



# LC/MS/MS Meta Library Version 1.0 for Cliquid<sup>®</sup> Software

## *iMethod<sup>™</sup> Application for LC/MS/MS Meta Library Version 1.0 for Cliquid<sup>®</sup> Software*

The following description outlines the 2340-compounds MRM catalogue and 2430-compounds spectral library that is available for use with AB SCIEX API or QTRAP<sup>®</sup> LC/MS/MS systems and Cliquid<sup>®</sup> Software. This library and MRM catalogue, created using certified reference materials, can be used alone to create custom screening and/or quantitation methods or in conjunction with the iMethod<sup>™</sup> application for drugs of abuse screening; pesticides screening; veterinary antibiotics screening and mycotoxin screening. The four iMethod<sup>™</sup> applications for screenings are sold separately and provides a pre-configured application for the screening using suitable extraction and cleanup techniques. This library is verified for use on AB SCIEX 3200 QTRAP<sup>®</sup>, 4000 QTRAP<sup>®</sup> and AB SCIEX QTRAP<sup>®</sup> 5500 LC/MS/MS Systems.

The MRM catalogue and spectral library contain information on the most common over 600 pesticides and their metabolites that need to be monitored in vegetables or other food products; over 1500 drugs of abuse and metabolites, over 160 veterinary antibiotics; and over 230 mycotoxins and metabolites. The MRM catalogue contains up to three transitions per compound. Each compound in the library has individual spectra acquired using three distinct collision energies (20 eV, 35 eV, 50 eV), as well as a single spectra representing the sum of all three collision

energies. A part of analytes have spectra acquired on multiple LC/MS/MS systems. If compounds ionize in both polarities, spectra for both are included, bringing the potential total number of spectra per compound to eight or more.

The MRM catalogue can be used to build methods without the need to re-infuse standards and optimize MRM transitions for a given compound. Screening and/or quantitation methods can be created for use with an MRM triggered EPI workflow, for use on QTRAP<sup>®</sup> instruments, or for traditional quantitation where the ratio of the response of two or more transitions is used for compound confirmation. The latter MRM approach can be performed on either an API triple quadrupole or a QTRAP<sup>®</sup> series instrument. Users simply need to select the compounds of interest as well as the number of transitions to be monitored from the MRM catalogue. Once selected, the Cliquid<sup>®</sup> Software automatically creates the acquisition and processing methods.

The following is a list of the 2430 pesticides currently in the library. Please note that this library is continuously being expanded to include additional compounds.

Compound	Formula	Formula Weight	CAS Number	# of Spectra
(-)-Trans-delta-9-THC carboxylic acid A	C22H30O4	358.2144	N/A	4
(6 $\alpha$ ,11 $\beta$ ,16 $\alpha$ ,17 $\beta$ )-6,9-difluoro-11,17-dihydroxy-16-methyl-3-oxoandrosta-1,4-diene-17-carboxylic acid	C21H26O5F2	396.1748	N/A	4
1-(3-chlorophenyl)piperazine	C10H13ClN2	196.0767	6640-24-0	4
1-(4-fluorophenyl)piperazine	C10H13FN2	180.1063	2252-63-3	4
1-(4-methoxyphenyl)piperazine	C11H16N2O	192.1263	38212-30-5	4
1-(4-trifluoromethylphenyl) piperazine	C11H13F3N2	230.1031	30459-17-7	4
1,4-androstadien-17 $\alpha$ -methyl-17 $\beta$ -ol-3-one	C20H28O2	300.2089	72-63-9	4
1,4-androstadien-17 $\alpha$ -methyl-6 $\beta$ ,17 $\beta$ -diol-3-one	C20H28O3	316.2038	N/A	4
1,4-androstadiene-3,17-dione	C19H24O2	284.1776	897-06-3	4
10-hydroxylated amitriptyline metabolite	C20H23NO	293.1780	64520-05-4	4
11-ketotestosterone	C19H26O3	302.1882	53187-98-7	4
11 $\alpha$ -hydroxymethyltestosterone	C20H30O3	318.2195	1807-02-9	4
15-Acetyl-deoxynivalenol	C17H22O7	338.1366	88337-96-6	4
15-Monoacetoxyscirpenol	C17H24O6	324.1573	2623-22-5	4
16-Ketoaspergillimide	C20H27N3O4	373.2002	199784-50-4	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
16 $\alpha$ -hydroxytestosterone	C19H28O3	304.2038	63-01-4	4
16 $\beta$ -hydroxystanozolol	C21H32N2O2	344.2464	N/A	4
17alpha-Hydroxyprogesterone	C21H30O3	330.2195	68-96-2	4
17-alpha-Methyltestosterone	C20H30O2	302.2246	58-18-4	4
17-epioxandrolone	C19H30O3	306.2195	26624-15-7	4
17 $\alpha$ -trenbolone acetate	C20H24O3	312.1725	49707-37-1	4
17 $\beta$ -carboxylic acid fluticasone propionate	C24H30O6F2	452.2010	65429-42-7	4
1-benzyl piperazine	C11H16N2	176.1313	860027-50-5	4
2-(1-hydroxyethyl)promazine	C19H24N2OS	328.1609	N/A	4
2,4-D	C8H6Cl2O3	219.9694	94-75-7	4
2,4-DB	C10H10Cl2O3	248.0007	94-82-6	4
2,6-dimethylaniline	C8H11N	121.0891	87-62-7	4
2-acetylphenothiazine	C14H11NOS	241.0561	6631-94-3	4
2-Amino-14,16-dimethyloctadecan-3-ol	C20H43ON	313.3345	540770-33-0	4
2-Amino-5-benzoylbenzimidazole	C14H11N3O	237.0902	52329-60-9	4
2-Amino-5-chlorobenzophenone	C13H10ClNO	231.0451	719-59-5	4
2-Amino-5-nitrobenzophenone	C13H10N2O3	242.0691	1775-95-7	8
2-Aminoflubendazole	C14H10FN3O	255.0808	82050-13-3	4
2-Benzyltetronic acid	C11H10O3	190.0630	3734-22-3	4
2-Hydroxyethylflurazepam	C17H14ClFN2O2	332.0728	20971-53-3	5
2-Hydroxymethyl-1-methyl-5-nitro-imidazol (HMMNI)	C5H7N3O3	157.0487	936-05-0	4
2-mercaptobenzimidazole	C7H6N2S	150.0252	583-39-1	4
2-Naphthoxyacetic acid	C12H10O3	202.0630	120-23-0	8
2-Nitrobenzaldehyde Semicarbazone	C8H8N4O3	208.0596	16004-43-6	4
2-Nitrobenzaldehyde Semicarbazone-15N2-C13	(13C 15N2) C7H8N2O3	211.0571	N/A	4
2-NP-AHD	C10H8N4O4	248.0546	623145-57-3	4
2-NP-AHD-13C3	13C3C7H8N4O4	251.0646	N/A	4
2-NP-AMAZ	C15H18N4O5	334.1277	183193-59-1	4
2-NP-AMAZ-D5	C15D5H13N4O5	339.1591		4
2-NP-AOZ	C10H9N3O4	235.0593	19687-73-1	4
2-NP-AOZ-D4	C10H5D4N3O4	239.0844		4
2-quinolinecarboxylic acid	C9H6N2O2	174.0429	879-65-2	4
3,4,5-Trimethacarb	C11H15NO2	193.1103	2686-99-9	9
3,4-Dimethoxyphenethylamine	C10H15NO2	181.1103	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	193.1103	42542-10-9	4
3,5-Diiodotyrosine	C9H9I2NO3	432.8672	66-02-4	4
3-Acetyl-deoxynivalenol	C17H22O7	338.1366	50722-38-8	8

Compound	Formula	Formula Weight	CAS Number	# of Spectra
3-Hydroxybromazepam	C14H10BrN3O2	330.9956	13132-73-5	4
3-Hydroxycarbofuran	C12H15NO4	237.1001	16655-82-6	8
3-hydroxydetomidine	C12H14N2O	202.1106	N/A	4
3-hydroxylicocaine	C14H22N2O2	250.1681	34604-55-2	4
3'-hydroxystanozolol	C21H32N2O2	344.2464	125709-39-9	4
3-Keto-carbofuran	C12H13NO4	235.0845	16709-30-1	8
3-Methylfentanyl	C23H30N2O	350.2358	42045-86-3	4
3-O-Methylviridicatin	C16H13NO2	251.0946	6152-51-4	4
4-androstene-3,17-dione	C19H26O2	286.1933	63-05-8	4
4-Benzamidosalicylic acid	C14H11NO4	257.0688	13898-58-3	8
4-chlorotestosterone	C19H27O2Cl	322.1700	1093-58-9	4
4-CPA	C8H7ClO3	186.0084	122-88-3	4
4-dimethylaminoantipyrine	C13H17N3O	231.1372	58-15-1	4
4-hydroxypropranolol	C16H21NO3	275.1521	10476-53-6	4
4-Methylumbelliferyl acetate	C12H10O4	218.0579	2747-05-9	4
4-pregnen-20 $\alpha$ -ol-3-one	C21H32O2	316.2402	145-14-2	4
5-(p-Methylphenyl)-phenylhydantoin	C16H14N2O2	266.1055	51169-17-6	4
5-Aminosalicylic acid	C7H7NO3	153.0426	89-57-6	4
5-Hydroxy-clethodim-sulfone	C17H26ClNO6S	407.1169	not available	8
5-Hydroxy-Clethodim-sulfone (-)	C17H26ClNO6S	407.1169	not available	4
5-Hydroxy-imidacloprid	C9H10ClN5O3	271.0472	not available	8
5-Hydroxy-thiabendazol	C10H7N3OS	217.0310	948-71-0	8
5-methoxy-N,N-dimethyltryptamine	C13H18N2O	218.1419	1019-45-0	4
6-Chlor-3-phenyl-pyridazin-4-ol	C10H7ClN2O	206.0247	40020-01-7	10
6-Chlorothymolsulfonic acid	C10H13ClO4S	264.0223	83732-70-1	4
6-dehydrotestosterone	C19H26O2	286.1933	2484-30-2	4
6-Mercaptourine	C5H4N4S	152.0157	50-44-2	8
6-naloxol	C19H23NO4	329.1627	20410-95-1	4
6-O-Monoacetylmorphine	C19H21NO4	327.1471	2784-73-8	6
6-phenyl-2-thiouracil	C10H8N2OS	204.0357	36822-11-4	4
6 $\beta$ ,17 $\alpha$ -hydroxyboldenone	C19H26O3	302.1882	N/A	4
6 $\beta$ -hydroxyfluoxymesterone	C20H29O4F	352.2050	88936-08-7	4
6 $\beta$ -hydroxytestosterone	C19H28O3	304.2038	62-99-7	4
6 $\beta$ -naloxol-3 $\beta$ -glucuronide	C25H31NO10	505.1948	24326-39-4	4
6 $\beta$ -naltrexol	C20H25NO4	343.1784	49625-89-0	4
7-Aminoclonazepam	C15H12ClN3O	285.0669	4959-17-5	4
7-Aminodesmethylflunitrazepam	C15H12FN3O	269.0964	894-76-8	4
7-Aminoflunitrazepam	C16H14FN3O	283.1121	34084-50-9	4
7-Aminonitrazepam	C15H13N3O	251.1059	4928-02-3	4
8-Chlorotheophylline	C7H7ClN4O2	214.0258	85-18-7	8

Compound	Formula	Formula Weight	CAS Number	# of Spectra
8-Hydroxyquinoline	C9H7NO	145.0528	148-24-3	4
9-Hydroxyrisperidone	C23H27FN4O3	426.2067	144598-75-4	4
9 $\alpha$ -Fluoro-17,17-dimethyl-18-norandrosta-4,13-diene-11 $\beta$ -ol-3-one	C20H27O2F	318.1995	N/A	4
9 $\alpha$ -fluoroprednisolone	C21H27FO5	378.1843	N/A	4
A23187	C29H37N3O6	523.2682	52665-69-7	8
AAL-TA1 Toxin	C25H47NO10	521.3200	79367-52-5	4
Acebutolol	C18H28N2O4	336.2049	37517-30-9	4
Acecarbromal	C9H15BrN2O3	278.0266	77-66-7	8
Aceclidine	C9H15NO2	169.1103	827-61-2	4
Aceclofenac	C16H13Cl2NO4	353.0222	89796-99-6	8
Acemetacin	C21H18ClNO6	415.0823	53164-05-9	4
Acenocoumarol	C19H15NO6	353.0899	152-72-7	8
Acephate	C4H10NO3PS	183.0119	30560-19-1	12
Acepromazine	C19H22N2OS	326.1453	61-00-7	4
Aceprometazine	C19H22N2OS	326.1453	13461-01-3	5
Acequinocyl	C24H32O4	384.2301	57960-19-7	4
Acetaminodantrolene	C16H14N4O4	326.1015	41515-09-7	4
Acetaminophen	C8H9NO2	151.0633	103-90-2	4
Acetamidrid	C10H11ClN4	222.0672	135410-20-7	8
acetanilide	C8H9NO	135.0684	103-84-4	4
Acetazolamide	C4H6N4O3S2	221.9881	59-66-5	4
Acetiamin	C16H22N4O4S	366.1362	28008-04-0	4
Acetochlor	C14H20ClNO2	269.1183	34256-82-1	14
acetoexamide	C15H20N2O4S	324.1144	968-81-0	4
Acetylaminonitroprophoxybenzene	C11H14N2O4	238.0954	553-20-8	8
Acetylsalicylamid	C9H9NO3	179.0582	487-48-9	8
Acetylsalicylic Acid	C9H8O4	180.0423	50-78-2	4
Acibenzolar-S-methyl	C8H6N2OS2	209.9922	135158-54-2	8
Aciclovir	C8H11N5O3	225.0862	59277-89-3	9
Acifluorfen	C14H7ClF3NO5	360.9965	50594-66-6	4
Acipimox	C6H6N2O3	154.0378	51037-30-0	4
Aclonifen	C12H9ClN2O3	264.0302	74070-46-5	12
Acrinathrin	C26H21F6NO5	541.1324	101007-06-1	4
Acrivastine	C22H24N2O2	348.1838	87848-99-5	4
Actinomycin D	C62H86N12O16	1254.6285	50-76-0	4
Actinoquinol	C11H11NO4S	253.0409	15301-40-3	8
Adefovir	C8H12N5O4P	273.0627	106941-25-7	4
Adenine	C5H5N5	135.0545	73-24-5	8
Adenosine	C10H13N5O4	267.0968	58-61-7	8

Compound	Formula	Formula Weight	CAS Number	# of Spectra
adiphenine	C20H25NO2	311.1885	64-95-9	4
Adrenalone	C9H11NO3	181.0739	99-45-6	8
Aflatoxin B1	C17H12O6	312.0634	1162-65-8	4
Aflatoxin B2	C17H14O6	314.0790	7220-81-7	4
Aflatoxin G1	C17H12O7	328.0583	1165-39-5	4
Aflatoxin G2	C17H14O7	330.0740	7241-98-7	4
Aflatoxin M1	C17H12O7	328.0583	6795-23-9	4
Aflatoxin M2	C17H14O7	330.0740	6885-57-0	4
Agroclavine	C16H18N2	238.1470	548-42-5	4
Ajmaline	C20H26N2O2	326.1994	4360-12-7	4
Alachlor	C14H20ClNO2	269.1183	15972-60-8	11
Alamethicin F30	C92H150N22O25	1963.1142	27061-78-5	4
Alanycarb	C17H25N3O4S2	399.1287	83130-01-2	8
Albendazole	C12H15N3O2S	265.0885	54965-21-8	4
Albendazole Sulfone	C12H15N3O4S	297.0783	76567-28-7	4
Albendazole Sulfoxide	C12H15N3O3S	281.0834	54029-12-8	4
Albendazole-2-aminosulfone	C10H13N3O2S	239.0728	80983-34-2	4
alclofenac	C11H11O3Cl	226.0397	22131-79-9	3
Alclometasone-17,21-dipropionate	C28H37ClO7	520.2228	66734-13-2	4
Alcuronium	C44H50N4O2	666.3934	23214-96-2	4
Aldicarb	C7H14N2O2S	190.0776	116-06-3	12
Aldicarb-sulfoxide	C7H14N2O3S	206.0725	1646-87-3	12
Aldoxycarb	C7H14N2O4S	222.0674	1646-88-4	12
alfadolone acetate	C23H34O5	390.2406	23930-37-2	4
Alfuzosine	C19H27N5O4	389.2063	81403-80-7	8
Alimemazine	C18H22N2S	298.1504	84-96-8	4
Alizapride	C16H21N5O2	315.1695	59338-93-1	8
Allopurinol	C5H4N4O	136.0385	315-30-0	9
Alloxydim	C17H25NO5	323.1733	55634-91-8	11
Almitrine	C26H29F2N7	477.2453	27469-53-0	4
alpha-Ethyl-1,3-benzodioxole-5-ethanamine	C11H15NO2	193.1103	107447-03-0	4
alpha-Hydroxyalprazolam	C17H13ClN4O	324.0778	37115-43-8	4
alpha-Hydroxymidazolam	C18H13ClFN3O	341.0731	59468-90-5	5
alpha-Hydroxytriazolam	C17H12Cl2N4O	358.0388	37115-45-0	8
alphaprodine	C16H23NO2	261.1729	77-20-3	4
alpha-Zearalenol	C18H24O5	320.1624	36455-72-8	8
alpha-Zearalenol-4-O-glucoside	C24H34O10	482.2152	135626-94-7	8
Alprazolam	C17H13ClN4	308.0829	28981-97-7	4
Alprenolol	C15H23NO2	249.1729	13655-52-2	4
Alprostadiil	C20H34O5	354.2406	745-65-3	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Altenuene	C15H16O6	292.0947	29752-43-0	8
Altenusin	C15H14O6	290.0790	31186-12-6	8
Alternariol	C14H10O5	258.0528	641-38-3	8
Alternariolmethylether	C15H12O5	272.0685	26894-49-5	8
Altersolanol	C16H16O7	320.0896	22268-16-2	8
Altertoxin-I	C20H16O6	352.0947	56258-32-3	4
althiazide	C11H14N3O4S3Cl	382.9835	5588-16-9	8
altrenogest	C21H26O2	310.1933	850-52-2	4
Altretamine	C9H18N6	210.1593	645-05-6	4
alverine	C20H27N	281.2144	150-59-4	4
Alypin	C16H26N2O2	278.1994	963-07-5	4
Amantadine	C10H17N	151.1361	768-94-5	4
Ambenonium	C28H42Cl2N4O2	536.2685	115-79-7	4
Ambroxol	C13H18Br2N2O	375.9786	18683-91-5	4
Ambucetamide	C17H28N2O2	292.2151	519-88-0	4
ambutonium	C20H27N2O	311.2123	14007-49-9	4
Amcinonide	C28H35FO7	502.2367	51022-69-6	4
Ametryn	C9H17N5S	227.1205	834-12-8	15
Amezinium	C11H12N3O	202.0980	30578-37-1	4
Amicarbazone	C10H19N5O2	241.1539	129909-90-6	8
Amidosulfuron	C9H15N5O7S2	369.0413	120923-37-7	8
Amidotrizoic Acid	C11H9I3N2O4	613.7697	117-96-4	4
Amiloride	C6H8ClN7O	229.0479	2609-46-3	4
aminacrine	C13H10N2	194.0844	90-45-9	4
amineptine	C22H27NO2	337.2042	57574-09-1	4
Aminocarb	C11H16N2O2	208.1212	2032-59-9	8
Aminodantrolene	C14H12N4O3	284.0909	14663-28-6	4
Aminoglutethimide	C13H16N2O2	232.1212	125-84-8	4
Aminophenazone	C13H17N3O	231.1372	58-15-1	8
Aminopromazine	C19H25N3S	327.1769	58-37-7	4
aminopterin	C19H20N8O5	440.1557	54-62-6	4
Aminopyralid	C6H4Cl2N2O2	205.9650	150114-71-9	8
Aminoquinuride	C21H20N6O	372.1699	3811-56-1	4
Aminorex	C9H10N2O	162.0793	2207-50-3	4
Amiodarone	C25H29I2NO3	645.0237	1951-25-3	7
Amiphenazole	C9H9N3S	191.0517	490-55-1	4
amisometradine	C9H13N3O2	195.1008	550-28-7	4
Amisulpride	C17H27N3O4S	369.1722	71675-85-9	4
Amitraz	C19H23N3	293.1892	33089-61-1	8
Amitriptylin	C20H23N	277.1830	50-48-6	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Amitriptylinoxide	C20H23NO	293.1780	4317-14-0	4
Amitrole	C2H4N4	84.0436	61-82-5	7
Amlodipine	C20H25CIN2O5	408.1452	88150-42-9	4
Ammoidin	C12H8O4	216.0423	298-81-7	4
Amobarbital	C11H18N2O3	226.1317	57-43-2	4
amodiaquine	C20H22N3OCl	355.1451	86-42-0	4
amopyroquine	C20H20N3OCl	353.1295	550-81-2	4
Amorolfine	C21H35NO	317.2719	78613-35-1	4
Amoxapine	C17H16CIN3O	313.0982	14028-44-5	4
Amoxicillin	C16H19N3O5S	365.1045	26787-78-0	16
AMPA (Aminomethyl phosphonic acid)	CH6O3PN	111.0085	1066-51-9	4
Amphetamine	C9H13N	135.1048	300-62-9	4
Amphotericin B	C47H73NO17	923.4879	1397-89-3	4
Ampicillin	C16H19N3O4S	349.1096	69-53-4	16
Amprolium	C14H19CIN4	278.1298	121-25-5	8
Amrinone	C10H9N3O	187.0746	60719-84-8	4
amylocaine	C14H21NO2	235.1572	644-26-8	4
anastrozole	C17H19N5	293.1640	120511-73-1	4
Anilazine	C9H5Cl3N4	273.9580	101-05-3	12
Anilofos	C13H19CINO3PS2	367.0233	64249-01-0	8
Anisomycin	C14H19NO4	265.1314	22862-76-6	4
Antazoline	C17H19N3	265.1579	91-75-8	4
Apalcillin	C25H23N5O6S	521.1369	63469-19-2	8
Apicidin	C34H49N5O6	623.3683	183506-66-3	8
apocodeine	C18H19NO2	281.1416	641-36-1	4
Apomorphine	C17H17NO2	267.1259	58-00-4	4
Apophedrin	C8H11NO	137.0841	7568-93-6	4
Apraclonidin	C9H10Cl2N4	244.0283	66711-21-5	4
Aprinidine	C22H30N2	322.2409	37640-71-4	4
Aprinocid	C12H9ClFN5	277.0531	55779-18-5	4
apronalide	C9H16N2O2	184.1212	528-92-7	4
Aramite	C15H23ClO4S	334.1006	140-57-8	11
Arecoline	C8H13NO2	155.0946	63-75-2	4
Aripiprazole	C23H27Cl2N3O2	447.1480	129722-12-9	8
arterenol	C8H11NO3	169.0739	51-41-2	4
Ascomycin	C43H69NO12	791.4820	104987-12-4	4
Aspercolorin	C25H28N4O5	464.2060	29123-52-2	8
Aspergillimide	C20H29N3O3	359.2209	195966-93-9	4
Asperlactone	C9H12O4	184.0736	76375-62-7	4
Asperloxine A	C21H19N3O5	393.1325	223130-52-7	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Aspinonene	C9H16O4	188.1049	157676-96-5	4
Aspon	C12H28O5P2S2	378.0853	3244-90-4	8
Aspyrone	C9H12O4	184.0736	17398-00-4	4
Astemizole	C28H31FN4O	458.2482	68844-77-9	4
Asterric acid	C17H16O8	348.0845	577-64-0	8
Asulam	C8H10N2O4S	230.0361	3337-71-1	4
Atenolol	C14H22N2O3	266.1630	29122-68-7	4
atipamezole	C14H16N2	212.1313	104054-27-5	4
atomoxetine	C17H21NO	255.1623	83015-26-3	4
Atorvastatin	C33H35FN2O5	558.2530	134523-00-5	8
Atpenin A5	C15H21Cl2NO5	365.0797	119509-24-9	8
Atraton	C9H17N5O	211.1433	1610-17-9	4
Atrazine	C8H14ClN5	215.0938	1912-24-9	12
Atrazine-2-hydroxy	C8H15N5O	197.1277	2163-68-0	8
Atrazine-desethyl	C6H10ClN5	187.0625	6190-65-4	12
Atrazine-desethyl-2-hydroxy	C6H11ON5	169.0964	6190-65-4	8
Atrazine-desisopropyl	C5H8N5Cl	173.0468	1007-28-9	8
Atropine	C17H23NO3	289.1678	51-55-8	4
Atropinmethylobromid	C18H26NO3	304.1913	2870-71-5	4
Atropin-N-octylbromide	C25H40NO3	402.3008	5843-82-3	4
Aureobasidin A	C60H92N8O11	1100.6886	127757-30-6	4
Aurofusarin	C30H18O12	570.0798	13191-64-5	8
Austdiol	C12H12O5	236.0685	53043-28-0	8
Austocystin A	C19H13ClO6	372.0401	55256-58-1	4
Avenacein Y	C15H10O8	318.0376	102426-44-8	4
Avermectin B1a	C48H72O14	872.4922	65195-55-3	4
Axeen	C10H14N2O4	226.0954	2537-29-3	4
Azaconazole	C12H11Cl2N3O2	299.0228	60207-31-0	8
azacyclonol	C18H21NO	267.1623	115-46-8	4
Azamethiophos	C9H10ClN2O5PS	323.9737	35575-96-3	8
azaperol	C19H24FN3O	329.1903	2804-05-9	4
azaperone	C19H22N3OF	327.1747	1649-18-9	4
azapetine	C17H17N	235.1361	146-36-1	4
Azapropazone	C16H20N4O2	300.1586	13539-59-8	8
Azatadine	C20H22N2	290.1783	3964-81-6	4
Azathioprine	C9H7N7O2S	277.0382	446-86-6	8
Azelaic Acid	C9H16O4	188.1049	123-99-9	4
Azelastine	C22H24ClN3O	381.1608	58581-89-8	4
Azidamphenicol	C11H13N5O5	295.0917	13838-08-9	4
Azidocillin	C16H17N5O4S	375.1001	17243-38-8	8



