	4

Compound	Formula	MW	CAS	# of spectra
Triadimefon	C14H16ClN3O2	293,0931	43121-43-3	4
Triadimenol	C14H18ClN3O2	295,1087	55219-65-3	4
Triallate	C10H16Cl3NOS	303,0018	2303-17-5	4
Triamcinolone	C21H27FO6	394,1791	124-94-7	8
Triamterene	C12H11N7	253,1075	396-01-0	4
Triasulfuron	C14H16ClN5O5S	401,056	82097-50-5	8
Triazolam	C17H12Cl2N4	342,0439	28911-01-5	4
Trifluperazine	C22H23F4NO2	409,1664	117-89-5	4
Trifluperidol	C22H23F4NO2	409,1664	749-13-3	4
Triflupromazine	C18H19F3N2S	352,1221	146-54-3	4
Trihexyphenidyl	C20H31NO	301,2405	114-11-6	4
Trimazosin	C20H29N5O6	435,2117	35795-16-5	4
Trimethobenzamide	C21H28N2O5	388,1998	138-56-7	4
Trimethoprim	C14H18N4O3	290,1378	738-70-5	4
Trimipramine	C20H26N2	294,2095	739-71-9	4
Tripelennamine	C16H21N3	255,1735	91-81-6	4
Triperiden	C21H29NO	311,2249	14617-17-5	4
Tripolidine	C19H22N2	278,1782	486-12-4	4
Tritoqualine	C26H32N2O8	500,2158	14504-73-5	4
Tromantadine	C16H28N2O2	280,215	53783-83-8	4
Tropisetron	C17H20N2O2	284,1524	89565-68-4	8
Trospium	C25H30NO3	392,2225	10405-02-4	4
Tryptamine	C10H12N2	160,1	61-54-1	4
Tulobuterol	C12H18ClNO	227,1076	41570-61-0	4
Urapidil	C20H29N5O3	387,2269	34661-75-1	4
Valacyclovir	C13H20N6O4	324,1546	124832-26-4	4
Valdecoxib	C16H14N2O3S	314,0725	181695-72-7	8
Valsartan	C24H29N5O3	435,227	137862-53-4	8
Vardenafil	C23H32N6O4S	488,2205	224785-90-4	4
Venlafaxine	C17H27NO2	277,2041	93413-69-5	4
Verapamil	C27H38N2O4	454,2831	52-53-9	4
Vetrabutine	C20H27NO2	313,2041	04/09/5974	4
Viloxazine	C13H19NO3	237,1364	46817-91-8	4
Viminol	C21H31ClN2O	362,2124	21363-18-8	4

Compound	Formula	MW	CAS	# of spectra
Vincamine	C21H26N2O3	354,1943	1617-90-9	4
Vinpocentine	C22H26N2O2	350,1994	42971-09-5	4
Viquidil	C20H24N2O2	324,1837	84-55-9	4
Warfarin	C19H16O4	308,1048	81-81-2	4
Xantanol	C13H21N5O4	311,1593	437-74-1	4
Xipamide	C15H15CIN2O4S	354,0441	14293-44-8	8
Xylometazoline	C16H24N2	244,1939	526-36-3	4
Yohimbine	C21H26N2O3	354,1943	146-48-5	4
Zimeldine	C16H17BrN2	316,0575	56775-88-3	4
Zolpidem	C19H21N3O	307,1684	82626-48-0	4
Zopiclone	C17H17CIN6O3	388,105	43200-80-2	4
Zotepine	C18H18CINOS	331,0797	26615-21-4	4
Zuclopenthixol	C22H25CIN2OS	400,1376	53772-83-1	4
α -Ethyl-1.3-benzodioxole-5-ethanamine	C11H15NO2	193,1102	107447-03-0	4

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