

Table S1: List of chemicals included in the accurate mass MS/MS spectral library

Compound Name	Formula	CAS	Polarity
(-)CP-47,497	C21H34O2	114753-51-4	-
(-)CP-55,940	C24H40O3	83002-04-4	+ -
(+)CP-47,497	C21H34O2	70434-82-1	+ -
(+)WIN-55212-2	C27H26N2O3	131543-22-1	+
(±)CP-47,497	C21H34O2	70434-82-1	+ -
(±)CP-47,497-C8-homolog	C22H36O2	70434-92-3	-
(±)CP-55,940	C24H40O3	83003-12-7	-
(±)JWH-018 N-(2-hydroxypentyl) metabolite	C24H23NO2		+ -
(±)JWH-018 N-(3-hydroxypentyl) metabolite	C24H23NO2		+ -
(±)JWH-073 N-(3-hydroxybutyl) metabolite	C23H21NO2		-
(±)WIN-55212	C27H26N2O3	137795-17-6	+
(S)-(+)-JWH-073 N-(3-hydroxybutyl) metabolite	C23H21NO2		-
α-MT / α-Methyltryptamine (Indopan)	C11H14N2	299-26-3	+
α-PBP / α-Pyrrolidinobutiophenone	C14H19NO	13415-82-2	+
α-PPP / α-Pyrrolidinopropiophenone	C13H17NO	19134-50-0	+
α-PVP / α-Pyrrolidinopentiophenone	C15H21NO	14530-33-7	+
1-(2,3-dihydroxypropyl)-Theobromine	C10H14N4O4	13460-96-3	+
1-(4-Fluorobenzyl) piperazine (1-(p-Fluorobenzyl) piperazine)	C11H15FN2	70931-28-1	+
1,1-Diphepanol	C20H25NO	510-07-6	+
1,2,3,4-Tetrahydroharmane-3-carboxylic acid	C13H14N2O2	5470-37-1	+
10-Hydroxycarbazepine	C15H14N2O2	29331-92-8	+
11a-Hydroxyprogesterone	C21H30O3	80-75-1	+
11-Ketotestosterone	C19H26O3	53187-98-7	+
12-Hydroxyibogamine (Noribogaine)	C19H24N2O	481-88-9	+
17a-Hydroxyprogesterone	C21H30O3	68-96-2	+
17alpha-Hydroxyprogesterone acetate	C23H32O4	17308-02-0	+
17beta-Estradiol	C18H24O2	50-28-2	-
1-Benzylimidazole	C10H10N2	4238-71-5	+
1-Dehydrotestosterone-benzoate	C26H30O3	19041-66-8	+
1'-Naphthoyl Indole (3-(1-Naphthoyl)indole)	C19H13NO	109555-87-5	+
2,2'-Bipyridyl	C10H8N2	366-18-7	+
2,2-Bis(ethylsulfonyl)butane	C8H18O4S2	76-20-0	+
2,2-propanedioldi-4,1-phenylene bis(phosphate)	C39H34O8P2	5945-33-5	+
2,3,5,6-Tetrachlorophenol	C6H2Cl4O	935-95-5	-
2,3-Dimercapto-1-propanesulfonic acid	C3H8O3S3	74-61-3	-
2,3-MDMC / 2,3-Methylenedioxy methcathinone	C11H13NO3		+
2,3-MDPEA / 2,3-Methylenedioxyphenethylamine	C9H11NO2		+
2,3-MDPV / 2,3-Methylenedioxy Pyrovalerone	C16H21NO3		+
2,3-MMDPEA / N-Methyl-2,3-methylenedioxyphenethylamine	C10H13NO2		+
2,3-Pentylone Isomer	C13H17NO3		+
2,4,5-T / 2,4,5-Trichlorophenoxyacetic acid	C8H5Cl3O3	93-76-5	-
2,4,5-TP / Silvex (Fenoprop)	C9H7Cl3O3	93-72-1	-
2,4-D / 2,4-Dichlorophenoxyacetic acid	C8H6Cl2O3	94-75-7	-
2,4-DB / 2,4-Dichlorophenoxybutyric acid	C10H10Cl2O3	94-82-6	-