Compound	Formula	Formula Weight	CAS Number	# of Spectra
Azimsulfuron	C13H16N10O5S	424.1026	120162-55-2	8
Azinphos-ethyl	C12H16N3O3PS2	345.0371	2642-71-9	8
Azinphos-methyl	C10H12N3O3PS2	317.0058	86-50-0	12
Azintamid	C10H14CIN3OS	259.0546	1830-32-6	4
Aziprotryne	C7H11N7S	225.0797	4658-28-0	4
Azithromycin	C38H72N2O12	748.5085	83905-01-5	4
Azoluron	C12H14N4O	230.1168	4058-90-6	4
Azosemide	C12H11CIN6O2S2	370.0073	27589-33-9	4
Azoxystrobin	C22H17N3O5	403.1168	131860-33-8	10
Aztreonam	C13H17N5O8S2	435.0519	78110-38-0	9
Bacampicillin	C21H27N3O7S	465.1570	50972-17-3	4
Bacitracin	C66H103N17O16S	1421.7489	22601-59-8	8
Baclofen	C10H12CINO2	213.0557	1134-47-0	4
Bafilomycin A1	C35H58O9	622.4081	88899-55-2	4
Bambuterol	C18H29N3O5	367.2107	81732-65-2	4
Bamethan	C12H19NO2	209.1416	3703-79-5	4
Bamifylline	C20H27N5O3	385.2114	2016-63-9	4
Bamipin	C19H24N2	280.1939	4945-47-5	4
Barbital	C8H12N2O3	184.0848	57-44-3	3
Barverin	C29H43N5O3	509.3366	1639-79-8	4
Beauvericin	C45H57N3O9	783.4095	26048-05-5	4
Beclamide	C10H12CINO	197.0607	501-68-8	4
Beclometasone dipropionate	C28H37CIO7	520.2228	5534-09-8	5
beclomethasone	C22H29CIO5	408.1704	4419-39-0	4
beclomethasone-17-propionate	C25H33O6Cl	464.1966	5534-18-9	8
Beflubutamid	C18H17F4NO2	355.1195	113614-08-7	12
Befunolol	C16H21NO4	291.1471	39552-01-7	4
Bemetizide	C15H16CIN3O4S2	401.0271	1824-52-8	4
Benactyzine	C20H25NO3	327.1834	302-40-9	4
Benalaxyl	C20H23NO3	325.1678	71626-11-4	9
benazepril	C24H28N2O5	424.1998	86541-75-5	4
Benazolin	C9H6CINO3S	242.9757	3813-05-6	16
Benazolin-ethyl	C11H10CINO3S	271.0070	25059-80-7	4
Bendamustine	C16H21Cl2N3O2	357.1011	16506-27-7	4
Bendiocarb	C11H13NO4	223.0845	22781-23-3	12
Bendroflumethiazide	C15H14F3N3O4S2	421.0378	73-48-3	4
Benfluorex	C19H20F3NO2	351.1446	23602-78-0	4
Benfotiamin	C19H23N4O6PS	466.1076	22457-89-2	8
Benfuracarb	C20H30N2O5S	410.1875	82560-54-1	12
Benfuresate	C12H16O4S	256.0769	68505-69-1	8

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Benodanil	C13H10INO	322.9807	15310-01-7	4
Benomyl	C14H18N4O3	290.1379	17804-35-2	12
Benorilate	C17H15NO5	313.0950	5003-48-5	4
Benoxacor	C11H11Cl2NO2	259.0167	98730-04-2	8
benoxaprofen	C16H12NO3Cl	301.0506	51234-28-7	4
Benperidole	C22H24FN3O2	381.1853	2062-84-2	4
Benproperine	C21H27NO	309.2093	2156-27-6	4
Benserazid	C10H15N3O5	257.1012	322-35-0	8
Bensulfuron-methyl	C16H18N4O7S	410.0896	83055-99-6	8
Bensulide	C14H24NO4PS3	397.0605	741-58-2	8
Bensultap	C17H21NO4S4	431.0353	17606-31-4	8
Bentazone	C10H12N2O3S	240.0569	25057-89-0	4
Benthiavalicarb-isopropyl	C18H24FN3O3S	381.1522	177406-68-7	8
Bentiromide	C23H20N2O5	404.1372	37106-97-1	8
Benzatropine	C21H25NO	307.1936	86-13-5	4
Benzethonium	C27H42NO2	412.3216	121-54-0	4
benzilonium	C22H28NO3	354.2069	1050-48-2	4
Benzocaine	C9H11NO2	165.0790	94-09-7	4
Benzoctamine	C18H19N	249.1517	17243-39-9	4
Benzododecinium	C21H38N	304.3004	139-07-1	4
Benzoximate	C18H18ClNO5	363.0874	29104-30-1	8
Benzoxonium	C23H42NO2	364.3216	19379-90-9	4
Benzoyllecgonine	C16H19NO4	289.1314	519-09-5	4
benzphetamine	C17H21N	239.1674	156-08-1	4
Benzquinamide	C22H32N2O5	404.2311	63-12-7	4
Benzthiazide	C15H14ClN3O4S3	430.9835	91-33-8	8
Benzthiazuron	C9H9N3OS	207.0466	1929-88-0	4
benztropine	C21H25NO	307.1936	86-13-5	4
Benzylamine	C19H23N3O	309.1841	642-72-8	4
Benzylpenicillin	C16H18N2O4S	334.0987	61-33-6	4
Benzyltetroneic acid	C11H10O3	190.0630	3734-22-3	8
Berberine	C20H18NO4	336.1236	2086-83-1	9
beta-Ergocryptine	C32H41N5O5	575.3108	511-09-1	4
beta-Ergocryptinine	C32H41N5O5	575.3108	511-10-4	4
Betaine	C5H11NO2	117.0790	107-43-7	4
Betamethasone	C22H29FO5	392.1999	378-44-9	4
Betamethasone 17-valerate	C27H37FO6	476.2574	2152-44-5	4
Betamethasone 21-phosphate	C22H30FO8P	472.1662	360-63-4	8
Betamethasone-17-benzoate	C29H33FO6	496.2261	22298-29-9	4
Betaxolol	C18H29NO3	307.2147	63659-18-7	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
beta-Zearalenol	C18H24O5	320.1624	71030-11-0	8
beta-Zearalenol-4-O-glucoside	C24H34O10	482.2152	135626-93-6	8
Bethanidine	C10H15N3	177.1266	55-73-2	4
Bevonium	C22H28NO3	354.2069	5205-82-3	4
Bezafibrate	C19H20ClNO4	361.1081	41859-67-0	8
Beziramide	C31H32HN4O2	493.2604	15301-48-1	4
bibenzonium	C19H26NO	284.2014	59866-76-1	4
Bicalutamide	C18H14F4N2O4S	430.0610	90357-06-5	4
Bidesmethylicalopram	C18H17N2OF	296.1325	N/A	4
Bietamiverine	C19H30N2O2	318.2307	479-81-2	4
Bifenazate	C17H20N2O3	300.1474	149877-41-8	8
Bifenox	C14H9Cl2NO5	340.9858	42576-02-3	11
Bifenthrin	C23H22ClF3O2	422.1260	82657-04-3	8
Bifonazole	C22H18N2	310.1470	60628-96-8	4
Bioallethrin	C19H26O3	302.1882	84030-86-4	13
Bioresmethrin	C22H26O3	338.1882	28434-01-7	12
Biotin	C10H16N2O3S	244.0882	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	337.1790	55179-31-2	13
bitolterol	C28H31NO5	461.2202	30392-40-6	4
bolasterone	C21H32O2	316.2402	1605-89-6	4
boldenone	C19H26O2	286.1933	846-48-0	4
Bopindolol	C23H28N2O3	380.2100	62658-63-3	4
Bornaprine	C21H31NO2	329.2355	20448-86-6	4
Boscalid	C18H12Cl2N2O	342.0327	188425-85-6	8
Bosentan	C27H29N5O6S	551.1839	147536-97-8	8
Brallobarbitol	C10H11BrN2O3	285.9953	561-86-4	4
Brefeldin A	C16H24O4	280.1675	20350-15-6	4
Brevicompanine B	C22H29N3O2	367.2260	215121-47-4	4
Brilliant green	C27H33N2	385.2644	633-03-4 (C.I. 42040)	4
Brimonidine	C11H10BrN5	291.0120	59803-98-4	4
Brivudine	C11H13BrN2O5	332.0008	69304-47-8	4
Brodifacoum	C31H23BrO3	522.0831	56073-10-0	16
Bromacil	C9H13BrN2O2	260.0160	314-40-9	21
Bromadiolone	C30H23BrO4	526.0780	28772-56-7	4
bromantan	C16H20NBr	305.0779	87913-26-6	4
Bromazepam	C14H10BrN3O	315.0007	1812-30-2	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Bromazine	C17H20BrNO	333.0728	118-23-0	4
Bromchlorophen	C13H8Br2Cl2O2	423.8268	15435-29-7	4
Bromhexine	C14H20Br2N2	375.9973	3572-43-8	4
bromisoval	C6H11N2O2Br	222.0004	496-67-3	4
Bromocriptine	C32H40BrN5O5	653.2213	25614-03-3	4
Bromophos	C8H8BrCl2O3PS	363.8492	2104-96-3	8
Bromophos-ethyl	C10H12BrCl2O3PS	391.8805	4824-78-6	4
Bromopride	C14H22BrN3O2	343.0895	4093-35-0	4
Bromoxynil	C7H3Br2NO	274.8581	1689-84-5	4
Bromperidol	C21H23BrFNO2	419.0896	10457-90-6	4
Brompheniramine	C16H19BrN2	318.0732	86-22-6	4
Bromuconazole	C13H12BrCl2N3O	374.9541	116255-48-2	8
Bromural	C6H11BrN2O2	222.0004	496-67-3	4
Bromurone	C9H11BrN2O	242.0055	3408-97-7	4
Brotizolam	C15H10BrClN4S	391.9498	57801-81-7	4
Brucine	C23H26N2O4	394.1893	357-57-3	4
Bucetin	C12H17NO3	223.1208	1083-57-4	8
buclizine	C28H33N2Cl	432.2332	82-95-1	4
Buclosamide	C11H14ClNO2	227.0713	575-74-6	8
Budesonide	C25H34O6	430.2355	51333-22-3	8
Budipine	C21H27N	293.2144	57982-78-2	4
Bufexamac	C12H17NO3	223.1208	2438-72-4	9
Bufloamedil	C17H25NO4	307.1784	55837-25-7	4
Bulbocapnin	C19H19NO4	325.1314	298-45-3	4
Bumadizone	C19H22N2O3	326.1630	3583-64-0	4
Bumetanide	C17H20N2O5S	364.1093	28395-03-1	4
Bunazosin	C19H27N5O3	373.2114	80755-51-7	4
Bunitrolol	C14H20N2O2	248.1525	34915-68-9	4
bunolol	C17H25NO3	291.1834	47141-42-4	4
Buphenine	C19H25NO2	299.1885	447-41-6	4
Bupirimate	C13H24N4O3S	316.1569	41483-43-6	8
Bupivacaine	C18H28N2O	288.2202	2180-92-9	4
Bupranolol	C14H22ClNO2	271.1339	14556-46-8	4
Buprenorphine	C29H41NO4	467.3036	52485-79-7	4
buprenorphine-3 $\beta$ -glucuronide	C35H49NO10	643.3356	N/A	4
Buprenorphine-D4	C29H37D4NO4	471.3287	136781-89-0	4
Buprofezin	C16H23N3OS	305.1562	69327-76-0	15
Bupropion	C13H18NOCl	239.1077	34841-39-9	8
Buspiron	C21H31N5O2	385.2478	36505-84-7	4
butacaine	C18H30N2O2	306.2307	149-16-6	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Butafenacil	C20H18ClF3N2O6	474.0805	134605-64-4	8
Butalamine	C18H28N4O	316.2263	22131-35-7	4
Butalbital	C11H16N2O3	224.1161	77-26-9	4
Butallylonal	C11H15BrN2O3	302.0266	1142-70-7	4
Butamirate	C18H29NO3	307.2147	18109-80-3	4
Butanilicain	C13H19ClN2O	254.1186	3785-21-5	4
Butaperazine	C24H31N3OS	409.2188	653-03-2	4
Butetamate	C16H25NO2	263.1885	14007-64-8	4
buthiazide	C11H16N3O4S2Cl	353.0271	2043-38-1	4
Butinoline	C20H21NO	291.1623	968-63-8	4
Butizide	C11H16ClN3O4S2	353.0271	2043-38-1	4
Butocarboxim-sulfoxide	C7H14N2O3S	206.0725	34681-24-8	12
butofilolol	C17H26FNO3	311.1897	58930-32-8	4
Butorphanol	C21H29NO2	327.2198	42408-82-2	8
Butoxycaine	C17H27NO3	293.1991	3772-43-8	4
Butoxycarboxim	C7H14N2O4S	222.0674	34681-23-7	9
Butralin	C14H21N3O4	295.1532	33629-47-9	10
Buturon	C12H13ClN2O	236.0716	3766-60-7	12
Butylate	C11H23NOS	217.1500	2008-41-5	8
Cabaril	C13H14N2O	214.1106	63-25-2	4
Cabergoline	C26H37N5O2	451.2947	81409-90-7	4
Cabral	C13H14N2O	214.1106	553-69-5	4
Cadusafos	C10H23O2PS2	270.0877	95465-99-9	8
Cafaminol	C11H17N5O3	267.1331	30924-31-3	4
Caffeine	C8H10N4O2	194.0804	58-08-2	4
Calphostin C	C44H38O14	790.2262	121263-19-2	8
Calteridol	C17H32N4O7	404.2271	121915-83-1	4
Cambendazole	C14H14N4O2S	302.0837	26097-80-3	4
Camyloline	C19H32N2O2	320.2464	54-30-8	4
Candesartan	C24H20N6O3	440.1597	139481-59-7	4
Canrenoic Acid	C22H30O4	358.2144	4138-96-9	8
canrenone	C22H28O3	340.2038	976-71-6	4
Capecitabine	C15H22FN3O6	359.1493	154361-50-9	8
Caproylresorcinol	C12H16O3	208.1099	70807-24-8	8
Captodiame	C21H29NS2	359.1741	486-17-9	4
Captopril	C9H15NO3S	217.0773	62571-86-2	8
caramiphen	C18H27NO2	289.2042	125-85-9	4
Carazolol	C18H22N2O2	298.1681	57775-29-8	4
Carbachol	C6H15N2O2	147.1134	51-83-2	4
Carbadox	C11H10N4O4	262.0702	6804-07-5	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Carbamazepine	C15H12N2O	236.0950	298-46-4	4
Carbamazepine 10,11-epoxide	C15H12N2O2	252.0899	36507-30-9	4
Carbaril	C12H11NO2	201.0790	63-25-2	4
Carbaryl	C12H11NO2	201.0790	63-25-2	8
Carbazochrom	C10H12N4O3	236.0909	69-81-8	4
Carbendazim	C9H9N3O2	191.0695	10605-21-7	12
Carbenoxolone	C34H50O7	570.3557	5697-56-3	8
Carbetamide	C12H16N2O3	236.1161	16118-49-3	8
Carbimazole	C7H10N2O2S	186.0463	22232-54-8	4
Carbinoxamine	C16H19CIN2O	290.1186	486-16-8	4
Carbofuran	C12H15NO3	221.1052	1563-66-2	8
Carbosulfan	C20H32N2O3S	380.2134	55285-14-8	11
Carboxin	C12H13NO2S	235.0667	5234-68-4	12
carbromal	C7H13BrN2O2	236.0160	77-65-6	4
Carbutamide	C11H17N3O3S	271.0991	339-43-5	8
Carbuterol	C13H21N3O3	267.1583	34866-47-2	4
carfentanil	C24H30N2O3	394.2256	59708-52-0	4
Carfentrazone-ethyl	C15H14Cl2F3N3O3	411.0364	128639-02-1	8
Carisoprodol	C12H24N2O4	260.1736	78-44-4	5
carphedone	C12H14N2O2	218.1055	77472-70-9	4
Carprofen	C15H12CINO2	273.0557	53716-49-7	8
Carpropamid	C15H18Cl3NO	333.0454	104030-54-8	13
Cartap	C7H15N3O2S2	237.0606	15263-52-2	4
Carteolol	C16H24N2O3	292.1787	51781-06-7	4
Carticain	C13H20N2O3S	284.1195	23964-58-1	4
Carvedilol	C24H26N2O4	406.1893	72956-09-3	4
Cefaclor	C15H14ClN3O4S	367.0394	70356-03-5	4
Cefadroxil	C16H17N3O5S	363.0889	53994-73-3	4
Cefalexin	C16H17N3O4S	347.0940	15686-71-2	4
Cefamandole	C18H18N6O5S2	462.0780	34444-01-4	4
Cefapirin	C17H17N3O6S2	423.0559	21593-23-7	4
Cefazedone	C18H15Cl2N5O5S3	546.9612	56187-47-4	4
Cefazolin	C14H14N8O4S3	454.0300	27164-46-1	4
Cefepime	C19H24N6O5S2	480.1250	88040-23-7	4
Cefetamet	C14H15N5O5S2	397.0515	65052-63-3	4
Cefixime	C16H15N5O7S2	453.0413	79350-37-1	4
Cefmenoxime	C16H17N9O5S3	511.0515	65085-01-0	8
Cefodizime	C20H20N6O7S4	584.0276	69739-16-8	4
Cefoperazone	C25H27N9O8S2	645.1424	62893-20-3	4
Cefotaxime	C16H17N5O7S2	455.0569	63527-52-6	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Cefotiam	C18H23N9O4S3	525.1035	61622-34-2	4
Cefpirome	C22H22N6O5S2	514.1093	84957-29-9	4
Ceftazidime	C22H22N6O7S2	546.0991	72558-82-8	4
Ceftiofur	C19H17N5O7S3	523.0290	80370-57-6	4
Ceftizoxime	C13H13N5O5S2	383.0358	68401-81-0	4
Ceftriaxone	C18H18N8O7S3	554.0461	73384-59-5	4
Cefuroxime	C16H16N4O8S	424.0689	55268-75-2	4
Celiprolol	C20H33N3O4	379.2471	56980-93-6	4
Cephalosporin C	C16H21N3O8S	415.1049	61-24-5	4
Cerivastatin	C26H34FNO5	459.2421	145599-86-6	4
Cerulenin	C12H17NO3	223.1208	17397-89-6	4
cetalkonium	C25H46N	360.3630	122-18-9	4
Cetirizine	C21H25ClN2O3	388.1554	83881-52-1	4
Cetobemidone	C15H21NO2	247.1572	469-79-4	8
Chaetocin	C30H28N6O6S4	696.0953	28097-03-2	8
Chaetoglobosin A	C32H36N2O5	528.2624	50335-03-0	4
Chanoclavine	C16H20N2O	256.1576	2390-99-0	4
Chetomin	C31H30O6N6S4	710.1110	1403-36-7	4
Chinomethionate	C10H6N2OS2	233.9922	2439-01-2	8
Chlamydosporol	C11H14O5	226.0841	135063-30-8	4
Chlorambucil	C14H19Cl2NO2	303.0793	305-03-3	3
Chloramphenicol	C11H12Cl2N2O5	322.0123	56-75-7	12
Chlorantraniliprole	C18H14BrCl2N5O2	480.9708	500008-45-7	4
Chlorazanil	C9H8ClN5	221.0468	500-42-5	4
Chlorbenzoxamine	C27H31ClN2O	434.2125	522-18-9	4
Chlorbromuron	C9H10BrClN2O2	291.9614	13360-45-7	8
Chlorbufam	C11H10ClNO2	223.0400	1967-16-4	8
Chlorcyclizine	C18H21ClN2	300.1393	82-93-9	4
Chlordiazepoxide	C16H14ClN3O	299.0825	58-25-3	4
Chlordimeform	C10H13ClN2	196.0767	6164-98-3	12
Chlorethoxyfos-oxon	C6H11Cl4O4P	317.9149	54593-83-8	8
Chlorfenvinphos	C12H14Cl3O4P	357.9695	470-90-6	8
Chlorfluazuron	C20H9Cl3F5N3O3	538.9630	71422-67-8	12
Chloridazon	C10H8ClN3O	221.0356	1698-60-8	16
Chlorimuron-ethyl	C15H15ClN4O6S	414.0401	90982-32-4	8
Chlormadinone Acetate	C23H29ClO4	404.1754	302-22-7	8
Chlormephos	C5H12ClO2PS2	233.9705	24934-91-6	8
Chlormequat	C5H13ClN	122.0737	999-81-5	4
Chlorophacinon	C23H15ClO3	374.0710	3691-35-8	4
Chlorophacinone	C23H15ClO3	374.0710	3691-35-8	12

Compound	Formula	Formula Weight	CAS Number	# of Spectra
chlorprocaine	C13H20Cl2N2O2	306.0902	133-16-4	4
Chloropyramine	C16H20ClN3	289.1346	59-32-5	4
Chloroquine	C18H26ClN3	319.1815	54-05-7	4
Chlorothiazide	C7H6ClN3O4S2	294.9488	58-94-6	4
Chlorotoluron	C10H13ClN2O	212.0716	15545-48-9	9
Chloroxuron	C15H15ClN2O2	290.0822	1982-47-4	8
chlorphenamine	C16H19ClN2	274.1237	132-22-9	4
Chlorphencyclan	C18H28ClNO	309.1859	5632-52-0	4
Chlorphenethiazine	C16H17N2SCl	304.0801	2095-24-1	4
Chlorpheniramine	C16H19ClN2	274.1237	132-22-9	4
Chlorphenoxamine	C18H22ClNO	303.1390	77-38-3	4
chlorphentermine	C10H14ClN	183.0815	461-78-9	4
Chlorpromazin-D3	C17H16Cl3N2S	321.1146	136765-28-1	4
Chlorpromazine	C17H19ClN2S	318.0957	50-53-3	4
Chlorpromazine Sulfoxide	C17H19ClN2OS	334.0907	969-99-3	4
chlorpropamide	C10H13N2O3SCl	276.0335	94-20-2	4
Chlorpropham	C10H12ClNO2	213.0557	101-21-3	4
Chlorprothixene	C18H18ClNS	315.0848	113-59-7	4
Chlorpyrifos	C9H11Cl3NO3PS	348.9263	2921-88-2	4
Chlorpyrifos-methyl	C7H7Cl3NO3PS	320.8950	5598-13-0	8
chlorquinaldol	C10H7NOCl2	226.9905	72-80-0	4
Chlorsulfuron	C12H12ClN5O4S	357.0299	64902-72-3	8
Chlortetracycline	C22H23ClN2O8	478.1143	57-62-5	4
chlorthalidone	C14H11ClN2O4S	338.0128	77-36-1	4
Chlorthenoxazine	C10H10ClNO2	211.0400	132-89-8	4
Chlorthiamid	C7H5Cl2NS	204.9520	1918-13-4	8
Chlorthiophos	C11H15Cl2O3PS2	359.9577	60238-56-4	8
Chlorzoxazone	C7H4ClNO2	168.9931	95-25-0	4
Ciclacillin	C15H23N3O4S	341.1409	3485-14-1	8
Cicletanine	C14H12ClNO2	261.0557	89943-82-8	8
Ciclonium Bromide	C22H34NO	328.2640	29546-59-6	4
Cilastatin	C16H26N2O5S	358.1562	82009-34-5	8
Cilazapril	C22H31N3O5	417.2264	88768-40-5	8
Cimetidine	C10H16N6S	252.1157	51481-61-9	8
Cinchocaine	C20H29N3O2	343.2260	85-79-0	4
Cinchonidine	C19H22N2O	294.1732	485-71-2	8
Cinchonine	C19H22N2O	294.1732	118-10-5	8
cinchophen	C16H11NO2	249.0790	132-60-5	4
Cinerin I	C20H28O3	316.2038	25402-06-6	4
Cinerin II	C21H28O5	360.1937	121-20-0	4



Compound	Formula	Formula Weight	CAS Number	# of Spectra
Cinidon-ethyl	C19H17Cl2NO4	393.0535	142891-20-1	8
Cinnarizine	C26H28N2	368.2252	298-57-7	4
Cinosulfuron	C15H19N5O7S	413.1005	94593-91-6	4
Cinoxacin	C12H10N2O5	262.0590	28657-80-9	8
Ciprofloxacin	C17H18FN3O3	331.1332	85721-33-1	8
Cisapride	C23H29ClFN3O4	465.1831	81098-60-4	4
Citalopram	C20H21FN2O	324.1638	59729-33-8	4
Citolone	C6H9NO2S	159.0354	1195-16-0	4
Citreoviridin	C23H30O6	402.2042	25425-12-1	4
Citrinin	C13H14O5	250.0841	518-75-2	8
Citromycetin	C14H10O7	290.0427	478-60-4	4
clanobutin	C18H18ClNO4	347.0924	30544-61-7	4
Clarithromycin	C38H69NO13	747.4769	81103-11-9	4
clefamide	C17H16N2O5Cl2	398.0436	3576-64-5	4
Clemastine	C21H26ClNO	343.1703	15686-51-8	4
Clemizole	C19H20ClN3	325.1346	442-52-4	4
Clenbuterol	C12H18Cl2N2O	276.0796	37148-27-9	4
Clethodim	C17H26ClNO3S	359.1322	99129-21-2	9
Clethodim-imin-sulfone	C14H23NO4S	301.1348	not available	8
Clethodim-imin-sulfoxide	C14H23NO3S	285.1399	not available	9
Clethodim-sulfone	C17H26ClNO5S	391.1220	not available	8
Clethodim-sulfoxide	C17H26ClNO4S	375.1271	not available	12
Clibucaine	C15H20Cl2N2O	314.0953	15302-10-0	4
clidinium	C22H26NO3	352.1913	7020-55-5	4
Climbazole	C15H17ClN2O2	292.0979	38083-17-9	4
Clindamycin	C18H33ClN2O5S	424.1799	18323-44-9	8
Clobazam	C16H13ClN2O2	300.0666	22316-47-8	4
Clobenzepam	C17H18ClN3O	315.1138	1159-93-9	4
Clobenzorex	C16H18ClN	259.1128	13364-32-4	4
Clobetasol-17-propionate	C25H32ClFO5	466.1922	25122-46-7	4
Clobetasol-butyrate	C26H32ClFO5	478.1922	25122-57-0	4
Clobutinol	C14H22ClNO	255.1390	14860-49-2	4
Clodinafop-propargyl	C17H13ClFN3O4	349.0517	105512-06-9	8
Clofedanol	C17H20ClNO	289.1233	791-35-5	4
Clofenamide	C6H7ClN2O4S2	269.9536	511-46-6	4
Clofentazine	C14H8Cl2N4	302.0126	74115-24-5	8
Clofexamide	C14H21ClN2O2	284.1292	1223-36-5	4
Clomazone	C12H14ClNO2	239.0713	81777-89-1	8
Clomeprop	C16H15Cl2NO2	323.0480	84496-56-0	8
Clomethiazole	C6H8ClNS	161.0066	533-45-9	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Clomiphene	C26H28ClNO	405.1859	911-45-5	4
Clomipramine	C19H23ClN2	314.1550	303-49-1	4
Clonazepam	C15H10ClN3O3	315.0411	1622-61-3	4
Clonidine	C9H9Cl2N3	229.0174	4205-90-7	4
clonixin	C13H11N2O2Cl	262.0509	17737-65-4	4
Clopramide	C14H20ClN3O3S	345.0914	636-54-4	8
Clopenthixol	C22H25ClN2OS	400.1376	982-24-1	4
Clopidogrel	C16H16ClNO2S	321.0590	113665-84-2	4
Clopidol	C7H7Cl2NO	190.9905	2971-90-6	4
Cloprednol	C21H25ClO5	392.1391	5251-34-3	8
Clopyralid	C6H3Cl2NO2	190.9541	1702-17-6	12
Cloquintocet-mexyl	C18H22ClNO3	335.1288	99607-70-2	8
clorexolone	C14H17N2O3SCl	328.0648	2127-01-7	4
Clorindione	C15H9ClO2	256.0291	1146-99-2	4
clorprenaline	C11H16NOCl	213.0920	3811-25-4	4
clorsulon	C8H8N3O4S2Cl3	378.9022	60200-06-8	4
Closantel	C22H14Cl2I2N2O2	661.8522	57808-65-8	4
Clothianidin	C6H8ClN5O2S	249.0087	210880-92-5	9
Clotiapine	C18H18ClN3S	343.0910	2058-52-8	4
Clotiazepam	C16H15ClN2OS	318.0594	33671-46-4	4
Clotrimazol	C22H17ClN2	344.1080	23593-75-1	4
Cloxacillin	C19H18ClN3O5S	435.0656	61-72-3	8
Cloxiquine	C9H6ClNO	179.0138	130-16-5	4
Clozapine	C18H19ClN4	326.1298	5786-21-0	8
Clozapine N-oxide	C18H19ClN4O	342.1247	34233-69-7	4
Cocaine	C17H21NO4	303.1471	50-36-2	4
Cochliodinol	C32H30N2O4	506.2206	11051-88-0	8
Codeine	C18H21NO3	299.1521	76-57-3	4
Colchicine	C22H25NO6	399.1682	64-86-8	4
Coniine	C8H17N	127.1361	458-88-8	4
Corticosterone	C21H30O4	346.2144	50-22-6	5
Cortisone	C21H28O5	360.1937	53-06-5	8
Cotinine	C10H12N2O	176.0950	486-56-6	4
Coumaphos	C14H16ClO5PS	362.0145	56-72-4	8
coumarin	C9H6O2	146.0368	91-64-5	4
Coumatetralyl	C19H16O3	292.1099	5836-29-3	12
Croconazole	C18H15ClN2O	310.0873	77175-51-0	4
Cromoglicic acid	C23H16O11	468.0693	16110-51-3	8
cropropamide	C13H24N2O2	240.1838	633-47-6	4
Crotetamide	C12H22N2O2	226.1681	6168-76-9	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Crotoxyphos	C14H19O6P	314.0919	7700-17-6	8
Cumyluron	C17H19CIN2O	302.1186	99485-76-4	8
Curvularin	C16H20O5	292.1311	10140-70-2	8
Cyamemazine	C19H21N3S	323.1456	3546-03-0	4
Cyanazine	C9H13CIN6	240.0890	21725-46-2	16
Cyanofenphos	C15H14NO2PS	303.0483	13067-93-1	12
Cyanophos	C9H10NO3PS	243.0119	2636-26-2	12
Cyazofamid	C13H13CIN4O2S	324.0448	120116-88-3	12
Cyclamic acid	C6H13NO3S	179.0616	100-88-9	4
Cyclanilide	C11H9Cl2NO3	272.9959	113136-77-9	4
Cyclicine	C18H22N2	266.1783	82-92-8	4
Cycloaspeptide A	C36H43N5O6	641.3213	109171-13-3	8
Cycloate	C11H21NOS	215.1344	1134-23-2	8
Cyclobenzaprine	C20H21N	275.1674	303-53-7	4
Cyclodrine	C19H29NO3	319.2147	52109-93-0	4
Cycloechinulin	C20H21N3O3	351.1583	143086-29-7	8
cycloguanil	C11H14N5Cl	251.0938	516-21-2	4
Cycloheximide	C15H23NO4	281.1627	66-81-9	8
cyclomethycaine	C22H33NO3	359.2460	139-62-8	4
Cyclopenin	C17H14N2O3	294.1004	19553-26-5	8
Cyclopentamine	C9H19N	141.1517	102-45-4	4
cyclopenthiiazide	C13H18N3O4S2Cl	379.0427	742-20-1	8
Cyclopentobarbital	C12H14N2O3	234.1004	76-68-6	4
Cyclopentolate	C17H25NO3	291.1834	512-15-2	4
Cyclopeptine	C17H16N2O2	280.1212	50886-63-0	4
Cyclophosphamide	C7H15Cl2N2O2P	260.0248	50-18-0	4
Cyclopiazonic acid	C20H20N2O3	336.1474	18172-33-3	8
Cyclosporin A	C62H111N11O12	1201.8414	59865-13-3	8
Cyclosporin C	C62H111N11O13	1217.8363	59787-61-0	4
Cyclosporin D	C63H113N11O12	1215.8570	63775-96-2	4
Cyclosporin H	C62H111N11O12	1201.8414	83602-39-5	4
cyclothiazide	C14H16N3O4S2Cl	389.0271	2259-96-3	4
Cyclovalone	C22H22O5	366.1467	579-23-7	4
Cycloxydim	C17H27NO3S	325.1712	101205-02-1	8
Cycluron	C11H22N2O	198.1732	2163-69-1	8
Cyflufenamid	C20H17F5N2O2	412.1210	180409-60-3	8
Cyfluthrin	C22H18Cl2FNO3	433.0648	68359-37-5	8
Cyhalofop-butyl	C20H20FNO4	357.1376	122008-85-9	8
Cymoxanil	C7H10N4O3	198.0753	57966-95-7	8
Cypermethrin	C22H19Cl2NO3	415.0742	52315-07-8	8

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Cyphenothrin	C24H25NO3	375.1834	39515-40-7	12
Cyproconazole	C15H18ClN3O	291.1138	113096-99-4	8
Cyprodinil	C14H15N3	225.1266	121552-61-2	8
Cyproheptadine	C21H21N	287.1674	129-03-3	4
Cyromazine	C6H10N6	166.0967	66215-27-8	8
Cytarabine	C9H13N3O5	243.0855	147-94-4	4
Cytochalasin A	C29H35O5N	477.2515	14110-64-6	4
Cytochalasin B	C29H37O5N	479.2672	14930-96-2	4
Cytochalasin C	C30H37O6N	507.2621	22144-76-9	4
Cytochalasin D	C30H37O6N	507.2621	22144-77-0	4
Cytochalasin E	C28H33O7N	495.2257	36011-19-5	4
Cytochalasin H	C30H39NO5	493.2828	53760-19-3	4
Cytochalasin J	C28H37NO4	451.2723	56144-22-0	4
D10-Psilocin	C12H6D10N2O	214.1890	N/A	4
D3-Atropin	C17H20D3NO3	292.1866	N/A	4
D3-Benzoyllecgonine	C16H16D3NO4	292.1502	115732-68-8	4
D3-Cocaine	C17H18D3NO4	306.1659	65266-73-1	4
D3-Codeine	C18H18D3NO3	302.1710	70420-71-2	4
D3-Doxepin	C19H18NOD3	282.1811	N/A	4
D3-Ecgonine methyl ester	C10H14D3NO3	202.1397	136765-34-9	4
D3-LSD	C20H22D3N3O	326.2186	136765-38-3	4
D3-Methadon	C21H24D3NO	312.2281	60263-63-0	4
D3-Morphine	C17H16D3NO3	288.1553	67293-88-3	4
D3-Morphine-3-beta-glucuronide	C23H24D3NO9	464.1874	N/A	12
D5-Amphetamin	C9H8D5N	140.1362	65538-33-2	4
D5-Diazepam	C16H8ClN2OD5	289.1030	N/A	4
D5-Fentanyl	C22H23D5N2O	341.2515	118357-29-2	4
D5-MBDB	C12H12D5NO2	212.1573	N/A	4
D5-MDA	C10H8D5NO2	184.1260	136765-42-9	4
D5-MDEA	C12H12D5NO2	212.1573	160227-43-0	4
D5-MDMA	C11H10D5NO2	198.1417	136765-43-0	4
D5-Metamphetamine	C10H10D5N	154.1518	60124-88-1	4
D7-7-Aminoflunitrazepam	C16H7D7FN3O	290.1560	N/A	4
D7-Flunitrazepam	C16H5D7FN3O3	320.1302	N/A	4
D9-Methadone	C21H18D9NO	318.2658	N/A	4
Dacarbazin	C6H10N6O	182.0916	4342-03-4	4
Daimuron	C17H20N2O	268.1576	42609-52-9	12
Daminozide	C6H12N2O3	160.0848	1596-84-5	10
Danazol	C22H27NO2	337.2042	17230-88-5	4
Danofloxacin	C19H20FN3O3	357.1489	112398-08-0	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
dantrolene	C14H10N4O5	314.0651	7261-97-4	4
Dapiprazole	C19H27N5	325.2266	72822-12-9	4
Dapsone	C12H12N2O2S	248.0619	80-08-0	8
Daunorubicin	C27H29NO10	527.1791	20830-81-3	4
Debrisoquine	C10H13N3	175.1109	1131-64-2	4
Decarestrictine	C10H16O5	216.0998	127393-89-9	4
Dechlorogriseofulvin	C17H18O6	318.1103	3680-32-8	4
Decoquinatate	C24H35NO5	417.2515	18507-89-6	4
Deepoxy-deoxynivalenol	C15H20O5	280.1311	88054-24-4	7
DEET	C12H17NO	191.1310	134-62-3	8
Deflazacort	C25H31NO6	441.2151	14484-47-0	4
Dehydrocholic acid	C24H34O5	402.2406	81-32-2	4
Delorazepam	C15H10Cl2N2O	304.0170	2894-67-9	4
Deltamethrin	C22H19Br2NO3	502.9732	52918-63-5	13
dembrexine	C13H17NO2Br2	376.9626	83200-09-3	4
Demecarium	C32H52N4O4	556.3989	56-94-0	4
Demeclocycline	C21H21ClN2O8	464.0986	127-33-3	8
Demeton-O	C8H19O3PS2	258.0513	298-03-3	4
Demeton-O-methyl	C6H15O3PS2	230.0200	867-27-6	4
Demeton-S-methyl	C6H15O3PS2	230.0200	919-86-8	7
Demeton-S-methyl-sulfone	C6H15O5PS2	262.0099	17040-19-6	12
Demoxepam	C15H11N2O2Cl	286.0509	963-39-3	4
Denaverine	C24H33NO3	383.2460	3579-62-2	4
Deoxybrevianamide E	C21H25N3O2	351.1947	34610-68-9	8
Deoxynivalenol	C15H20O6	296.1260	51481-10-8	6
Deoxynivalenol-3-glucoside	C21H30O11	458.1788	131180-21-7	8
depropine	C23H27NO	333.2093	604-51-3	4
dequalinium	C30H40N4	456.3253	6707-58-0	4
Desalkylflurazepam	C15H10N2OFCI	288.0466	2886-65-9	8
Desethylene Ciprofloxacin	C15H16FN3O3	305.1176	103222-12-4	4
Desipramine	C18H22N2	266.1783	50-47-5	4
Desmedipham	C16H16N2O4	300.1110	13684-56-5	16
Desmethylcitalopram	C19H19N2OF	310.1481	144010-85-5	4
Desmethylclobazam	C15H11ClN2O2	286.0509	22316-55-8	8
Desmethylclomipramine	C18H21ClN2	300.1393	303-48-0	4
Desmethyl-formamido-pirimiticarb	C11H16N4O3	252.1222	59333-83-4	8
desmethylpapaverine	C19H19NO4	325.1314	18813-60-0	4
Desmethyl-pirimiticarb	C10H16N4O2	224.1273	30614-22-3	8
desmethylreserpine	C32H38N2O9	594.2577	N/A	4
Desmetryne	C8H15N5S	213.1048	1014-69-3	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
desonide	C24H32O6	416.2199	638-94-8	8
Desoximethasone	C22H29FO4	376.2050	382-67-2	8
Desoxycortone 21-(3-phenylpropionate)	C30H38O4	462.2770	14007-50-2	4
Desoxycortone enantate	C28H42O4	442.3083	N/A	4
despropionyl fentanyl	C19H24N2	280.1939	21409-26-7	4
Detajmium	C27H42N3O3	456.3226	33774-52-6	4
detomidine	C12H14N2	186.1157	76631-46-4	4
detomidine carboxylic acid	C12H12N2O2	216.0899	115664-39-6	4
Dexamethasone	C22H29FO5	392.1999	50-02-2	5
Dexamethasone 21-Acetate	C24H31FO6	434.2105	1177-87-3	8
Dexamethasone 21-isonicotinate	C28H32FNO6	497.2214	2265-64-7	4
dexamethasone phenylpropionate	C31H37FO6	524.2574	1879-72-7	4
Dexfenfluramine	C12H16F3N	231.1235	3239-44-9	4
dexpanthenol	C9H19NO4	205.1314	62507-76-0	4
Dextromethorphan	C18H25NO	271.1936	125-71-3	4
Dextromoramide	C25H32N2O2	392.2464	357-56-2	4
Dextropropoxyphene	C22H29NO2	339.2198	469-62-5	9
Diacetoxyscirpenol	C19H26O7	366.1679	2270-40-8	4
Dialifos	C14H17ClNO4PS2	393.0025	10311-84-9	8
Di-allate	C10H17Cl2NOS	269.0408	2303-16-4	9
Diamidafos	C8H13N2O2P	200.0715	1754-58-1	8
diamorphine	C21H23NO5	369.1576	561-27-3	4
Diaveridine	C13H16N4O2	260.1273	5355-16-8	8
Diazepam	C16H13ClN2O	284.0716	439-14-5	4
Diazinon	C12H21N2O3PS	304.1011	333-41-5	8
Diazoxide	C8H7ClN2O2S	229.9917	364-98-7	8
Dibenzepin	C18H21N3O	295.1685	4498-32-2	4
Dibutyl adipate	C14H26O4	258.1831	105-99-7	4
Dichlofenthion	C10H13Cl2O3PS	313.9700	97-17-6	8
Dichlofluanid	C9H11Cl2FN2O2S2	331.9623	1085-98-9	8
Dichlorophen	C13H10Cl2O2	268.0058	97-23-4	4
Dichlorprop	C9H8Cl2O3	233.9850	120-36-5	4
Dichlorvos	C4H7Cl2O4P	219.9459	62-73-7	8
Diclobutrazol	C15H19Cl2N3O	327.0905	75736-33-3	8
Diclofenac	C14H11Cl2NO2	295.0167	15307-86-5	12
Diclofop-methyl	C16H14Cl2O4	340.0269	51338-27-3	12
Dicloran	C6H4Cl2N2O2	205.9650	99-30-9	4
Diclosulam	C13H10Cl2FN5O3S	404.9865	145701-21-9	8
Dicloxacillin	C19H17Cl2N3O5S	469.0266	3116-76-5	4
Dicrotophos	C8H16NO5P	237.0766	3735-78-3	8

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Dicyclanil	C8H10N6	190.0967	112636-83-6	12
Dicycloverine	C19H35NO2	309.2668	77-19-0	4
Didanosine	C10H12N4O3	236.0909	69655-05-6	8
didesmethylchlorpromazine	C15H15N2SCL	290.0644	2095-17-2	4
Dienestrol	C18H18O2	266.1307	84-17-3	4
Dienogest	C20H25NO2	311.1885	65928-58-7	4
Diethazine	C18H22N2S	298.1504	60-91-3	4
Diethofencarb	C14H21NO4	267.1471	87130-20-9	8
Diethylcarbamazine	C10H21N3O	199.1685	90-89-1	4
diethylpropion	C13H19NO	205.1467	90-84-6	4
Difenacoum	C31H24O3	444.1725	56073-07-5	8
Difenoconazole	C19H17Cl2N3O3	405.0647	119446-68-3	12
Difenoxuron	C16H18N2O3	286.1317	14214-32-5	12
Difenzoquat	C17H17N2	249.1392	43222-48-6	12
Diflorasone diacetate	C26H32F2O7	494.2116	33564-31-7	4
Difloxacin	C21H19F2N3O3	399.1394	98106-17-3	4
Diflubenzuron	C14H9ClF2N2O2	310.0321	35367-38-5	8
Diflucortolone	C22H28F2O4	394.1956	2607-06-9	4
Diflufenican	C19H11F5N2O2	394.0741	83164-33-4	4
Diflufenzopyr	C15H12F2N4O3	334.0877	109293-97-2	8
digoxin	C41H64O14	780.4296	20830-75-5	4
Dihydralazine	C8H10N6	190.0967	484-23-1	4
Dihydrocodeine	C18H23NO3	301.1678	125-28-0	4
Dihydroergocristin	C35H41N5O5	611.3108	17479-19-5	4
Dihydroergokryptine	C32H43N5O5	577.3264	25447-66-9	8
Dihydroergosine	C30H39N5O5	549.2951	7288-61-1	4
Dihydroergotamine	C33H37N5O5	583.2795	511-12-6	8
Dihydrolysergol	C16H20N2O	256.1576	18051-16-6	4
Dihyprylone	C9H15NO2	169.1103	77-03-2	4
Dilazep	C31H44N2O10	604.2996	35898-87-4	4
Diltiazem	C22H26N2O4S	414.1613	42399-41-7	4
dimeflin	C20H21NO3	323.1521	1165-48-6	4
Dimefuron	C15H19ClN4O3	338.1146	34205-21-5	17
Dimephenopan	C11H17N	163.1361	17279-39-9	4
Dimepiperate	C15H21NOS	263.1344	61432-55-1	8
Dimetacrine	C20H26N2	294.2096	4757-55-5	4
Dimethachlor	C13H18ClNO2	255.1026	50563-36-5	12
Dimethametryn	C11H21N5S	255.1518	22936-75-0	8
Dimethenamide	C12H18ClNO2S	275.0747	87674-68-8	8
Dimethoate	C5H12NO3PS2	228.9996	60-51-5	8

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Dimethomorph	C21H22ClNO4	387.1237	110488-70-5	12
Dimetilan	C10H16N4O3	240.1222	644-64-4	8
Dimetindene	C20H24N2	292.1939	5636-83-9	4
Dimetotiazine	C19H25N3O2S2	391.1388	7456-24-8	4
Dimetridazole	C5H7N3O2	141.0538	551-92-8	8
Dimoxystrobin	C19H22N2O3	326.1630	149961-52-4	8
Diniconazole	C15H17Cl2N3O	325.0749	83657-24-3	12
Dinoprost	C20H34O5	354.2406	551-11-1	4
Dinoseb	C10H12N2O5	240.0746	88-85-7	4
Dinotefuran	C7H14N4O3	202.1066	165252-70-0	8
Dinoterb	C10H12N2O5	240.0746	1420-07-1	4
Dioxacarb	C11H13NO4	223.0845	6988-21-2	8
Dioxathion	C12H26O6P2S4	456.0088	78-34-2	12
Dioxethedrin	C11H17NO3	211.1208	497-75-6	8
Diphacinone	C23H16O3	340.1099	82-66-6	8
Diphenamid	C16H17NO	239.1310	957-51-7	12
Diphenhydramine	C17H21NO	255.1623	58-73-1	4
Diphenidol	C21H27NO	309.2093	972-02-1	4
Diphenylamine	C12H11N	169.0891	122-39-4	8
Diphenylpyraline	C19H23NO	281.1780	147-20-6	4
dipipanone	C24H31NO	349.2406	467-83-4	4
Dipipoverine	C20H30N2O2	330.2307	117-30-6	4
Diponium	C20H38NO2	324.2903	58875-33-5	4
diprenorphine	C26H35NO4	425.2566	14357-78-9	4
Diprophylline	C10H14N4O4	254.1015	479-18-5	4
Dipyridamole	C24H40N8O4	504.3173	58-32-2	4
Dipyron	C13H16N3NaO4S	333.0759	68-89-3	4
Diquat	C12H12N2	184.1000	2764-72-9	12
Disopyramide	C21H29N3O	339.2311	3737-09-5	4
Distigmin	C22H32N4O4	416.2424	15876-67-2	4
Disulfiram	C10H20N2S4	296.0509	97-77-8	4
Disulfoton	C8H19O2PS3	274.0285	298-04-4	8
Dithianon	C14H4N2O2S2	295.9714	3347-22-6	4
Dithiopyr	C15H16F5NO2S2	401.0543	97886-45-8	8
Diuron	C9H10Cl2N2O	232.0170	330-54-1	8
Dixyrazine	C24H33N3O2S	427.2293	2470-73-7	4
DNOC	C7H6N2O5	198.0277	534-52-1	4
Dobutamine	C18H23NO3	301.1678	34368-04-2	8
Dodemorph	C18H35NO	281.2719	1593-77-7	8
Dodine	C15H33N3O2	287.2573	2439-10-3	8



Compound	Formula	Formula Weight	CAS Number	# of Spectra
Dolasetron	C19H20N2O3	324.1474	115956-12-2	8
Domperidone	C22H24ClN5O2	425.1619	57808-66-9	8
Dopamin	C8H11NO2	153.0790	51-61-6	8
Dopexamine	C22H32N2O2	356.2464	86197-47-9	4
Dormovit	C12H14N2O4	250.0954	1146-21-0	4
Dorzolamide	C10H16N2O4S3	324.0272	120279-96-1	8
Dosulepin	C19H21NS	295.1395	113-53-1	4
Doxapram	C24H30N2O2	378.2307	309-29-5	4
Doxazosin	C23H25N5O5	451.1856	74191-85-8	4
Doxepin	C19H21NO	279.1623	1668-19-5	4
Doxorubicin	C27H29NO11	543.1741	23214-92-8	4
Doxycycline	C22H24N2O8	444.1533	564-25-0	4
Doxylamine	C17H22N2O	270.1732	469-21-6	4
Drazoloxon	C10H8ClN3O2	237.0305	5707-69-7	4
Drofenine	C20H31NO2	317.2355	1679-76-1	4
droperidol	C22H22N3O2F	379.1696	548-73-2	4
Dropropizine	C13H20N2O2	236.1525	17692-31-8	4
Drospirenone	C24H30O3	366.2195	67392-87-4	4
duloxetine	C18H19NOS	297.1187	116539-58-3	4
Ecgonin-D3	C9H12D3NO3	188.1240	N/A	8
Ecgoninemethylester	C10H17NO3	199.1208	7143-09-1	4
EDDP	C20H23N	277.1830	30223-73-5	4
EDDP-D3	C20H21D3N	281.2097	136765-23-6	4
Edifenphos	C14H15O2PS2	310.0251	17109-49-8	8
Eldoral	C11H17N3O3	239.1270	509-87-5	4
Elymoclavine	C16H18N2O	254.1419	548-43-6	4
Elymoclavine fructoside	C22H28N2O6	416.1947	12379-50-9	4
Emamectin B1a	C49H75NO13	885.5238	123997-28-4	4
Emamectin B1b	C48H73NO13	871.5082	137335-79-6	4
embramine	C18H22NOBr	347.0885	3565-72-8	4
Embutramide	C17H27NO3	293.1991	15687-14-6	4
Emepronium	C20H28N	282.2222	3614-30-0	4
Emetine	C29H40N2O4	480.2988	483-18-1	4
Emodin	C15H10O5	270.0528	518-82-1	12
Enalapril	C20H28N2O5	376.1998	75847-73-3	4
Endomide	C17H28N2O2	292.2151	4582-18-7	4
Endosulfansulfate	C9H6Cl6O4S	419.8118	1031-07-8	4
Enniatin A	C36H63N3O9	681.4564	144446-20-8	4
Enniatin A1	C35H61N3O9	667.4408	4530-21-6	4
Enniatin B	C33H57N3O9	639.4095	917-13-5	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Enniatin B1	C34H59N3O9	653.4251	19914-20-6	4
Enniatin B2	C32H55N3O9	625.3938	632-91-7	4
Enniatin B3	C31H53N3O9	611.3782	864-99-3	4
Enoxacin	C15H17FN4O3	320.1285	74011-58-8	4
Enoximone	C12H12N2O2S	248.0619	77671-31-9	4
Enrofloxacin	C19H22FN3O3	359.1645	93106-60-6	4
Ephedrine	C10H15NO	165.1154	299-42-3	4
Epinephrine	C9H13NO3	183.0895	51-43-4	8
epi-Tetracycline	C22H24N2O8	444.1533	60-54-8	4
epithiazide	C10H11N3O4F3S3Cl	424.9552	1764-85-8	4
EPN	C14H14NO4PS	323.0381	2104-64-5	8
Epoxiconazole	C17H13ClFN3O	329.0731	106325-08-0	8
Eprazinone	C24H32N2O2	380.2464	10402-90-1	4
Eprosartan	C23H24N2O4S	424.1457	133040-01-4	4
EPTC	C9H19NOS	189.1187	759-94-4	8
Equisetin	C22H31NO4	373.2253	57749-43-6	8
Ergine	C16H17N3O	267.1372	478-94-4	4
Erginine	C16H17N3O	267.1372		4
Ergocornine	C31H39N5O5	561.2951	564-36-3	4
Ergocorninine	C31H39N5O5	561.2951	564-37-4	4
Ergocristine	C35H39N5O5	609.2951	511-08-0	4
Ergocristinine	C35H39N5O5	609.2951	511-07-9	4
Ergocryptine	C32H41N5O5	575.3108	511-09-1	4
Ergocryptinine	C32H41N5O5	575.3108	511-10-4	4
ergometrine	C19H23N3O2	325.1790	60-79-7	8
Ergometrinine	C19H23N3O2	325.1790	479-00-5	4
Ergosine	C30H37N5O5	547.2795	561-94-4	4
Ergosinine	C30H37N5O5	547.2795	596-88-3	4
Ergotamine	C33H35N5O5	581.2638	113-15-5	4
Ergotaminine	C33H35N5O5	581.2638	639-81-6	4
Ergovaline	C29H35N5O5	533.2638	2873-38-3	4
Erythromycin	C37H67NO13	733.4612	114-07-8	16
Erythromycin-13C2	(13C)2C35H67NO13	735.4680	N/A	4
Esculin	C15H16O9	340.0794	531-75-9	8
Esfenvalerate	C25H22ClNO3	419.1288	66230-04-4	16
Esmolol	C16H25NO4	295.1784	103598-03-4	4
Esprocarb	C15H23NOS	265.1500	85785-20-2	8
Estazolam	C16H11ClN4	294.0672	29975-16-4	5
estr-4-ene-3,17-dione	C18H24O2	272.1776	734-32-7	4
Etaconazole	C14H15Cl2N3O2	327.0541	60207-93-4	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Etafedrine	C12H19NO	193.1467	48141-64-6	4
Etafenone	C21H27NO2	325.2042	90-54-0	4
Etamiphyllin	C13H21N5O2	279.1695	314-35-2	4
Etamivan	C12H17NO3	223.1208	304-84-7	4
Ethaboxam	C14H16N4OS2	320.0766	162650-77-3	8
Ethacridine	C15H15N3O	253.1215	442-16-0	4
Ethacrylic Acid	C13H12Cl2O4	302.0113	58-54-8	8
Ethambutol	C10H24N2O2	204.1838	74-55-5	4
Ethametsulfuron-methyl	C15H18N6O6S	410.1009	97780-06-8	8
Ethaverine	C24H29NO4	395.2097	486-47-5	4
Ethenzamide	C9H11NO2	165.0790	938-73-8	4
ethiazide	C9H12N3O4S2Cl	324.9958	1824-58-4	4
Ethidimuron	C7H12N4O3S2	264.0351	30043-49-3	8
Ethiofencarb	C11H15NO2S	225.0824	29973-13-5	12
Ethiofencarb-sulfone	C11H15NO4S	257.0722	53380-23-7	12
Ethiofencarb-sulfoxide	C11H15NO3S	241.0773	53380-22-6	8
Ethion	C9H22O4P2S4	383.9876	563-12-2	8
Ethion monoxon	C9H22O5P2S3	368.0105	17356-42-2	8
Ethionamide	C8H10N2S	166.0565	536-33-4	8
Ethiprole	C13H9Cl2F3N4OS	395.9826	181587-01-9	8
Ethirimol	C11H19N3O	209.1528	23947-60-6	8
ethisterone	C21H28O2	312.2089	434-03-7	4
Ethofumesate	C13H18O5S	286.0875	26225-79-6	12
Ethoprophos	C8H19O2PS2	242.0564	13194-48-4	8
Ethosuximide	C7H11NO2	141.0790	77-67-8	5
ethotoin	C11H12N2O2	204.0899	86-35-1	4
Ethoxyquin	C14H19NO	217.1467	91-53-2	4
Ethoxysulfuron	C15H18N4O7S	398.0896	126801-58-9	8
Ethyl glucuronide	C8H14O7	222.0740	17685-04-0	4
Ethyl glucuronide-D5	C8H9D5O7	227.1053	N/A	4
Ethyl sulfate	C2H6O4S	125.9987	540-82-9	4
Ethyl sulfate-D5	C2HD5O4S	131.0301	N/A	4
Ethylbenzhydramine	C19H25NO	283.1936	642-58-0	4
Ethylthiourea	C3H6N2S	102.0252	96-45-7	12
ethylmorphine	C19H23NO3	313.1678	76-58-4	4
Ethylparathion	C10H14NO5PS	291.0330	56-38-2	4
Etidocaine	C17H28N2O	276.2202	36637-18-0	4
Etifelmin	C17H19N	237.1517	341-00-4	4
Etilamfetamine	C11H17N	163.1361	457-87-4	4
Etilefrine	C10H15NO2	181.1103	709-55-7	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Etiroxate	C18H17I4NO4	818.7337	17365-01-4	8
Etobenzanid	C16H15Cl2NO3	339.0429	79540-50-4	8
Etodolac	C17H21NO3	287.1521	41340-25-4	12
Etodroxizine	C23H31ClN2O3	418.2023	17692-34-1	4
Etofenamate	C18H18F3NO4	369.1188	30544-47-9	4
Etofenprox	C25H28O3	376.2038	80844-07-1	8
Etofibrate	C18H18ClNO5	363.0874	31637-97-5	4
Etofyllinclofibrate	C19H21ClN4O5	420.1200	54504-70-0	4
Etofylline	C9H12N4O3	224.0909	519-37-9	4
Etoloxamine	C19H25NO	283.1936	1157-87-5	4
Etomidate	C14H16N2O2	244.1212	33125-97-2	4
Etophylline	C9H12N4O3	224.0909	519-37-9	4
Etoposide	C29H32O13	588.1843	33419-42-0	8
Etozazole	C21H23F2NO2	359.1697	153233-91-1	8
Etrimfos	C10H17N2O4PS	292.0647	38260-54-7	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
Famoxadone	C22H18N2O4	374.1267	131807-57-3	8
Famphur	C10H16NO5PS2	325.0208	52-85-7	8
Famprofazone	C24H31N3O	377.2467	22881-35-2	4
Febantel	C20H22N4O6S	446.1260	58306-30-2	4
Fedrilate	C20H29NO4	347.2097	23271-74-1	4
Felbamate	C11H14N2O4	238.0954	25451-15-4	4
Felodipine	C18H19Cl2NO4	383.0691	72509-76-3	8
Fenamidone	C17H17N3OS	311.1092	161326-34-7	8
Fenamiphos	C13H22NO3PS	303.1058	22224-92-6	8
Fenarimol	C17H12Cl2N2O	330.0327	60168-88-9	16
Fenazaquin	C20H22N2O	306.1732	120928-09-8	8
Fenbendazole	C15H13N3O2S	299.0728	43210-67-9	4
Fenbendazole Sulfone	C15H13N3O4S	331.0627	54029-20-8	4
Fenbendazole Sulfoxide	C15H13N3O3S	315.0678	53716-50-0	4
Fenbuconazole	C19H17ClN4	336.1142	114369-43-6	8
fenbufen	C16H14O3	254.0943	36330-85-5	4
Fenbutrazate	C23H29NO3	367.2147	4378-36-3	4
fencamfamine	C15H21N	215.1674	1209-98-9	4
fenclozic acid	C11H8ClNO2S	252.9964	17969-20-9	4
Fendiline	C23H25N	315.1987	13042-18-7	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Fenetylline	C18H23N5O2	341.1852	3736-08-1	4
Fenfluramine	C12H16F3N	231.1235	458-24-2	4
Fenfuram	C12H11NO2	201.0790	24691-80-3	12
Fenhexamid	C14H17Cl2NO2	301.0636	126833-17-8	8
Fenitrothion	C9H12NO5PS	277.0174	122-14-5	12
Fenobucarb	C12H17NO2	207.1259	3766-81-2	12
Fenofibrate	C20H21ClO4	360.1128	49562-28-9	4
Fenoprofen	C15H14O3	242.0943	31879-05-7	4
Fenoprop	C9H7Cl3O3	267.9461	93-72-1	4
Fenoterol	C17H21NO4	303.1471	13392-18-2	4
Fenothiocarb	C13H19NO2S	253.1137	62850-32-2	8
Fenoxanil	C15H18Cl2N2O2	328.0745	115852-48-7	8
Fenoxaprop-P-ethyl	C18H16ClNO5	361.0717	71283-80-2	8
Fenoxazoline	C13H18N2O	218.1419	4846-91-7	4
Fenoxycarb	C17H19NO4	301.1314	79127-80-3	8
fenzolone	C11H12N2O2	204.0899	15302-16-6	4
Fenpiclonil	C11H6Cl2N2	235.9908	74738-17-3	9
Fenpipramide	C21H26N2O	322.2045	77-01-0	4
Fenpiprane	C20H25N	279.1987	3329-14-4	4
Fenpropathrin	C22H23NO3	349.1678	39515-41-8	8
Fenpropidin	C19H31N	273.2457	67306-00-7	8
Fenpropimorph	C20H33NO	303.2562	67306-03-0	8
Fenproporex	C12H16N2	188.1313	15686-61-0	4
Fenpyroximate	C24H27N3O4	421.2002	111812-58-9	8
fenspiride	C15H20N2O2	260.1525	5053-06-5	4
Fentanyl	C22H28N2O	336.2202	437-38-7	7
Fenthion	C10H15O3PS2	278.0200	55-38-9	8
fenticlor	C12H8O2SCl2	285.9622	97-24-5	4
Fenticonazole	C24H20Cl2N2OS	454.0673	72479-26-6	4
Fentin	C18H15Sn	351.0196	668-34-8	12
Fenuron	C9H12N2O	164.0950	101-42-8	8
Fenvalerate	C25H22ClNO3	419.1288	51630-58-1	12
feprazone	C20H20N2O2	320.1525	30748-29-9	4
Festuclavine	C16H20N2	240.1626	569-26-6	4
Fexofenadine	C32H39NO4	501.2879	83799-24-0	4
Finasteride	C23H36N2O2	372.2777	98319-26-7	4
Fipronil	C12H4Cl2F6N4OS	435.9387	120068-37-3	9
Fipronil-desulfinyl	C12H4Cl2F6N4	387.9717	205650-65-3	4
Fipronil-sulfide	C12H4Cl2F6N4S	419.9438	120067-83-6	4
Fipronil-sulfone	C12H4Cl2F6N4O2S	451.9336	120068-36-2	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
FK 506	C44H69NO12	803.4820	104987-11-3	8
Flamprop-M-isopropyl	C19H19CIFNO3	363.1037	63782-90-1	12
Flamprop-M-methyl	C17H15CIFNO3	335.0724	63729-98-6	8
Flavoxate	C24H25NO4	391.1784	15301-69-6	4
Flazasulfuron	C13H12F3N5O5S	407.0511	104040-78-0	8
Flecainide	C17H20F6N2O3	414.1378	54143-55-4	4
Fleroxacin	C17H18F3N3O3	369.1300	79660-72-3	4
Flocoumafen	C33H25F3O4	542.1705	90035-08-8	8
Floctafenine	C20H17F3N2O4	406.1140	23779-99-9	4
Flonicamid	C9H6F3N3O	229.0463	158062-67-0	8
Florasulam	C12H8F3N5O3S	359.0300	145701-23-1	4
Florfenicol	C12H14Cl2FN04S	357.0005	73231-34-2	4
Florfenicol Amine	C10H14FN03S	247.0678	76639-93-5	4
Fluanisone	C21H25FN2O2	356.1900	1480-19-9	4
Fluazifop (free acid)	C15H12F3NO4	327.0718	83066-88-0	8
Fluazifop-butyl	C19H20F3NO4	383.1344	69806-50-4	12
Fluazinam	C13H4Cl2F6N4O4	463.9514	79622-59-6	4
Flubendazole	C16H12FN3O3	313.0863	31430-15-6	4
Flucarbazono	C12H11F3N4O6S	396.0351	145026-88-6	6
Flucloxacillin	C19H17ClFN3O5S	453.0561	5250-39-5	8
Fluconazole	C13H12F2N6O	306.1041	86386-73-4	4
Flucycloxuron	C25H20ClF2N3O3	483.1161	113036-88-7	8
Flucythrinate	C26H23F2NO4	451.1595	70124-77-5	8
Fludioxonil	C12H6F2N2O2	248.0397	131341-86-1	13
fludrocortisone	C21H29O5F	380.1999	127-31-1	8
Fludrocortisone Acetate	C23H31FO6	422.2105	514-36-3	4
fludroxycortide	C24H33FO6	436.2261	1524-88-5	8
Flufenacet	C14H13F4N3O2S	363.0665	142459-58-3	8
Flufenamic Acid	C14H10F3NO2	281.0664	530-78-9	8
Flufenoxuron	C21H11ClF6N2O3	488.0362	101463-69-8	8
Flumazenil	C15H14FN3O3	303.1019	78755-81-4	4
Flumequine	C14H12FNO3	261.0801	42835-25-6	4
flumethasone	C22H28F2O5	410.1905	2135-17-3	8
Flumetsulam	C12H9F2N5O2S	325.0445	98967-40-9	8
Flumioxazin	C19H15FN2O4	354.1016	103361-09-7	4
Flunarizine	C26H26F2N2	404.2064	52468-60-7	4
flunisolide	C24H31FO6	434.2105	3385-03-3	8
Flunitrazepam	C16H12FN3O3	313.0863	1622-62-4	4
Flunixin	C14H11N2O2F3	296.0773	38677-85-9	8
Fluocinolone Acetonide	C24H30F2O6	452.2010	67-73-2	8

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Fluocinonide	C26H32F2O7	494.2116	356-12-7	8
Fluocortin Butyl	C26H35FO5	446.2469	41767-29-7	8
Fluocortolone	C22H29FO4	376.2050	152-97-6	4
Fluometuron	C10H11F3N2O	232.0823	2164-17-2	8
Fluoroglycofene-ethyl	C18H13ClF3NO7	447.0333	77501-90-7	8
fluorometholone	C22H29O4F	376.2050	426-13-1	4
fluoroprednisolone acetate	C23H29O6F	420.1948	338-98-7	4
Fluorouracil	C4H3FN2O2	130.0179	51-21-8	4
Fluoxastrobin	C21H16ClFN4O5	458.0793	361377-29-9	8
Fluoxetine	C17H18NOF3	309.1340	54910-89-3	4
fluoxymesterone	C20H29O3F	336.2101	76-43-7	4
Flupentixol	C23H25F3N2OS	434.1640	2709-56-0	4
Fluphenazine	C22H26F3N3OS	437.1749	69-23-8	4
Flupirtine	C15H17FN4O2	304.1336	56995-20-1	4
fluprednisolone	C21H27O5F	378.1843	53-34-9	8
Fluprednylidene 21-Acetate	C24H29FO6	432.1948	1255-35-2	8
Flupyrsulfuron-methyl	C15H14F3N5O7S	465.0566	144740-54-5	8
Fluquinconazole	C16H8Cl2FN5O	375.0090	136426-54-5	8
Flurazepam	C21H23ClFN3O	387.1514	17617-23-1	4
Flurbiprofen	C15H13FO2	244.0900	5104-49-4	4
Flurenol	C14H10O3	226.0630	467-69-6	4
Fluridone	C19H14F3NO	329.1027	59756-60-4	12
Flurochloridone	C12H10Cl2F3NO	311.0092	61213-25-0	13
Fluroxypyr	C7H5Cl2FN2O3	253.9661	69377-81-7	8
Fluroxypyr-meptyl	C15H21Cl2FN2O3	366.0913	81406-37-3	9
Flurprimidole	C15H15F3N2O2	312.1086	56425-91-3	8
Flurtamone	C18H14F3NO2	333.0977	96525-23-4	8
Flusilazole	C16H15F2N3Si	315.1003	85509-19-9	8
Fluspirilen	C29H31F2N3O	475.2435	1841-19-6	8
Flusulfamide	C13H7Cl2F3N2O4S	413.9456	106917-52-6	4
Flutamide	C11H11F3N2O3	276.0722	13311-84-7	4
Fluthiacet-methyl	C15H15ClFN3O3S2	403.0227	117337-19-6	9
Fluticasone Propionate	C25H31F3O5S	500.1844	80474-14-2	9
Flutolanil	C17H16F3NO2	323.1133	66332-96-5	8
Flutriafol	C16H13F2N3O	301.1027	76674-21-0	8
Fluvastadine	C24H26FNO4	411.1846	93957-54-1	8
Fluvoxamine	C15H21F3N2O2	318.1555	54739-18-3	4
Fluxofenim	C12H11ClF3NO3	309.0380	88485-37-4	12
Fomesafen	C15H10ClF3N2O6S	437.9900	72178-02-0	8
Fominoben	C21H24ClN3O3	401.1506	18053-31-1	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Fomocain	C20H25NO2	311.1885	17692-39-6	4
Fonofos	C10H15OPS2	246.0302	944-22-9	12
Foramsulfuron	C17H20N6O7S	452.1114	173159-57-4	9
Forchlorfenuron	C12H10CIN3O	247.0512	68157-60-8	8
Formetanate	C11H15N3O2	221.1164	22259-30-9	9
formoterol	C19H24N2O4	344.1736	73573-87-2	4
Formylsulfamethine	C13H14N4O3S	306.0787	795-13-1	8
Fosinopril	C30H46NO7P	563.3012	98048-97-6	8
Fosthiazate	C9H18NO3PS2	283.0466	98886-44-3	4
Fuberidazole	C11H8N2O	184.0637	3878-19-1	16
Fulvic acid	C14H12O8	308.0532	479-66-3	8
Fumagillin	C26H34O7	458.2305	23110-15-8	8
Fumigaclavine A	C18H22N2O2	298.1681	6879-59-0	4
Fumitremorgin C	C22H25N3O3	379.1896	118974-02-0	4
Fumonisin B1	C34H59NO15	721.3885	116355-83-0	8
Fumonisin B2	C34H59NO14	705.3936	116355-84-1	8
Fumonisin B3	C34H59NO14	705.3936	136379-59-4	8
Furalaxyl	C17H19NO4	301.1314	57646-30-7	12
Furaltadone	C13H16N4O6	324.1070	139-91-3	4
Furathiocarb	C18H26N2O5S	382.1562	65907-30-4	8
Furazolidone	C8H7N3O5	225.0386	67-45-8	4
Furosemid	C12H11CIN2O5S	330.0077	54-31-9	4
Fusaproliferin	C27H40O5	444.2876	152469-17-5	4
Fusarenon-X	C17H22O8	354.1315	23255-69-8	8
Fusarielin A	C25H38O4	402.2770	132341-17-5	4
Fusidic acid	C31H48O6	516.3451	6990-06-3	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	110.0850	N/A	4
Geldanamycin	C29H40N2O9	560.2734	30562-34-6	4
Gemcitabine	C9H11F2N3O4	263.0718	95058-81-4	4
Gemfibrozil	C15H22O3	250.1569	25812-30-0	4
Gentian Violet	C25H30N3	372.2440	548-62-9 (C.I. 42555)	4
gentisic acid	C7H6O4	154.0266	490-79-9	4
Geodin	C17H12Cl2O7	397.9960	427-63-4	8
Gepefrine	C9H13NO	151.0997	18840-47-6	4
Gestodene	C21H26O2	310.1933	60282-87-3	4



Compound	Formula	Formula Weight	CAS Number	# of Spectra
gestrinone	C21H24O2	308.1776	16320-04-0	4
Gibberelic acid	C19H22O6	346.1416	77-06-5	4
Gibberellic acid	C19H22O6	346.1416	77-06-5	8
Gitoxigenin	C23H34O5	390.2406	545-26-6	4
Glafenin	C19H17ClN2O4	372.0877	3820-67-5	4
Glibenclamide	C23H28ClN3O5S	493.1438	10238-21-8	4
Glibornuride	C18H26N2O4S	366.1613	26944-48-9	4
Gliclazide	C15H21N3O3S	323.1304	21187-98-4	4
Glimepiride	C24H34N4O5S	490.2250	93479-97-1	8
Glitoxin	C13H14O4N2S2	326.0395	67-99-2	4
Glipizide	C21H27N5O4S	445.1784	29094-61-9	4
Gliquidone	C27H33N3O6S	527.2090	33342-05-1	8
Glisoxepide	C20H27N5O5S	449.1733	25046-79-1	8
Glucosamine	C6H13NO5	179.0794	3416-24-8	4
Glufosinate	C5H12NO4P	181.0504	77182-82-2	8
glutethimide	C13H15NO2	217.1103	77-21-4	3
glycopyrronium	C19H28NO3	318.2069	596-51-0	4
Glymidine	C13H15N3O4S	309.0783	3459-20-9	4
Granisetron	C18H24N4O	312.1950	109889-09-0	4
Grepafloxacin	C19H22FN3O3	359.1645	161967-81-3	4
Griseofulvin	C17H17ClO6	352.0714	126-07-8	8
Guafecainol	C16H27NO4	297.1940	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	245.0123	29110-47-2	8
guanoclor	C9H12N4OCl2	262.0388	5001-32-1	4
Guanoxan	C10H13N3O2	207.1008	2165-19-7	4
Halcinonide	C24H32ClFO5	454.1922	3093-35-4	8
Halfenprox	C24H23BrF2O3	476.0799	111872-58-3	8
Halofantrine	C26H30Cl2F3NO	499.1657	69756-53-2	4
Halofenozide	C18H19ClN2O2	330.1135	112226-61-6	12
Halofuginone	C16H17BrClN3O3	413.0142	55837-20-2	12
Halometasone	C22H27ClF2O5	444.1515	50629-82-8	4
Haloperidol	C21H23ClFNO2	375.1401	52-86-8	4
Haloperidol-D4	C21H19ClD4FNO2	379.1652	136765-35-0	4
Halosulfuron-methyl	C13H15ClN6O7S	434.0411	100784-20-1	9
haloxon	C14H14O6PCl3	413.9594	321-55-1	4
Haloxypop ethoxyethyl ester	C19H19ClF3NO5	433.0904	87237-48-7	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Haloxyfop-etotyl	C19H19ClF3NO5	433.0904	87237-48-7	8
Haloxyfop-P	C15H11ClF3NO4	361.0329	95977-29-0	4
Haloxyfop-P-methyl	C16H13ClF3NO4	375.0485	72619-32-0	8
Hapargoside	C24H30O11	494.1788	19210-12-9	8
HC-Toxin	C21H32N4O6	436.2322	83209-65-8	8
Heptaminol	C8H19NO	145.1467	372-66-7	4
Heptenophos	C9H12ClO4P	250.0162	23560-59-0	8
Heroin	C21H23NO5	369.1576	561-27-3	4
Hesperidin	C28H34O15	610.1898	520-26-3	4
Hexacarbacholine	C18H40N4O4	376.3050	306-41-2	4
Hexachlorophene	C13H6Cl6O2	403.8499	70-30-4	4
Hexaconazole	C14H17Cl2N3O	313.0749	79983-71-4	8
Hexaflumuron	C16H8Cl2F6N2O3	459.9816	86479-06-3	12
Hexamethonium	C12H30N2	202.2409	60-26-4	4
Hexamidine	C20H26N4O2	354.2056	3811-75-4	4
Hexazinone	C12H20N4O2	252.1586	51235-04-2	12
Hexobendine	C30H44N2O10	592.2996	54-03-5	4
Hexythiazox	C17H21ClN2O2S	352.1012	78587-05-0	8
Histamine	C5H9N3	111.0796	51-45-6	4
Histapyrrodine	C19H24N2	280.1939	493-80-1	4
Histidine	C6H9N3O2	155.0695	71-00-1	4
HMMA	C11H17NO2	195.1259	117652-28-5	4
Homatropine	C16H21NO3	275.1521	87-00-3	4
homidium	C21H20N3	314.1657	3546-21-2	4
Homofenazine	C23H28F3N3OS	451.1905	1256-01-5	4
Hordenine	C10H15NO	165.1154	539-15-1	4
HT-2-Toxin	C22H32O8	424.2097	26934-87-2	4
Hydralazine	C8H8N4	160.0749	86-54-4	4
Hydramethylnon	C25H24F6N4	494.1905	67485-29-4	8
hydrastine	C21H21NO6	383.1369	118-08-1	4
Hydrochlorothiazide	C7H8ClN3O4S2	296.9645	58-93-5	4
Hydrocodone	C18H21NO3	299.1521	125-29-1	5
Hydrocortisone	C21H30O5	362.2093	50-23-7	5
Hydrocortisone 21-acetate	C23H32O6	404.2199	50-03-3	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
hydrolyzed Fumonisin B1	C22H47NO5	405.3454	145040-09-1	4
Hydromorphone	C17H19NO3	285.1365	466-99-9	4
Hydroxychlorquine	C18H26ClN3O	335.1764	118-42-3	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Hydroxymebendazole	C16H15N3O3	297.1113	60254-95-7	4
Hydroxymethylpyridine	C6H7NO	109.0528	N/A	4
hydroxyprogesterone acetate	C23H32O4	372.2301	302-23-8	4
hydroxyprogesterone caproate	C27H40O4	428.2927	630-56-8	4
Hydroxythiabendazole	C10H7N3OS	217.0310	948-71-0	4
Hydroxyzine	C21H27ClN2O2	374.1761	68-88-2	4
Hymecromone	C10H8O3	176.0473	90-33-5	8
hyoscine	C17H21NO4	303.1471	51-34-3	4
Hyoscyamine	C17H23NO3	289.1678	101-31-5	4
Ibogaine	C20H26N2O	310.2045	83-74-9	4
Ibuprofen	C13H18O2	206.1307	15687-27-1	5
Idarubicin	C26H27NO9	497.1686	58957-92-9	4
Idoxuridine	C9H11N2O5	353.9713	54-42-2	4
Ifosfamide	C7H15Cl2N2O2P	260.0248	3778-73-2	4
Imazalil	C14H14Cl2N2O	296.0483	35554-44-0	8
Imazamethabenz-methyl	C16H20N2O3	288.1474	81405-85-8	8
Imazapic	C14H17N3O3	275.1270	104098-48-8	12
Imazapyr	C13H15N3O3	261.1113	81334-34-1	9
Imazaquin	C17H17N3O3	311.1270	81335-37-7	8
Imazethapyr	C15H19N3O3	289.1426	81335-77-5	8
Imazosulfuron	C14H13ClN6O5S	412.0357	122548-33-8	4
Imibenconazole	C17H13Cl3N4S	409.9927	86598-92-7	8
Imiclozapine	C25H32ClN5OS	485.2016	7224-08-0	4
Imidacloprid	C9H10ClN5O2	255.0523	138261-41-3	12
Imidacloprid-Olefin	C9H8ClN5O2	253.0367	not available	12
Imidapril	C20H27N3O6	405.1900	89371-37-9	4
Iminostilbene	C14H11N	193.0891	256-96-2	4
Imipramine	C19H24N2	280.1939	50-49-7	4
Imiquimod	C14H16N4	240.1375	99011-02-6	4
Imolamine	C14H20N4O	260.1637	318-23-0	4
Inabenfide	C19H15ClN2O2	338.0822	82211-24-3	8
Indanazoline	C12H15N3	201.1266	40507-78-6	4
indapamide	C16H16ClN3O3S	365.0601	26807-65-8	4
Indapamine	C16H16ClN3O3S	365.0601	26807-65-8	4
Indinavir	C36H47N5O4	613.3628	150378-17-9	4
Indomethacin	C19H16ClNO4	357.0768	53-86-1	9
Indoprofen	C17H15NO3	281.1052	31842-01-0	4
Indoramin	C22H25N3O	347.1998	26844-12-2	4
Indoxacarb	C22H17ClF3N3O7	527.0707	173584-44-6	8
Inosine	C10H12N4O5	268.0808	58-63-9	8

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Iobitridol	C20H28I3N3O9	834.8960	136949-58-1	4
Iodosulfuron-methyl	C14H13IN5O6S	505.9631	185119-76-0	8
Ioglicic acid	C13H12I3N3O5	670.7911	49755-67-1	4
Ionomycin	C41H72O9	708.5176	56092-82-1	4
Iopodic acid	C12H13I3N2O2	597.8111	5587-89-3	4
Ioxynil	C7H3I2NO	370.8304	1689-83-4	4
Ipconazole	C18H24CIN3O	333.1608	125225-28-7	8
Ipratropium	C20H30NO3	332.2226	22254-24-6	4
Iprazochrome	C12H16N4O3	264.1222	7248-21-7	8
Iprindole	C19H28N2	284.2252	5560-72-5	4
Iprobenfos	C13H21O3PS	288.0949	26087-47-8	4
Iprodione	C13H13Cl2N3O3	329.0334	36734-19-7	10
iproniazid	C9H13N3O	179.1059	54-92-2	4
Ipronidazole	C7H11N3O2	169.0851	14885-29-1	4
Ipronidazole-OH	C7H11N3O3	185.0800	35175-14-5	4
Ipronidazole-OH-D3	C7H8D3N3O3	188.0989		4
Iprovalicarb	C18H28N2O3	320.2100	140923-17-7	8
Irbesartan	C25H28N6O	428.2325	138402-11-6	4
Isazofos	C9H17CIN3O3PS	313.0417	42509-80-8	8
Isoaminile	C16H24N2	244.1939	77-51-0	4
Isocarbamid	C8H15N3O2	185.1164	30979-48-7	8
Isocarboxazid	C12H13N3O2	231.1008	59-63-2	4
Isochlortetracycline	C22H23CIN2O8	478.1143	514-53-4	4
Isoconazole	C18H14Cl4N2O	413.9860	24168-96-5	4
isoetarine	C13H21NO3	239.1521	530-08-5	4
Isofenphos	C15H24NO4PS	345.1164	25311-71-1	8
Isofenphos-oxon	C15H24NO5P	329.1392	31120-85-1	12
isoflupredone	C21H27O5F	378.1843	338-95-4	4
isometamidium	C28H26N7	460.2250	20438-03-3	4
Isoniazide	C6H7N3O	137.0589	54-85-3	4
Isoprenaline	C11H17NO3	211.1208	7683-59-3	8
Isoprocarb	C11H15NO2	193.1103	2631-40-5	8
isopropamide	C23H33N2O	353.2593	7492-32-2	4
Isoprothiolane	C12H18O4S2	290.0647	50512-35-1	8
Isoproturon	C12H18N2O	206.1419	34123-59-6	16
Isothipendyl	C16H19N3S	285.1300	482-15-5	4
Isoxaben	C18H24N2O4	332.1736	82558-50-7	8
Isoxadifen-ethyl	C18H17NO3	295.1208	163520-33-0	12
Isoxaflutole	C15H12F3NO4S	359.0439	141112-29-0	8
Isoxathion	C13H16NO4PS	313.0538	18854-01-8	8

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Isoxicam	C14H13N3O5S	335.0576	34552-84-6	8
Isoxsuprine	C18H23NO3	301.1678	395-28-8	4
Isradipine	C19H21N3O5	371.1481	75695-93-1	4
Jasmolin I	C21H30O3	330.2195	4466-14-2	4
Jasmolin II	C22H30O5	374.2093	1172-63-0	4
Josamycin	C42H69NO15	827.4667	16846-24-5	4
K252a	C27H21N3O5	467.1481	97161-97-2	4
K252b	C26H19N3O5	453.1325	99570-78-2	8
Kavain	C14H14O3	230.0943	500-64-1	4
Ketamine	C13H16CINO	237.0920	6740-88-1	4
Ketazolam	C20H17CIN2O3	368.0928	27223-35-4	4
ketocaine	C18H29NO2	291.2198	1092-46-2	4
Ketoconazole	C26H28Cl2N4O4	530.1488	65277-42-1	4
Ketoprofen	C16H14O3	254.0943	22071-15-4	8
Ketorolac	C15H13NO3	255.0895	74103-06-3	4
Ketotifen	C19H19NOS	309.1187	34580-13-7	4
Ketotriclabendazole	C13H7Cl3N2O2	327.9573		4
Khellin	C14H12O5	260.0685	82-02-0	4
Kojic acid	C6H6O4	142.0266	501-30-4	4
Kresoxim-methyl	C18H19NO4	313.1314	143390-89-0	9
Labetalol	C19H24N2O3	328.1787	36894-69-6	4
Lacidipine	C26H33NO6	455.2308	103890-78-4	8
Lactitol	C12H24O11	344.1319	585-86-4	4
Lactofen	C19H15ClF3NO7	461.0489	77501-63-4	8
Laidlomycin propionate -Ammonium	C40H69O13N	771.4769	84799-02-0	4
lambda-Cyhalothrin	C23H19ClF3NO3	449.1006	91465-08-6	12
Lamivudine	C8H11N3O3S	229.0521	134678-17-4	4
Lamotrigine	C9H7Cl2N5	255.0079	84057-84-1	4
Lasalocid	C34H54O8	590.3819	25999-31-9	8
Lauroguadine	C20H36N6O	376.2951	135-43-3	4
Leflunomide	C12H9F3N2O2	270.0616	75706-12-6	4
Lenacil	C13H18N2O2	234.1368	2164-08-1	8
Lercanidipine	C36H41N3O6	611.2995	100427-26-7	4
letrozole	C17H11N5	285.1014	112809-51-5	4
Leucogentian violet	C25H31N3	373.2518	603-48-5	4
Leucomalachite green	C23H26N2	330.2096	129-73-7	4
Leucomalachite green-D5	C23H21D5N2	335.2410		4
Levallorphan	C19H25NO	283.1936	152-02-3	4
Levobunolol	C17H25NO3	291.1834	47141-41-4	4
Levocabastine	C26H29FN2O2	420.2213	79516-68-0	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Levodopa	C9H11NO4	197.0688	59-92-7	8
Levomepromazine	C19H24N2OS	328.1609	60-99-1	4
levophacetoperane	C14H19NO2	233.1416	24558-01-8	4
Levopropylhexedrin	C10H21N	155.1674	6192-97-8	4
Lidocaine	C14H22N2O	234.1732	137-58-6	4
lidoflazine	C30H35F2N3O	491.2748	3416-26-0	4
Lincomycin	C18H34N2O6S	406.2138	154-21-2	12
Linuron	C9H10Cl2N2O2	248.0119	330-55-2	8
Liothyronine	C15H12I3NO4	650.7901	6893-02-3	8
Lisinopril	C21H31N3O5	405.2264	76547-98-3	4
Lisurid	C20H26N4O	338.2107	18016-80-3	4
Lobeline	C22H27NO2	337.2042	90-69-7	4
Lofepramine	C26H27ClN2O	418.1812	23047-25-8	4
lofedidine	C11H12Cl2N2O	258.0327	31036-80-3	4
Lolitre B	C42H55NO7	685.3979	81771-19-9	8
Lomefloxacin	C17H19F2N3O3	351.1394	98079-51-7	4
Lonazolac	C17H13ClN2O2	312.0666	53808-88-1	4
Loperamide	C29H33ClN2O2	476.2231	53179-11-6	4
loprazolam	C23H21N6O3Cl	464.1364	61197-73-7	4
Loracarbef	C16H16ClN3O4	349.0829	76470-66-1	4
Loratadine	C22H23ClN2O2	382.1448	79794-75-5	4
Lorazepam	C15H10Cl2N2O2	320.0119	846-49-1	5
Lormetazepam	C16H12Cl2N2O2	334.0276	848-75-9	4
Lornoxicam	C13H10ClN3O4S2	370.9801	70374-39-9	8
Losartan	C22H23ClN6O	422.1622	114798-39-9	4
Lovastatin	C24H36O5	404.2563	75330-75-5	4
Loxapine	C18H18ClN3O	327.1138	1977-10-2	4
lucanthone	C20H24N2OS	340.1609	479-50-5	4
Lufenuron	C17H8Cl2F8N2O3	509.9784	103055-07-8	8
Lysergide	C20H25N3O	323.1998	50-73-3	4
Lysergol	C16H18N2O	254.1419	602-85-7	4
Macrosporin	C16H12O5	284.0685	22225-67-8	8
Maduramycin	C47H80O17	916.5396	84878-61-5	4
Mafenide	C7H10N2O2S	186.0463	138-39-6	4
Malachite green	C23H25N2	329.2018	10309-95-2	4
Malaoxon	C10H19O7PS	314.0589	1634-78-2	8
Malathion	C10H19O6PS2	330.0361	121-75-5	11
Maleic hydrazide	C4H4N2O2	112.0273	123-33-1	11
Malformin C	C23H39N5O5S2	529.2393	59926-78-2	4
Mandipropamid	C23H22ClNO4	411.1237	374726-62-2	13

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Maprotiline	C20H23N	277.1830	10262-69-8	4
Marbofloxacin	C17H19FN4O4	362.1390	115550-35-1	4
Marcfortine A	C28H35N3O4	477.2628	75731-43-0	4
Mazindol	C16H13ClN2O	284.0716	22232-71-9	4
MCPA	C9H9ClO3	200.0240	94-74-6	4
MCPA-2-Ethylhexylester	C17H25ClO3	312.1492	29450-45-1	8
MCPA-butotyl	C15H21ClO4	300.1128	19480-43-4	8
MCPB	C11H13ClO3	228.0553	94-81-5	4
Mebendazole	C16H13N3O3	295.0957	31431-39-7	8
Mebeverine	C25H35NO5	429.2515	3625-06-7	4
mebhydrolin	C19H20N2	276.1626	524-81-2	4
Mecarbam	C10H20NO5PS2	329.0521	2595-54-2	12
Meclofenamic acid	C14H11Cl2NO2	295.0167	644-62-2	8
Meclofenoxate	C12H16NO3Cl	257.0819	51-68-3	4
Mecloxamine	C19H24ClNO	317.1546	5668-06-4	4
Meclozine	C25H27ClN2	390.1863	569-65-3	8
meconine	C10H10O4	194.0579	569-31-3	4
Mecoprop-P	C10H11ClO3	214.0397	16484-77-8	4
Medazepam	C16H15ClN2	270.0924	2898-12-6	4
medetomidine	C13H16N2	200.1313	86347-14-0	4
medetomidine carboxylic acid	C13H14N2O2	230.1055	N/A	4
Medroxyprogesterone 17-acetate	C24H34O4	386.2457	71-58-9	4
medroxyprogesterone acetate	C24H34O4	386.2457	71-58-9	4
Mefenacet	C16H14N2O2S	298.0776	73250-68-7	12
Mefenamic acid	C15H15NO2	241.1103	61-68-7	8
Mefenorex	C12H18ClN	211.1128	17243-57-1	4
Mefenpyr-diethyl	C16H18Cl2N2O4	372.0644	135590-91-9	8
Mefexamide	C15H24N2O3	280.1787	1227-61-8	4
Mefloquine	C17H16F6N2O	378.1167	53230-10-7	4
Mefruside	C13H19ClN2O5S2	382.0424	7195-27-9	8
megestrol acetate	C24H32O4	384.2301	51154-23-5	8
Melatonin	C13H16N2O2	232.1212	73-31-4	8
Meleagrins	C23H23N5O4	433.1750	71751-77-4	8
melengestrol	C23H30O3	354.2195	5633-18-1	4
melengestrol acetate	C25H32O4	396.2301	2919-66-6	8
Melengestrol acetate-D3	C25H29O4D3	399.2489		4
Melitracen	C21H25N	291.1987	5118-29-6	4
Meloxicam	C14H13N3O4S2	351.0347	71125-38-7	4
Melperone	C16H22FNO	263.1685	3575-80-2	4
Melphalan	C13H18Cl2N2O2	304.0745	148-82-3	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Mepacrine	C23H30ClN3O	399.2077	83-89-6	4
Mepanipyrim	C14H13N3	223.1109	110235-47-7	8
mepazine	C19H22N2S	310.1504	60-89-9	4
mepenzolate	C21H26NO3	340.1913	25990-43-6	4
Meperidine	C15H21NO2	247.1572	125-29-1	4
Meperidine-D4	C15H17D4NO2	251.1823	53484-73-4	4
mephenoxalone	C11H13NO4	223.0845	70-07-5	4
Mephentermine	C11H17N	163.1361	100-92-5	4
Mepindolol	C15H22N2O2	262.1681	23694-81-7	4
Mepiquat	C7H16N	114.1283	24307-26-4	4
Mepivacaine	C15H22N2O	246.1732	96-88-8	4
Meprobamate	C9H18N2O4	218.1267	57-53-4	5
Mepronil	C17H19NO2	269.1416	55814-41-0	8
Meptazinol	C15H23NO	233.1780	54340-58-8	4
mepyramine	C17H23N3O	285.1841	91-84-9	4
Mequitazine	C20H22N2S	322.1504	29216-28-2	4
mesalazine	C7H7NO3	153.0426	89-57-6	4
Mescaline	C11H17NO3	211.1208	54-04-6	4
mesocarb	C18H18N4O2	322.1430	34262-84-5	4
Mesoridazine	C21H26N2OS2	386.1487	5588-33-0	4
Mesosulfuron-methyl	C17H21N5O9S2	503.0781	208465-21-8	8
Mesotrione	C14H13NO7S	339.0413	104206-82-8	12
mesterolone	C20H32O2	304.2402	1424-00-6	4
Mesuximide	C12H13NO2	203.0946	77-41-8	4
Metaclazepam	C18H18BrClN2O	392.0291	65517-27-3	4
Metaflumizone	C24H16F6N4O2	506.1177	139968-49-3	4
Metalaxyl	C15H21NO4	279.1471	57837-19-1	8
Metamfepramone	C11H15NO	177.1154	15351-09-4	4
Metamitron	C10H10N4O	202.0855	41394-05-2	20
Metamizol	C13H17N3O4S	311.0940	68-89-3	8
metaraminol	C9H13NO2	167.0946	54-49-9	4
metaxalone	C12H15NO3	221.1052	1665-48-1	4
Metazachlor	C14H16ClN3O	277.0982	67129-08-2	13
Metconazole	C17H22ClN3O	319.1451	125116-23-6	8
Metenolone acetate	C22H32O3	344.2351	434-05-9	4
Metformin	C4H11N5	129.1014	657-24-9	4
Methabenzthiazuron	C10H11N3OS	221.0623	18691-97-9	16
Methacrifos	C7H13O5PS	240.0221	30864-28-9	8
Methadone	C21H27NO	309.2093	76-99-3	4
Methamidophos	C2H8NO2PS	141.0013	10265-92-6	12



Compound	Formula	Formula Weight	CAS Number	# of Spectra
Methamphetamine	C10H15N	149.1204	537-46-2	4
Methamphetamine-D11	C10H4D11N	160.1895	152477-88-8	4
Methamphetamine-D8	C10H7D8N	157.1707	136765-40-7	4
Methanthelinium	C21H26NO3	340.1913	53-46-3	4
Methaphenilene	C15H20N2S	260.1347	493-78-7	4
Methapyrilene	C14H19N3S	261.1300	91-80-5	4
Methaqualone	C16H14N2O	250.1106	72-44-6	4
Methazolamide	C5H8N4O3S2	236.0038	554-57-4	8
Methfuroxam	C14H15NO2	229.1103	28730-17-8	12
Methidathion	C6H11N2O4PS3	301.9619	950-37-8	8
Methiocarb	C11H15NO2S	225.0824	2032-65-7	8
Methiocarb-sulfoxide	C11H15NO3S	241.0773	2635-10-1	4
Methocarbamol	C11H15NO5	241.0950	532-03-6	4
Methohexital	C14H18N2O3	262.1317	151-83-7	3
Methohexital-D5	C14H13D5N2O3	267.1631	160227-45-2	4
Methomyl	C5H10N2O2S	162.0463	16752-77-5	9
Methomyl-oxime	C3H7NOS	105.0248	13749-94-5	8
Methoprotryne	C11H21N5OS	271.1467	841-06-5	12
Methotrexate	C20H22N8O5	454.1713	59-05-2	4
Methoxyfenozide	C22H28N2O3	368.2100	161050-58-4	8
methoxyphenamine	C11H17NO	179.1310	93-30-1	4
methoxypromazine	C18H22N2OS	314.1453	61-01-8	4
methyclothiazide	C9H11N3O4S2Cl2	358.9568	135-07-9	4
Methyl nicotinate	C7H7NO2	137.0477	93-60-7	4
Methyl dopa	C10H13NO4	211.0845	555-30-6	8
Methylephedrine	C11H17NO	179.1310	552-79-4	4
Methylphenidate	C14H19NO2	233.1416	113-45-1	4
Methylprednisolone	C22H30O5	374.2093	83-43-2	12
methylprednisolone acetate	C24H32O6	416.2199	53-36-1	4
Methylscopolamine	C18H23NO4	317.1627	155-41-9	4
Methylthiouracil	C5H6N2OS	142.0201	56-04-2	8
Methysergide	C21H27N3O2	353.2103	361-37-5	8
meticrane	C10H13NO4S2	275.0286	1084-65-7	4
Metipranolol	C17H27NO4	309.1940	22664-55-7	4
Metixene	C20H23NS	309.1551	4969-02-2	4
Metobromuron	C9H11BrN2O2	258.0004	3060-89-7	8
Metoclopramide	C14H22ClN3O2	299.1401	364-62-5	4
Metofenazate	C31H36ClN3O5S	597.2064	388-51-2	4
Metolachlor	C15H22ClNO2	283.1339	51218-45-2	8
metolazone	C16H16N3O3SCl	365.0601	17560-51-9	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Metolcarb	C9H11NO2	165.0790	1129-41-5	12
Metoprolol	C15H25NO3	267.1834	37350-58-6	4
Metosulam	C14H13Cl2N5O4S	417.0065	139528-85-1	8
Metoxuron	C10H13ClN2O2	228.0666	19937-59-8	8
Metrafenone	C19H21BrO5	408.0572	220899-03-6	8
Metribuzin	C8H14N4OS	214.0888	21087-64-9	12
Metronidazole	C6H9N3O3	171.0644	443-48-1	8
Metronidazole-OH	C6H9N3O4	187.0593	4812-40-2	4
Metsulfuron-methyl	C14H15N5O6S	381.0743	74223-64-6	16
Metyrapone	C14H14N2O	226.1106	54-36-4	4
Mevastatin	C23H34O5	390.2406	73573-88-3	4
Mevinolin	C24H36O5	404.2563	75330-75-5	4
Mevinphos	C7H13O6P	224.0450	7786-34-7	13
Mexacarbate	C12H18N2O2	222.1368	315-18-4	8
Mexiletine	C11H17NO	179.1310	31828-71-4	4
Mezlocillin	C21H25N5O8S2	539.1145	51481-65-3	4
Mianserin	C18H20N2	264.1626	24219-97-4	4
mibolerone	C20H30O2	302.2246	3704-09-4	4
Miconazole	C18H14Cl4N2O	413.9860	22916-47-8	4
Midazolam	C18H13ClFN3	325.0782	59467-70-8	4
Midodrine	C12H18N2O4	254.1267	42794-76-3	4
Milrinone	C12H9N3O	211.0746	78415-72-2	8
Miltefosine	C21H46NO4P	407.3164	58066-85-6	4
Minocycline	C23H27N3O7	457.1849	10118-90-8	8
Minoxidil	C9H15N5O	209.1277	38304-91-5	4
Mirtazapine	C17H19N3	265.1579	61337-67-5	4
Mithramycin	C52H76O24	1084.4727	18378-89-7	4
Mitomycin C	C15H18N4O5	334.1277	50-07-7	4
Mizolastine	C24H25FN6O	432.2074	108612-45-9	4
Moclobemide	C13H17ClN2O2	268.0979	71320-77-9	4
Modafinil	C15H15NO2S	273.0824	68693-11-8	4
Mofebutazone	C13H16N2O2	232.1212	68693-11-8	8
Molinate	C9H17NOS	187.1031	2212-67-1	9
Molindone	C16H24N2O2	276.1838	7416-34-4	4
Molsidomine	C9H14N4O4	242.1015	25717-80-0	4
Monactin	C41H66O12	750.4554	7182-54-9	4
Monensin	C36H62O11	670.4292	17090-79-8	8
monethylglycine xylidide	C12H18N2O	206.1419	N/A	4
Monocrotophos	C7H14NO5P	223.0610	6923-22-4	12
Monolinuron	C9H11ClN2O2	214.0509	1746-81-2	15

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Monuron	C9H11ClN2O	198.0560	150-68-5	12
Moperone	C22H26FNO2	355.1948	1050-79-7	4
Morantel	C12H16N2S	220.1034	20574-50-9	4
Morazone	C23H27N3O2	377.2103	6536-18-1	4
Morphine	C17H19NO3	285.1365	57-27-2	8
Morphine-3-beta-D-glucuronide	C23H27NO9	461.1686	20290-09-9	4
Moxaverine	C20H21NO2	307.1572	10539-19-2	4
Moxidectin	C37H53NO8	639.3771	113507-06-5	12
Moxisylyte	C16H25NO3	279.1834	54-32-0	4
Moxonidine	C9H12ClN5O	241.0730	75438-57-2	4
MTPAP	C14H13N2OF3	282.0980	N/A	4
Myclobutanil	C15H17ClN4	288.1142	88671-89-0	8
Mycophenolic acid	C17H20O6	320.1260	24280-93-1	7
Myriocin	C21H39NO6	401.2777	35891-70-4	4
N,N-Diethyl-m-toluamide	C12H17NO	191.1310	134-62-3	4
N,N-dimethyltryptamine	C12H16N2	188.1313	61-50-7	4
N2-Ethylguanin	C7H9N5O	179.0807	19545-00-7	8
Nabumetone	C15H16O2	228.1150	42924-53-8	4
Nadolol	C17H27NO4	309.1940	42200-33-9	4
nadoxolol	C14H16N2O3	260.1161	54063-51-3	4
Nafcillin	C21H22N2O5S	414.1249	147-52-4	4
Naftidrofuryl	C24H33NO3	383.2460	31329-57-4	4
Naftifine	C21H21N	287.1674	65472-88-0	4
nalbuphine	C21H27NO4	357.1940	20594-83-6	4
Naled	C4H7Br2Cl2O4P	377.7826	300-76-5	12
Nalidixic acid	C12H12N2O3	232.0848	389-08-2	8
Nalorphine	C19H21NO3	311.1521	62-67-9	4
Naloxone	C19H21NO4	327.1471	465-65-6	4
naloxone-3-glucuronide	C25H29NO10	503.1791	22135-79-1	4
Naltrexone	C20H23NO4	341.1627	16590-41-3	4
Nandrolone	C18H26O2	274.1933	434-22-0	4
Naphazoline	C14H14N2	210.1157	835-31-4	4
Napropamide	C17H21NO2	271.1572	15299-99-7	12
Naproxen	C14H14O3	230.0943	22204-53-1	16
Narasin	C43H72O11	764.5075	55134-13-9	8
Natamycin	C33H47NO13	665.3047	7681-93-8	4
N-Despropylpropafenone	C18H21NO3	299.1521	86383-21-3	4
Nebivolol	C22H25F2NO4	405.1752	99200-09-6	4
Neburon	C12H16Cl2N2O	274.0640	555-37-3	8
Nefazodone	C25H32ClN5O2	469.2245	83366-66-9	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Nefopam	C17H19NO	253.1467	13669-70-0	4
Neosolaniol	C19H26O8	382.1628	36519-25-2	4
Neoxaline	C23H25N5O4	435.1907	71812-10-7	8
NG012	C32H38O15	662.2211	141731-76-2	8
nialamide	C16H18N4O2	298.1430	51-12-7	4
Nicametate	C12H18N2O2	222.1368	3099-52-3	4
Nicarbazin	C19H18N6O6	426.1288	330-95-0	4
Nicarbazin (1,3- N,N'-bis(4-nitrophenyl)urea)	C13H10N4O5	302.0651	330-95-0	4
Nicardipine	C26H29N3O6	479.2056	5598-32-5	4
Nicergoline	C24H26BrN3O3	483.1158	27848-84-6	4
Niclosamide	C13H8Cl2N2O4	325.9861	50-65-7	4
Nicosulfuron	C15H18N6O6S	410.1009	111991-09-4	4
Nicotinamide	C6H6N2O	122.0480	98-92-0	5
Nicotinamide N-oxide	C6H6N2O2	138.0429	1986-81-8	4
Nicotine	C10H14N2	162.1157	54-11-5	20
Nidulin	C20H17Cl3O5	442.0142	10089-10-8	4
Nifedipine	C17H18N2O6	346.1165	21829-25-4	4
nifenalol	C11H16N2O3	224.1161	5054-57-9	4
Nifenazone	C17H16N4O2	308.1273	2139-47-1	4
Niflumic acid	C13H9F3N2O2	282.0616	4394-00-7	8
Nigericin	C40H68O11	724.4762	28643-80-3	4
nikethamide	C10H14N2O	178.1106	59-26-7	4
Nilvadipine	C19H19N3O6	385.1274	75530-68-6	4
Nimodipine	C21H26N2O7	418.1740	66085-59-4	4
Nimorazole	C9H14N4O3	226.1066	6506-37-2	4
Nimustine	C9H13ClN6O2	272.0789	42471-28-3	4
Nisoldipine	C20H24N2O6	388.1634	63675-72-9	4
N-Isopropylsalicylamide	C10H13NO2	179.0946	551-35-9	8
Nitenpyram	C11H15ClN4O2	270.0884	120738-89-8	9
Nitrazepam	C15H11N3O3	281.0800	146-22-5	4
Nitrendipine	C18H20N2O6	360.1321	39562-70-4	4
Nivalenol	C15H20O7	312.1209	23282-20-4	8
Nizatidine	C12H21N5O2S2	331.1137	76963-41-2	4
N-Methyl-1-(1,3-benzodioxol-5-yl)-2-butanamine	C12H17NO2	207.1259	103818-46-8	4
N-Methylephedrine	C11H17NO	179.1310	552-79-4	4
Nomifensine	C16H18N2	238.1470	24526-64-5	4
Nonactin	C40H64O12	736.4398	6833-84-7	4
Nonivamide	C17H27NO3	293.1991	2444-46-4	4
Norbuprenorphine	C25H35NO4	413.2566	78715-23-8	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
norbuprenorphine-3β-glucuronide	C31H43NO10	589.2887	N/A	4
Norbuprenorphine-D3	C25H32D3NO4	416.2754	N/A	4
Nordiazepam	C15H11CIN2O	270.0560	1088-11-5	4
Nordiazepam N-ethyl	C17H15N2OCl	298.0873	N/A	4
Nordiazepam-D5	C15H6CID5N2O	275.0874	65891-80-7	4
Norephedrine	C9H13NO	151.0997	14838-15-4	4
Norepinephrine	C8H11NO3	169.0739	51-41-2	4
norethandrolone	C20H30O2	302.2246	52-78-8	4
Norethisterone	C20H26O2	298.1933	68-22-4	4
Norethisterone acetate	C22H28O3	340.2038	51-98-9	4
Norfenefrine	C8H11NO2	153.0790	536-21-0	4
Norfentanyl	C14H20N2O	232.1576	1609-66-1	4
Norfloracin	C16H18FN3O3	319.1332	70458-96-7	8
Norfloracin-D5	C16H13D5FN3O3	324.1646		4
Norflurazon	C12H9ClF3N3O	303.0386	27314-13-2	8
Norflurazon-desmethyl	C11H7ClF3N3O	289.0230	23576-24-1	8
norgestrel	C21H28O2	312.2089	6533-00-2	4
Normeperidine	C14H19NO2	233.1416	77-17-8	6
normethandrone	C19H28O2	288.2089	514-61-4	4
Normorphine	C16H17NO3	271.1208	466-97-7	4
Nornidulin	C19H15Cl3O5	427.9985	33403-37-1	4
Noroxycodone	C17H19NO4	301.1314	57664-96-7	8
Norpropoxyphene	C21H27NO2	325.2042	3376-94-1	8
Norpropoxyphene degradant	C21H26NO	308.2014	N/A	8
Norpseudoephedrine	C9H13NO	151.0997	492-39-7	8
Nortriptyline	C19H21N	263.1674	72-69-5	4
Noscapine	C22H23NO7	413.1475	128-62-1	4
Novaluron	C17H9ClF8N2O4	492.0123	116714-46-6	12
Novobiocin	C31H36N2O11	612.2319	303-81-1	4
Nuarimol	C17H12ClFN2O	314.0622	63284-71-9	12
Obidoxime	C14H16N4O3	288.1222	7683-36-5	12
Ochratoxin A	C20H18NO6Cl	403.0823	303-47-9	8
Ochratoxin alpha	C11H9ClO5	256.0139	19165-63-0	7
Ochratoxin B	C20H19NO6	369.1212	4825-86-9	8
octacaine	C14H22N2O	234.1732	13912-77-1	4
Octopamine	C8H11NO2	153.0790	104-14-3	4
Ofloxacin	C18H20FN3O4	361.1438	82419-36-1	8
Ofurace	C14H16ClNO3	281.0819	58810-48-3	8
Olanzapine	C17H20N4S	312.1409	132539-06-1	4
Oligomycin A	C45H74O11	790.5231	579-13-5	8

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Oligomycin B	C45H72O12	804.5024	11050-94-5	4
Olsalazine	C14H10N2O6	302.0539	15772-48-2	4
Omeprazole	C17H19N3O3S	345.1147	73590-58-6	4
Omethoate	C5H12NO4PS	213.0225	1113-02-6	8
O-Methylsterigmatocystin	C19H14O6	338.0790	17878-69-2	4
Ondansetron	C18H19N3O	293.1528	99614-02-5	4
Ophiobolin A	C25H36O4	400.2614	4611-05-6	4
Ophiobolin B	C25H38O4	402.2770	5601-74-1	8
Opipramol	C23H29N3O	363.2311	315-72-0	4
opromazine	C17H19CIN2OS	334.0907	969-99-3	4
Orbencarb	C12H16CINOS	257.0641	34622-58-7	8
Orbifloxacin	C19H20F3N3O3	395.1457	113617-63-3	4
Orciprenaline	C11H17NO3	211.1208	586-06-1	4
Ormetoprim	C14H18N4O2	274.1430	6981-18-6	4
Ornidazole	C7H10CIN3O3	219.0411	16773-42-5	4
Orphenadrine	C18H23NO	269.1780	83-98-7	4
Oxacillin	C19H19N3O5S	401.1045	66-79-5	4
Oxadiargyl	C15H14Cl2N2O3	340.0381	39807-15-3	8
Oxadiazon	C15H18Cl2N2O3	344.0694	19666-30-9	8
Oxadixyl	C14H18N2O4	278.1267	77732-09-3	17
oxaflumazine	C26H32N3O2F3S	507.2167	16498-21-8	4
Oxamyl	C7H13N3O3S	219.0678	23135-22-0	12
Oxamyl-oxime	C5H10N2O2S	162.0463	30558-43-1	8
Oxaspirodion	C13H14O5	250.0841	774538-95-3	4
Oxasulfuron	C17H18N4O6S	406.0947	144651-06-9	8
Oxatomide	C27H30N4O	426.2420	60607-34-3	4
Oxazepam	C15H11CIN2O2	286.0509	604-75-1	7
Oxcarbazepine	C15H12N2O2	252.0899	28721-07-5	4
Oxedrine	C9H13NO2	167.0946	94-07-5	4
Oxeladin	C20H33NO3	335.2460	468-61-1	4
Oxetacaine	C28H41N3O3	467.3148	126-27-2	4
Oxfendazole	C15H13N3O3S	315.0678	53716-50-0	4
Oxfendazole Sulfone	C15H13N3O4S	331.0627	54029-20-8	4
Oxibendazole	C12H15N3O3	249.1113	20559-55-1	4
Oxiconazole	C18H13Cl4N3O	426.9813	64211-45-6	4
oxidized Elymoclavine	N/A	258.1	N/A	4
oxidized Luol	N/A	290.5	N/A	4
Oxilofrine	C10H15NO2	181.1103	365-26-4	4
Oxitriptan	C11H12N2O3	220.0848	4350-09-8	8
Oxitropium	C19H26NO4	332.1862	30286-75-0	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
oxolamine	C14H19N3O	245.1528	959-14-8	4
Oxolinic Acid	C13H11NO5	261.0637	14698-29-4	4
Oxomemazine	C18H22N2O2S	330.1402	3689-50-7	4
Oxprenolol	C15H23NO3	265.1678	6452-71-7	4
Oxybuprocaine	C17H28N2O3	308.2100	99-43-4	4
Oxybutynin	C22H31NO3	357.2304	5633-20-5	4
Oxycarboxin	C12H13NO4S	267.0565	5259-88-1	4
Oxycodone	C18H21NO4	315.1471	76-42-6	6
Oxydemeton-methyl	C6H15O4PS2	246.0149	301-12-2	8
Oxyfedrine	C19H23NO3	313.1678	15687-41-9	4
Oxyfluorfen	C15H11ClF3NO4	361.0329	42874-03-3	8
oxymesterone	C20H30O3	318.2195	145-12-0	4
Oxymetazoline	C16H24N2O	260.1889	1491-59-4	4
Oxymorphone	C17H19NO4	301.1314	76-41-5	4
Oxypendyl	C20H26N4OS	370.1827	17297-82-4	4
Oxypertine	C23H29N3O2	379.2260	153-87-7	4
oxyphenbutazone	C19H20N2O3	324.1474	129-20-4	8
Oxytetracycline	C22H24N2O9	460.1482	79-57-2	8
p-(Aminomethyl)benzoic acid	C8H9NO2	151.0633	56-91-7	4
Paclobutrazol	C15H20ClN3O	293.1295	76738-62-0	8
pancuronium	C35H60N2O4	572.4553	15500-66-0	4
Papaverine	C20H21NO4	339.1471	58-74-2	4
Paracetamol	C8H9NO2	151.0633	103-90-2	4
Paraherquamide A	C28H35N3O5	493.2577	77392-58-6	6
paramethasone acetate	C24H31O6F	434.2105	1597-82-6	4
Paraoxon	C10H14NO6P	275.0559	311-45-5	12
Paraoxon-methyl	C8H10NO6P	247.0246	950-35-6	8
Parathion	C10H14NO5PS	291.0330	56-38-2	8
Parathion-methyl	C8H10NO5PS	263.0017	298-00-0	10
paraxanthine	C7H8N4O2	180.0647	611-59-6	4
Paroxetine	C19H20FNO3	329.1427	61869-08-7	4
Paspaline	C28H39NO2	421.2981	11024-56-9	4
Paspalinine	C27H31NO4	433.2253	63722-91-8	8
Paspalitre A	C32H39NO4	501.2879	63722-90-7	4
Paspalitre B	C32H39NO5	517.2828	63764-58-9	4
Paxilline	C27H33NO4	435.2410	57186-25-1	8
p-bromophenethylamine	C8H10NBr	198.9997	73918-56-6	4
Pebulate	C10H21NOS	203.1344	1114-71-2	12
pemoline	C9H8N2O2	176.0586	2152-34-3	4
pempidine	C10H21N	155.1674	79-55-0	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Penbutolol	C18H29NO2	291.2198	38363-40-5	4
Penconazole	C13H15Cl2N3	283.0643	66246-88-6	8
Pencycuron	C19H21ClN2O	328.1342	66063-05-6	8
Pendimethalin	C13H19N3O4	281.1376	40487-42-1	9
Penfluridol	C28H27ClF5NO	523.1701	26864-56-2	4
Penicillic acid	C8H10O4	170.0579	90-65-3	4
Penicillin G	C16H18N2O4S	334.0987	61-33-6	12
Penicillin G-D7	C16H10D7N2O4S	340.1348	N/A	4
Penicillin V	C16H18N2O5S	350.0936	87-08-1	8
Penigequinolone A	C27H33NO6	467.2308	180045-91-4	8
Penitrem A	C37H44O6NCl	633.2857	12627-35-9	8
Penoxsulam	C16H14F5N5O5S	483.0636	219714-96-2	8
Pentamidine	C19H24N4O2	340.1899	100-33-4	4
Pentazocine	C19H27NO	285.2093	359-83-1	8
pentetrazol	C6H10N4	138.0905	54-95-5	4
pentifylline	C13H20N4O2	264.1586	8060-62-6	4
Pentobarbital	C11H18N2O3	226.1317	76-74-4	3
Pentobarbital-D5	C11H13D5N2O3	231.1631	52944-66-8	4
Pentoxifylline	C13H18N4O3	278.1379	6493-05-6	8
Pentoxyverine	C20H31NO3	333.2304	77-23-6	4
Perazine	C20H25N3S	339.1769	84-97-9	4
Pergolide	C19H26N2S	314.1817	66104-22-1	4
Periciazine	C21H23N3OS	365.1562	2622-26-6	4
perimethazine	C22H28N2O2S	384.1872	13093-88-4	4
Perindopril	C19H32N2O5	368.2311	82834-16-0	4
perindoprilat	C17H28N2O5	340.1998	95153-31-4	4
Permethrin	C21H20Cl2O3	390.0790	52645-53-1	8
Perphenazine	C21H26ClN3OS	403.1485	58-39-9	4
Pestalotin	C11H18O4	214.1205	34565-32-7	4
Pethidine	C15H21NO2	247.1572	57-42-1	4
Pethoxamid	C16H22ClNO2	295.1339	106700-29-2	8
Phenacetin	C10H13NO2	179.0946	62-44-2	4
phenazocine	C22H27NO	321.2093	127-35-5	4
Phenazone	C11H12N2O	188.0950	60-80-0	4
Phenazopyridine	C11H11N5	213.1014	94-78-0	4
Phencyclidine	C17H25N	243.1987	77-10-1	8
phendimetrazine	C12H17NO	191.1310	21784-30-5	4
Phenelzine	C8H12N2	136.1000	51-71-8	4
Phenethylamin	C8H11N	121.0891	64-04-0	4
phenindamine	C19H19N	261.1517	82-88-2	4



Compound	Formula	Formula Weight	CAS Number	# of Spectra
Phenindione	C15H10O2	222.0681	83-12-5	8
pheniprazine	C9H14N2	150.1157	55-52-7	4
Pheniramine	C16H20N2	240.1626	86-21-5	4
Phenmedipham	C16H16N2O4	300.1110	13684-63-4	12
Phenobarbital	C12H12N2O3	232.0848	50-06-6	4
Phenobarbital-D5	C12H7D5N2O3	237.1162	72793-46-5	3
Phenothiazine	C12H9NS	199.0456	92-84-2	4
Phenoxyethylpenicillin	C16H18N2O5S	350.0936	87-08-1	8
Phenprobamate	C10H13NO2	179.0946	673-31-4	4
Phenprocoumon	C18H16O3	280.1099	435-97-2	4
phentermine	C10H15N	149.1204	122-09-8	4
Phenthoate	C12H17O4PS2	320.0306	2597-03-7	12
Phentolamine	C17H19N3O	281.1528	50-60-2	4
phenyl aminosaliclylate	C13H11NO3	229.0739	133-11-9	4
Phenylbutazone	C19H20N2O2	308.1525	50-33-9	8
Phenylephrine	C9H13NO2	167.0946	59-42-7	4
Phenylpropanolamine	C9H13NO	151.0997	14838-15-4	4
Phenyltoloxamine	C17H21NO	255.1623	92-12-6	4
Phenytoin	C15H12N2O2	252.0899	57-41-0	4
Pholedrine	C10H15NO	165.1154	370-14-9	4
Phomopsin A	C36H45CIN6O12	788.2784	64925-80-0	6
Phorate	C7H17O2PS3	260.0128	298-02-2	8
Phorate-sulfone	C7H17O4PS3	292.0027	2588-04-7	8
Phorate-sulfoxide	C7H17O3PS3	276.0077	2588-03-6	8
Phosalone	C12H15CINO4PS2	366.9869	2310-17-0	8
Phosmet	C11H12NO4PS2	316.9945	732-11-6	11
Phosphamidon	C10H19CINO5P	299.0689	13171-21-6	8
Phoxim	C12H15N2O3PS	298.0541	14816-18-3	12
Phthalylsulfathiazole	C17H13N3O5S2	403.0297	85-73-4	8
Physcion	C16H12O5	284.0685	521-61-9	8
Physostigmine	C15H21N3O2	275.1634	57-47-6	4
Picolinafen	C19H12F4N2O2	376.0835	137641-05-5	8
Picoxystrobin	C18H16F3NO4	367.1031	117428-22-5	8
Pilocarpine	C11H16N2O2	208.1212	92-13-7	4
Pimozide	C28H29F2N3O	461.2279	2062-78-4	4
Pindolol	C14H20N2O2	248.1525	13523-86-9	4
Pioglitazone	C19H20N2O3S	356.1195	111025-46-8	4
pipamazine	C21H24N3OSCI	401.1329	84-04-8	4
Pipamperone	C21H30FN3O2	375.2322	1893-33-0	4
Pipemidic acid	C14H17N5O3	303.1331	51940-44-4	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Piperacillin	C23H27N5O7S	517.1631	61477-96-1	4
piperidione	C9H15NO2	169.1103	77-03-2	4
piperidolate	C21H25NO2	323.1885	82-98-4	4
piperocaine	C16H23NO2	261.1729	32248-37-6	4
Piperonyl-butoxide	C19H30O5	338.2093	51-03-6	8
Piperophos	C14H28NO3PS2	353.1248	24151-93-7	8
piperoxan	C14H19NO2	233.1416	59-39-2	4
pipradol	C18H21NO	267.1623	467-60-7	4
Piprozolin	C14H22N2O3S	298.1351	17243-64-0	4
Piracetam	C6H10N2O2	142.0742	7491-74-9	4
Pirbuterol	C12H20N2O3	240.1474	38677-81-5	4
Pirenzepine	C19H21N5O2	351.1695	28797-61-7	4
Piretanide	C17H18N2O5S	362.0936	55837-27-9	8
Pirimicarb	C11H18N4O2	238.1430	23103-98-2	8
Pirimiphos-ethyl	C13H24N3O3PS	333.1276	23505-41-1	8
Pirimiphos-methyl	C11H20N3O3PS	305.0963	29232-93-7	8
Piritramide	C27H34N4O	430.2733	302-41-0	4
Piroxicam	C15H13N3O4S	331.0627	36322-90-4	4
pirprofen	C13H14NO2Cl	251.0713	31793-07-4	4
Pizotifen	C19H21NS	295.1395	15574-96-6	4
Polythiazide	C11H13ClF3N3O4S3	438.9709	346-18-9	4
Practolol	C14H22N2O3	266.1630	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	383.1594	19216-56-9	4
Prednisolone	C21H28O5	360.1937	50-24-8	12
prednisolone acetate	C23H30O6	402.2042	52-21-1	8
prednisolone pivalate	C26H36O6	444.2512	1107-99-9	4
Prednisone	C21H26O5	358.1780	53-03-2	12
Prenylamine	C24H27N	329.2144	390-64-7	4
Prilocaine	C13H20N2O	220.1576	721-50-6	4
Primaquine	C15H21N3O	259.1685	90-34-6	4
Primidone	C12H14N2O2	218.1055	125-33-7	4
Primisulfuron-methyl	C15H12F4N4O7S	468.0363	86209-51-0	4
probarbital	C9H14N2O3	198.1004	76-76-6	4
Procainamide	C13H21N3O	235.1685	51-06-9	4
Procaine	C13H20N2O2	236.1525	59-46-1	4
procarbazine	C12H19N3O	221.1528	671-16-9	4
Prochloraz	C15H16Cl3N3O2	375.0308	67747-09-5	9

Compound	Formula	Formula Weight	CAS Number	# of Spectra
prochlorperazine	C20H24N3SCI	373.1379	58-38-8	4
Prochlorperazine	C20H24CIN3S	373.1379	58-38-8	4
Procyclidine	C19H29NO	287.2249	77-37-2	4
Procymidone	C13H11CI2NO2	283.0167	32809-16-8	12
Profenamine	C19H24N2S	312.1660	522-00-9	4
Profenofos	C11H15BrClO3PS	371.9351	41198-08-7	8
Progesterone	C21H30O2	314.2246	57-83-0	4
Prohexadione	C10H12O5	212.0685	88805-35-0	12
prolintane	C15H23N	217.1830	493-92-5	4
Promazine	C17H20N2S	284.1347	58-40-2	4
Promecarb	C12H17NO2	207.1259	2631-37-0	8
Promethazine	C17H20N2S	284.1347	60-87-7	4
Prometon	C10H19N5O	225.1590	1610-18-0	8
Prometryn	C10H19N5S	241.1361	7287-19-6	12
Propachlor	C11H14ClNO	211.0764	1918-16-7	8
Propafenone	C21H27NO3	341.1991	54063-53-5	4
Propallylonal	C10H13BrN2O3	288.0110	545-93-7	4
Propamocarb	C9H20N2O2	188.1525	24579-73-5	8
Propanil	C9H9Cl2NO	217.0061	709-98-8	13
propantheline	C23H30NO3	368.2226	298-50-0	4
Propaquizafop	C22H22CIN3O5	443.1248	111479-05-1	8
Propargite	C19H26O4S	350.1552	2312-35-8	8
Propazin-2-hydroxy	C9H17N5O	211.1433	not available	8
Propazine	C9H16CIN5	229.1094	139-40-2	8
Propetamphos	C10H20NO4PS	281.0851	31218-83-4	9
Propham	C10H13NO2	179.0946	122-42-9	12
Propiconazole	C15H17Cl2N3O2	341.0698	60207-90-1	12
propiomazine	C20H24N2OS	340.1609	362-29-8	4
Propionylpromazine	C20H24N2OS	340.1609	3568-24-9	4
Propipocaine	C17H25NO2	275.1885	3670-68-6	4
Propiverine	C23H29NO3	367.2147	60569-19-9	4
propoxur	C11H15NO3	209.1052	114-26-1	12
Propoxycarbazono	C15H18N4O7S	398.0896	181274-15-7	8
Propranolol	C16H21NO2	259.1572	525-66-6	4
Propyphenazone	C14H18N2O	230.1419	479-92-5	4
Propyzamide	C12H11Cl2NO	255.0218	23950-58-5	12
proquazone	C18H18N2O	278.1419	22760-18-5	4
Prosulfocarb	C14H21NOS	251.1344	52888-80-9	8
Prosulfuron	C15H16F3N5O4S	419.0875	94125-34-5	8
Prothioconazole	C14H15Cl2N3OS	343.0313	178928-70-6	8

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Prothioconazole Desthiometabolite	C14H15Cl2N3O	311.0592	not available	8
Prothiofos	C11H15Cl2O2PS2	343.9628	34643-46-4	8
Prothiopendyl	C16H19N3S	285.1300	303-69-5	4
Protionamide	C9H12N2S	180.0721	14222-60-7	8
Protriptyline	C19H21N	263.1674	438-60-8	4
Proximpam	C10H12N2O2	192.0899	2828-42-4	4
proxyphylline	C10H14N4O3	238.1066	603-00-9	4
Pseudoephedrine	C10H15NO	165.1154	90-82-4	4
Pseurotin A	C22H25NO8	431.1580	58523-30-1	7
Psilocin	C12H16N2O	204.1263	520-53-6	4
Puromycin	C22H29N7O5	471.2230	53-79-2	4
Pymetrozine	C10H11N5O	217.0964	123312-89-0	8
Pyracarbolid	C13H15NO2	217.1103	24691-76-7	8
Pyraclufos	C14H18ClN2O3PS	360.0464	89784-60-1	8
Pyraclostrobin	C19H18ClN3O4	387.0986	175013-18-0	8
Pyraflufen-ethyl	C15H13Cl2F3N2O4	412.0204	129630-17-7	8
Pyranocoumarin	C20H18O4	322.1205	518-20-7	4
Pyrazophos	C14H20N3O5PS	373.0861	13457-18-6	8
Pyrenophorol	C16H24O6	312.1573	22248-41-5	4
Pyrethrin I	C21H28O3	328.2038	121-21-1	12
Pyrethrin II	C22H28O5	372.1937	121-29-9	4
Pyribenzamine	C16H21N3	255.1735	91-81-6	4
Pyridaben	C19H25ClN2OS	364.1376	96489-71-3	8
Pyridalyl	C18H14Cl4F3NO3	488.9680	179101-81-6	8
Pyridaphenthion	C14H17N2O4PS	340.0647	119-12-0	8
Pyridate	C19H23ClN2O2S	378.1169	55512-33-9	8
Pyridoxine	C8H11NO3	169.0739	65-23-6	4
Pyrifenox	C14H12Cl2N2O	294.0327	88283-41-4	8
Pyrilamine	C17H23N3O	285.1841	91-84-9	4
Pyrimethamine	C12H13ClN4	248.0829	58-14-0	4
Pyrimethanil	C12H13N3	199.1109	53112-28-0	8
Pyriproxyfen	C20H19NO3	321.1365	95737-68-1	8
Pyripyropene A	C31H37NO10	583.2417	147444-03-9	4
Pyritinol	C16H20N2O4S2	368.0865	1098-97-1	8
Pyroquilon	C11H11NO	173.0841	57369-32-1	8
Pyroxulam	C14H13F3N6O5S	434.0620	422556-08-9	8
pyrrobutamine	C20H22NCl	311.1441	91-82-7	4
Pyrvinium	C26H28N3	382.2283	548-84-5	4
Quetiapine	C21H25N3O2S	383.1667	111974-72-2	4
Quinalphos	C12H15N2O3PS	298.0541	13593-03-8	8

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Quinapril	C25H30N2O5	438.2155	85441-61-8	4
Quinaprilat	C23H26N2O5	410.1842	82768-85-2	8
quinic acid	C7H12O6	192.0634	77-95-2	4
Quinidine	C20H24N2O2	324.1838	56-54-2	4
Quinine	C20H24N2O2	324.1838	130-95-0	8
Quinmerac	C11H8ClNO2	221.0244	90717-03-6	8
Quinoclamine	C10H6ClNO2	207.0087	2797-51-5	8
Quinoxifen	C15H8Cl2FNO	306.9967	124495-18-7	8
Quizalofop-ethyl	C19H17ClN2O4	372.0877	76578-14-8	8
Quizalofop-P (free acid)	C17H13ClN2O4	344.0564	94051-08-8	9
ractopamine	C18H23NO3	301.1678	97825-25-7	8
Radicicol	C18H17ClO6	364.0714	12772-57-5	8
Rafoxanide	C19H11Cl2I2NO3	624.8206	22662-39-1	5
raloxifene	C28H27NO4S	473.1661	84449-90-1	4
Ramifenazone	C14H19N3O	245.1528	3615-24-5	4
Ramipril	C23H32N2O5	416.2311	87333-19-5	4
Ranitidine	C13H22N4O3S	314.1413	66357-35-5	4
Rapamycin	C51H79NO13	913.5551	53123-88-9	8
Raubasine	C21H24N2O3	352.1787	483-04-5	4
Raupin	C19H22N2O2	310.1681	482-68-8	4
Reboxetine	C19H23NO3	313.1678	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
Reserpine	C33H40N2O9	608.2734	50-55-5	4
Resmethrin	C22H26O3	338.1882	10453-86-8	8
Rifampicin	C43H58N4O12	822.4051	13292-46-1	4
Riluzole	C8H5F3N2OS	234.0075	1744-22-5	4
rimeterol	C12H17NO3	223.1208	32953-89-2	4
Rimsulfuron	C14H17N5O7S2	431.0569	122931-48-0	9
Risperidone	C23H27FN4O2	410.2118	106266-06-2	4
Ritodrine	C17H21NO3	287.1521	26652-09-5	4
Rizatriptan	C15H19N5	269.1640	145202-66-0	4
Rocuronium	C32H53N2O4	529.4005	119302-91-9	4
romifidine	C9H9N3FBr	256.9964	65896-16-4	4
Ronidazole	C6H8N4O4	200.0546	7681-76-7	4
Ropinirole	C16H24N2O	260.1889	91374-21-9	4
Ropivacaine	C17H26N2O	274.2045	84057-95-4	4
Roquefortine C	C22H23N5O2	389.1852	58735-64-1	8
Roridin A	C29H40O9	532.2672	14729-29-4	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Rosiglitazon	C18H19N3O3S	357.1147	122320-73-4	4
Rotenone	C23H22O6	394.1416	83-79-4	8
Roxithromycin	C41H76N2O15	836.5246	80214-83-1	4
Rubellin D	C30H22O10	542.1213	121325-49-3	8
Rugulosin	C30H22O10	542.1213	23537-16-8	8
Salbutamol	C13H21NO3	239.1521	18559-94-9	5
Salicylamide	C7H7NO2	137.0477	65-45-2	8
Salinomycin	C42H70O11	750.4918	53003-10-4	4
Salmeterol	C25H37NO4	415.2723	89365-50-4	4
Salsalate	C14H10O5	258.0528	552-94-3	4
Sarafloxacin	C20H17F2N3O3	385.1238	98105-99-8	4
Scopolamine	C17H21NO4	303.1471	51-34-3	4
Sebuthylazine	C9H16CIN5	229.1094	7286-69-3	12
Sebuthylazine-desethyl	C7H12CIN5	201.0781	not available	9
Secalonic acid	C32H30O14	638.1636	56283-72-8	8
Secbumeton	C10H19N5O	225.1590	26259-45-0	8
Secbutabarbital	C10H16N2O3	212.1161	125-40-6	3
Selegilin	C13H17N	187.1361	14611-51-9	4
Semduramicin	C45H76O16	872.5133	113378-31-7	4
Serotonin	C10H12N2O	176.0950	50-67-9	4
Sertindole	C24H26CIFN4O	440.1779	106516-24-9	4
Sertraline	C17H17Cl2N	305.0738	79559-97-0	4
Sethoxydim	C17H29NO3S	327.1868	74051-80-2	8
Setosusin	C29H38O8	514.2567	182926-45-0	4
Sibutramin	C17H26CIN	279.1754	106650-56-0	4
Siduron	C14H20N2O	232.1576	1982-49-6	8
Sildenafil	C22H30N6O4S	474.2049	139755-83-2	4
Silthiofam	C13H21NOSSi	267.1113	175217-20-6	4
Simazine	C7H12CIN5	201.0781	122-34-9	12
Simazine-2-hydroxy	C7H13N5O	183.1120	2599-11-3	12
Simetryn	C8H15N5S	213.1048	1014-70-6	8
Simvastatin	C25H38O5	418.2719	79902-63-9	4
Sotalol	C12H20N2O3S	272.1195	959-24-0	4
Spinetoram A	C42H69NO10	747.4921	187166-40-1	8
Spinetoram B	C43H69NO10	759.4921	187166-15-0	8
Spinosyn A	C41H65NO10	731.4608	131929-60-7	7
Spinosyn D	C42H67NO10	745.4765	131929-63-0	11
Spiramycin	C43H74N2O14	842.5140	8025-81-8	4
Spirapril	C22H30N2O5S2	466.1596	83647-97-6	8
Spirodiclofen	C21H24Cl2O4	410.1052	148477-71-8	8

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Spiromesifen	C23H30O4	370.2144	283594-90-1	8
spironolactone	C24H32O4S	416.2021	52-01-7	4
Spirotetramat	C21H27NO5	373.1889	203313-25-1	8
Spiroxamine	C18H35NO2	297.2668	118134-30-8	8
Stachybotrylactam	C23H31NO4	385.2253	163391-76-2	4
Stanozolol	C21H32N2O	328.2515	10418-03-8	4
Staurosporine	C28H26N4O3	466.2005	62996-74-1	4
Sterigmatocystin	C18H12O6	324.0634	10048-13-2	4
strychnine	C21H22N2O2	334.1681	57-24-9	4
Sulcotrione	C14H13ClO5S	328.0172	99105-77-8	12
Sulfabenzamide	C13H12N2O3S	276.0569	127-71-9	12
Sulfacetamide	C8H10N2O3S	214.0412	144-80-9	8
Sulfachloropyridazine	C10H9ClN4O2S	284.0135	80-32-0	4
Sulfacloamide	C12H13ClN4O2S	312.0448	4015-18-3	8
Sulfaclozine	C10H9ClN4O2S	284.0135	102-65-8	4
Sulfadiazine	C10H10N4O2S	250.0524	68-35-9	8
Sulfadicramide	C11H14N2O3S	254.0725	115-68-4	8
Sulfadimethoxine	C12H14N4O4S	310.0736	122-11-2	4
Sulfadoxine	C12H14N4O4S	310.0736	2447-57-6	12
Sulfaethidole	C10H12N4O2S2	284.0402	94-19-9	8
Sulfaguanidine	C7H10N4O2S	214.0524	57-67-0	8
Sulfalene	C11H12N4O3S	280.0630	152-47-6	4
Sulfamerazine	C11H12N4O2S	264.0681	127-79-7	8
Sulfameter	C11H12N4O3S	280.0630	651-06-9	4
Sulfamethazine	C12H14N4O2S	278.0837	57-68-1	4
Sulfamethazine-D4	C12H10D4N4O2S	282.1089	N/A	4
Sulfamethizole	C9H10N4O2S2	270.0245	144-82-1	12
Sulfamethoxazole	C10H11N3O3S	253.0521	723-46-6	12
Sulfamethoxazole-D4	C10H7D4N3O3S	257.0772	N/A	4
Sulfamethoxypyridazine	C11H12N4O3S	280.0630	80-35-3	8
Sulfamonomethoxine	C11H12N4O3S	280.0630	1220-83-3	4
Sulfamoxole	C11H13N3O3S	267.0678	729-99-7	4
Sulfanilamide	C6H8N2O2S	172.0306	63-74-1	4
Sulfanilic Acid	C6H7NO3S	173.0147	121-57-3	4
Sulfanitran	C14H13N3O5S	335.0576	122-16-7	4
Sulfaphenazole	C15H14N4O2S	314.0837	526-08-9	4
Sulfapyridine	C11H11N3O2S	249.0572	144-83-2	8
Sulfaquinoxaline	C14H12N4O2S	300.0681	59-40-5	12
Sulfasalazine	C18H14N4O5S	398.0685	599-79-1	9
Sulfathiazole	C9H9N3O2S2	255.0136	42-14-0	12

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Sulfathiazole-D4	C9H5D4N3O2S2	259.0387	N/A	4
Sulfentrazone	C11H10Cl2F2N4O3S	385.9819	122836-35-5	12
Sulfinpyrazone	C23H20N2O3S	404.1195	57-96-5	4
Sulfisomidine	C12H14N4O2S	278.0837	515-64-0	4
Sulfisoxazole	C11H13N3O3S	267.0678	127-69-5	4
Sulfometuron-methyl	C15H16N4O5S	364.0841	74222-97-2	8
Sulfosulfuron	C16H18N6O7S2	470.0678	141776-32-1	8
Sulfotep	C8H20O5P2S2	322.0227	3689-24-5	8
Sulindac	C20H17FO3S	356.0882	38194-50-2	4
Sulochrin	C17H16O7	332.0896	519-57-3	8
Sulpiride	C15H23N3O4S	341.1409	15676-16-1	4
Sulprofos	C12H19O2PS3	322.0285	35400-43-2	8
Sultiame	C10H14N2O4S2	290.0395	61-56-3	8
Sumatriptan	C14H21N3O2S	295.1354	103628-46-2	4
Suxibuzone	C24H26N2O6	438.1791	27470-51-5	8
T2-Tetraol	C15H22O6	298.1416	34114-99-3	4
T2-Toxin	C24H34O9	466.2203	21259-20-1	4
T2-Triol	C20H30O7	382.1992	34114-98-2	4
Tacrine	C13H14N2	198.1157	321-64-2	4
Tadalafil	C22H19N3O4	389.1376	171596-29-5	4
Talinolol	C20H33N3O3	363.2522	57460-41-0	4
Tamoxifen	C26H29NO	371.2249	10540-29-1	4
tau-Fluvalinate	C26H22ClF3N2O3	502.1271	102851-06-9	8
Taxol	C47H51NO14	853.3310	33069-62-4	8
Tebuconazole	C16H22ClN3O	307.1451	107534-96-3	12
Tebufenozide	C22H28N2O2	352.2151	112410-23-8	8
Tebufenpyrad	C18H24ClN3O	333.1608	119168-77-3	8
Tebupirimfos	C13H23N2O3PS	318.1167	96182-53-5	8
Tebutam	C15H23NO	233.1780	35256-85-0	4
Tebuthiuron	C9H16N4OS	228.1045	34014-18-1	8
Teflubenzuron	C14H6Cl2F4N2O2	379.9742	83121-18-0	12
Telmisartan	C33H30N4O2	514.2369	144701-48-4	4
Temazepam	C16H13ClN2O2	300.0666	846-50-4	8
Temephos	C16H20O6P2S3	465.9897	3383-96-8	8
tenamfetamine	C10H13NO2	179.0946	4764-17-4	4
Teniposide	C32H32O13S	656.1564	29767-20-2	4
Tenocixam	C13H11N3O4S2	337.0191	59804-37-4	4
Tentoxin	C22H30N4O4	414.2267	28540-82-1	8
Tenuazonic acid	C10H15O3N	197.1052	610-88-8	8
TEPP	C8H20O7P2	290.0684	107-49-3	8



Compound	Formula	Formula Weight	CAS Number	# of Spectra
Tepraloxidim	C17H24ClNO4	341.1394	149979-41-9	4
Terazosine	C19H25N5O4	387.1907	63590-64-7	4
Terbacil	C9H13ClN2O2	216.0666	5902-51-2	4
Terbinafine	C21H25N	291.1987	91161-71-6	4
Terbufos	C9H21O2PS3	288.0441	13071-79-9	8
Terbumeton	C10H19N5O	225.1590	33693-04-8	12
Terbutaline	C12H19NO3	225.1365	23031-25-6	4
Terbutylazine	C9H16ClN5	229.1094	5915-41-3	12
Terbutylazine-2-hydroxy	C9H17N5O	211.1433	not available	8
Terbutylazine-desethyl	C7H12ClN5	201.0781	30125-63-4	8
Terbutryn	C10H19N5S	241.1361	886-50-0	12
Terconazole	C26H31Cl2N5O3	531.1804	67915-31-5	4
Terfenadine	C32H41NO2	471.3137	50679-08-8	4
Terphenyllin	C20H18O5	338.1154	52452-60-5	8
Territrem B	C29H34O9	526.2203	70407-20-4	4
Tertalolol	C16H25NO2S	295.1606	34784-64-0	4
Testosterone	C19H28O2	288.2089	58-22-0	4
Testosterone benzoate	C26H32O3	392.2351	2088-71-3	4
testosterone-D3	C19D3H25O2	291.2278	77546-39-5	4
Tetracaine	C15H24N2O2	264.1838	94-24-6	5
Tetrachlorvinphos	C10H9Cl4O4P	363.8993	22248-79-9	8
Tetraconazole	C13H11Cl2F4N3O	371.0215	112281-77-3	8
Tetracycline	C22H24N2O8	444.1533	60-54-8	16
Tetramethrin	C19H25NO4	331.1784	7696-12-0	13
tetramisole	C11H12N2S	204.0721	5036-02-2	8
Tetrazepam	C16H17ClN2O	288.1029	10379-14-3	4
Tetroxoprim	C16H22N4O4	334.1641	53808-87-0	4
Tetryzoline	C13H16N2	200.1313	84-22-0	4
THC	C21H30O2	314.2246	7683-36-5	5
THC-COOH	C21H28O4	344.1988	23978-85-0	8
THC-OH	C21H30O3	330.2195	366557-05-08	8
Thebacon	C20H23NO4	341.1627	466-90-0	4
Thenalidine	C17H22N2S	286.1504	86-12-4	4
thenyldiamine	C14H19N3S	261.1300	91-79-2	4
Theobromine	C7H8N4O2	180.0647	83-67-0	4
Theodrenaline	C17H21N5O5	375.1543	13460-98-5	4
Theophylline	C7H8N4O2	180.0647	58-55-9	4
Thiabendazole	C10H7N3S	201.0361	148-79-8	16
Thiabendazole-13C6	C4H7(13C)6N3S	207.0562	N/A	4
Thiacloprid	C10H9ClN4S	252.0236	111988-49-9	8

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Thiamazole	C4H6N2S	114.0252	60-56-0	4
Thiamethoxam	C8H10ClN5O3S	291.0193	153719-23-4	12
Thiamine	C12H17N4OS	265.1123	59-43-8	4
Thiamphenicol	C12H15Cl2NO5S	355.0048	15318-45-3	4
thiamylal	C12H18N2O2S	254.1089	77-27-0	4
Thiazaflurone	C6H7F3N4OS	240.0293	25366-23-8	8
Thiazinamium	C18H23N2S	299.1582	2338-21-8	4
Thidiazuron	C9H8N4OS	220.0419	51707-55-2	8
Thiencarbazone-methyl	C12H14N4O7S2	390.0304	317815-83-1	12
Thiethylperazine	C22H29N3S2	399.1803	1420-55-9	4
Thifensulfuron-methyl	C12H13N5O6S2	387.0307	79277-27-3	8
Thiobencarb	C12H16ClNOS	257.0641	28249-77-6	8
Thiobutabarbital	C10H16N2O2S	228.0932	2095-57-0	4
Thiodicarb	C10H18N4O4S3	354.0490	59669-26-0	12
Thiofanox	C9H18N2O2S	218.1089	39196-18-4	17
Thiofanox-sulfone	C9H18N2O4S	250.0987	39184-59-3	12
Thiofanox-sulfoxide	C9H18N2O3S	234.1038	39184-27-5	17
Thioguanine	C5H5N5S	167.0266	154-42-7	4
Thiolutin	C8H8N2O2S2	228.0027	87-11-6	4
Thiometon	C6H15O2PS3	245.9972	640-15-3	4
Thiopental	C11H17N2O2S	241.1011	76-75-5	4
Thiophanate	C14H18N4O4S2	370.0769	23564-06-9	8
Thiophanate-methyl	C12H14N4O4S2	342.0456	23564-05-8	8
Thiopropazate	C23H28ClN3O2S	445.1591	84-06-0	4
Thiopropazine	C22H30N4O2S2	446.1810	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	286.1794	91-85-0	4
thozalinone	C11H12N2O2	204.0899	655-05-0	4
Thymopentin	C30H49N9O9	679.3653	69558-55-0	4
Tiagabine	C20H25NO2S2	375.1327	115103-54-3	4
Tiamulin	C28H47NO4S	493.3226	55297-95-5	4
Tiapride	C15H24N2O4S	328.1457	51012-32-9	4
tiaprofenic acid	C14H12O3S	260.0507	33005-95-7	4
Ticlopidine	C14H14ClNS	263.0535	55142-85-3	4
Tiemonium	C18H24NO2S	318.1528	144-12-7	4
Tilidine	C17H23NO2	273.1729	20380-58-9	4
Tilmicosin	C46H80N2O13	868.5660	108050-54-0	8
Timolol	C13H24N4O3S	316.1569	26839-75-8	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Tinidazole	C8H13N3O4S	247.0627	19387-91-8	4
Tiocarlide	C23H32N2O2S	400.2185	910-86-1	8
tiotixene	C23H29N3O2S2	443.1701	5591-45-7	4
Tiracizine	C21H25N3O3	367.1896	83275-56-3	4
Tizanidine	C9H8ClN5S	253.0189	51322-75-9	4
Tocainide	C11H16N2O	192.1263	41708-72-9	4
tofenacin	C17H21NO	255.1623	15301-93-6	4
Tolazamide	C14H21N3O3S	311.1304	1156-19-0	8
Tolazoline	C10H12N2	160.1000	59-98-3	4
Tolbutamide	C12H18N2O3S	270.1038	64-77-7	4
Tolclofos-methyl	C9H11Cl2O3PS	299.9544	57018-04-9	8
Tolfenamic acid	C14H12ClNO2	261.0557	13710-19-5	4
Toliprolol	C13H21NO2	223.1572	2933-94-0	4
Tolmetin	C15H15NO3	257.1052	26171-23-3	4
Tolnaftate	C19H17NOS	307.1031	2398-96-1	4
Tolpropamine	C18H23N	253.1830	5632-44-0	4
Tolycaine	C15H22N2O3	278.1630	3686-58-6	4
Tolyfluanid	C10H13Cl2FN2O2S2	345.9780	731-27-1	8
Topotecan	C23H23N3O5	421.1638	123948-87-8	4
Torasemide	C16H20N4O3S	348.1256	56211-40-6	8
toremifene	C26H28NOCl	405.1859	89778-26-7	4
Tralkoxydim	C20H27NO3	329.1991	87820-88-0	8
Tramadol	C16H25NO2	263.1885	27203-92-5	8
tramazoline	C13H17N3	215.1422	1082-57-1	4
Tranexamic acid	C8H15NO2	157.1103	1197-18-8	4
Tranlycypromine	C9H11N	133.0891	155-09-9	4
Trapidil	C10H15N5	205.1327	15421-84-8	4
Trazodone	C19H22ClN5O	371.1513	19794-93-5	4
trenbolone	C18H22O2	270.1620	10161-33-8	4
Triadimefon	C14H16ClN3O2	293.0931	43121-43-3	12
Triadimenol	C14H18ClN3O2	295.1088	55219-65-3	12
Triallate	C10H16Cl3NOS	303.0018	2303-17-5	4
Tri-allate	C10H16Cl3NOS	303.0018	2303-17-5	8
Triamcinolone	C21H27FO6	394.1792	124-94-7	8
triamcinolone acetonide	C24H31O6F	434.2105	76-25-5	12
triamcinolone diacetate	C25H31FO8	478.2003	67-78-7	4
triamcinolone hexacetonide	C30H41FO7	532.2836	5611-51-8	8
triamcinolone-16,21-diacetate	C25H31O8F	478.2003	67-78-7	4
Triamterene	C12H11N7	253.1076	396-01-0	4
Triasulfuron	C14H16ClN5O5S	401.0561	82097-50-5	15

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Triazamate	C13H22N4O3S	314.1413	112143-82-5	8
Triazolam	C17H12Cl2N4	342.0439	28911-01-5	4
Triazophos	C12H16N3O3PS	313.0650	24017-47-8	8
Triazoxide	C10H6ClN5O	247.0261	72459-58-6	8
Tribenuron-methyl	C15H17N5O6S	395.0900	101200-48-0	8
Trichlorfon	C4H8Cl3O4P	255.9226	52-68-6	12
trichlormethiazide	C8H8N3O4S2Cl3	378.9022	133-67-5	4
Trichodermin	C17H24O4	292.1675	4682-50-2	4
Trichostatin A	C17H22N2O3	302.1630	58880-19-6	4
Triclabendazole	C14H9Cl3N2OS	357.9501	68786-66-3	4
Triclabendazole Sulfone	C14H9Cl3N2O3S	389.9400	100648-14-4	4
Triclabendazole Sulfoxide	C14H9Cl3N2O2S	375.9422	100648-13-3	4
Triclopyr	C7H4Cl3NO3	254.9257	55335-06-3	4
Tricyclazole	C9H7N3S	189.0361	41814-78-2	8
Tridemorph	C19H39NO	297.3032	24602-86-6	8
Trietazine	C9H16ClN5	229.1094	1912-26-1	12
Trifloxystrobin	C20H19F3N2O4	408.1297	141517-21-7	8
Triflumizole	C15H15ClF3N3O	345.0856	68694-11-1	12
Triflumuron	C15H10ClF3N2O3	358.0332	64628-44-0	8
trifluomeprazine	C19H21N2F3S	366.1378	2622-37-9	4
Trifluoperazine	C21H24F3N3S	407.1643	117-89-5	8
Trifluoperidol	C22H23F4NO2	409.1665	749-13-3	4
Triflupromazine	C18H19F3N2S	352.1221	146-54-3	4
Triflusulfuron-methyl	C17H19F3N6O6S	492.1039	126535-15-7	8
Trihexyphenidyl	C20H31NO	301.2406	114-11-6	4
Trimazosin	C20H29N5O6	435.2118	35795-16-5	4
trimeprazine	C18H22N2S	298.1504	84-96-8	4
trimetazidine	C14H22N2O3	266.1630	5011-34-7	4
Trimethobenzamide	C21H28N2O5	388.1998	138-56-7	4
Trimethoprim	C14H18N4O3	290.1379	738-70-5	8
Trimipramine	C20H26N2	294.2096	739-71-9	4
Trinexapac-ethyl	C13H16O5	252.0998	95266-40-3	4
tripamide	C16H20N3O3SCL	369.0914	73803-48-2	4
Tripelennamine	C16H21N3	255.1735	91-81-6	4
Triperiden	C21H29NO	311.2249	14617-17-5	4
Triphenylphosphate	C18H15O4P	326.0708	115-86-6	12
Tripolidine	C19H22N2	278.1783	486-12-4	4
Tris-(1,3-dichloro-isopropyl)-phosphate	C9H15Cl6O4P	427.8839	13674-87-8	8
Triticonazole	C17H20ClN3O	317.1295	131983-72-7	8
Tritoqualine	C26H32N2O8	500.2159	14504-73-5	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Tritosulfuron	C13H9F6N5O4S	445.0279	142469-14-5	8
Tromantadine	C16H28N2O2	280.2151	53783-83-8	4
Tropisetron	C17H20N2O2	284.1525	89565-68-4	8
Trospium	C25H30NO3	392.2226	10405-02-4	4
Tryprostatin A	C22H27N3O3	381.2052	171864-80-5	4
Tryptamine	C10H12N2	160.1000	61-54-1	4
tuaminoheptane	C7H17N	115.1361	123-82-0	4
tubocurarine	C37H42N2O6	610.3043	57-95-4	4
Tulobuterol	C12H18ClNO	227.1077	41570-61-0	4
tybamate	C13H26N2O4	274.1893	4268-36-4	4
Tylosin	C46H77NO17	915.5192	1401-69-0	4
Uniconazole	C15H18ClN3O	291.1138	83657-22-1	9
Urapidil	C20H29N5O3	387.2270	34661-75-1	4
Ustiloxin A	C28H43N5O12S	673.2629	143557-93-1	4
Ustiloxin B	C26H39N5O12S	645.2316	151841-41-7	4
Ustiloxin D	C23H34N4O8	494.2377	158243-18-6	8
Valacyclovir	C13H20N6O4	324.1546	124832-26-4	4
Valdecoxib	C16H14N2O3S	314.0725	181695-72-7	8
Valinomycin	C54H90N6O18	1110.6312	2001-95-8	8
valnoctamide	C8H17NO	143.1310	4171-13-5	4
Valsartan	C24H29N5O3	435.2270	137862-53-4	8
Vamidothion	C8H18NO4PS2	287.0415	2275-23-2	8
Vancomycin	C66H75Cl2N9O24	1447.4302	1404-93-9	4
Vardenafil	C23H32N6O4S	488.2206	224785-90-4	4
vecuronium	C34H57N2O4	557.4318	50700-72-6	4
Venlafaxine	C17H27NO2	277.2042	93413-69-5	4
Verapamil	C27H38N2O4	454.2832	52-53-9	4
Verrucarin A	C27H34O9	502.2203	3148-09-2	4
Verrucarol	C15H22O4	266.1518	2198-92-7	4
Verrucofortine	C24H31N3O3	409.2365	113706-21-1	4
Verruculogen	C27H33O7N3	511.2319	12771-72-1	8
Vetrabutine	C20H27NO2	313.2042	5974-09-4	4
Viloxazine	C13H19NO3	237.1365	46817-91-8	4
Viminol	C21H31ClN2O	362.2125	21363-18-8	4
Vincamine	C21H26N2O3	354.1943	1617-90-9	4
Vinpocentine	C22H26N2O2	350.1994	42971-09-5	4
Viomellein	C30H24O11	560.1319	55625-78-0	8
Viquidil	C20H24N2O2	324.1838	84-55-9	4
Viridicatin	C15H11NO2	237.0790	129-24-8	4
Warfarin	C19H16O4	308.1049	81-81-2	12

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Wortmannin	C23H24O8	428.1471	19545-26-7	4
Xantinal	C13H21N5O4	311.1594	437-74-1	4
xenysalate	C19H23NO3	313.1678	3572-52-9	4
Xipamide	C15H15CIN2O4S	354.0441	14293-44-8	8
xylazine	C12H16N2S	220.1034	7361-61-7	4
Xylometazoline	C16H24N2	244.1939	526-36-3	4
Yohimbine	C21H26N2O3	354.1943	146-48-5	4
Zearalenone	C18H22O5	318.1467	17924-92-4	8
Zearalenone-4-glucoside	C24H32O10	480.1995	105088-14-0	8
Zearalenone-4-sulfate	C18H22O8S	398.1035	132505-04-5	4
zeranol	C18H26O5	322.1780	26538-44-3	4
Zimeldine	C16H17BrN2	316.0575	56775-88-3	4
ziprasidone	C21H21CIN4OS	412.1125	146939-27-7	4
Ziram	C6H12N2S4Zn	303.9175	137-30-4	4
Zolpidem	C19H21N3O	307.1685	82626-48-0	4
Zopiclone	C17H17CIN6O3	388.1051	43200-80-2	4
Zotepine	C18H18CINOS	331.0798	26615-21-4	4
Zoxamide	C14H16C13NO2	335.0247	156052-68-5	12
Zuclopenthixol	C22H25CIN2OS	400.1376	53772-83-1	4

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