Compound Name	Formula	CAS	Polarity
2,4-Dinitrophenol	C6H4N2O5	51-28-5	-
2,4-DP / Dichloroprop	C9H8Cl2O3	120-36-5	-
2',5-Dichloro-2-(methylamino)benzophenone	C14H11Cl2NO	5621-86-3	+
2,5-DMA / Dimethoxyamphetamine (Dimethoxyamfetamine)	C11H17NO2	2801-68-5	+
2,6-di-tert-butyl-p-Cresol (BHT)	C15H24O	128-37-0	-
2,6-Xanthine	C5H4N4O2	69-89-6	+ -
25-Desacetyl rifampicin	C41H56N4O11	16783-99-6	+
25I-NBOMe	C18H22INO3	919797-19-6	+
2-Al / 2-Aminoindane	C9H11N	2975-41-9	+
2-Amino-5-chlorobenzophenone	C13H10ClNO	719-59-5	+
2-Amino-5-nitrobenzophenone	C13H10N2O3	1775-95-7	-
2-Amino-5-nitrophenol	C6H6N2O3	121-88-0	-
2-Brom-2-ethylbutanamide	C6H12BrNO	511-70-6	+
2C-B (BDMPEA)	C10H14BrNO2	66142-81-2	+
2C-B-BZP (1-(4-Bromo-2,5-dimethoxybenzyl)piperazine)	C13H19BrN2O2	1094424-37-9	+
2C-B-Fly	C12H14BrNO2	178557-21-6	+
2C-C / 2,5-Dimethoxy-4-chlorophenethylamine	C10H14ClNO2	88441-15-0	+
2C-D / 2,5-Dimethoxy-4-methylphenethylamine	C11H17NO2	24333-19-5	+
2C-E / 2,5-Dimethoxy-4-ethylphenethylamine	C12H19NO2	71539-34-9	+
2C-H / 2,5-Dimethoxyphenethylamine (Benzeneethanamine)	C10H15NO2	3600-86-0	+
2C-I / 2,5-Dimethoxy-4-iodophenethylamine	C10H14INO2	69587-11-7	+
2C-N / 2,5-Dimethoxy-4-nitrophenethylamine	C10H14N2O4	261789-00-8	+
2C-P / 2,5-Dimethoxy-4-propylphenethylamine	C13H21NO2	207740-22-5	+
2C-T-2 / 2,5-Dimethoxy-4-ethylthiophenethylamine	C12H19NO2S	207740-24-7	+
2C-T-4 / 2,5-Dimethoxy-4-isopropylthiophenethylamine	C13H21NO2S	207740-25-8	+
2C-T-7 / 2,5-Dimethoxy-4-propylthiophenethylamine	C13H21NO2S	207740-26-9	+
2-DPMP / Desoxy pipradrol	C18H21N	519-74-4	+
2-EEC / 2-Ethylethcathinone	C13H19NO		+
2-EMC / 2-Ethylmethcathinone	C12H17NO		+
2-ethylhexyl-diphenyl phosphate	C20H27O4P	1241-94-7	+
2-FA / 2-Fluoroamphetamine (2-Fluoroamfetamine)	C9H12FN	1716-60-5	+
2-FEC / 2-Fluoroethcathinone	C11H14FNO		+
2-FMA / 2-Fluoromethamphetamine (2-Fluoromethamfetamine)	C10H14FN	1017176-48-5	+
2-FMC / 2-Fluoromethcathinone	C10H12FNO	1186137-35-8	+
2-Hydroxyethyl salicylate	C9H10O4	87-28-5	-
2-hydroxy-Hydroquinone	C6H6O3	533-73-3	-
2-MEC / 2-Methylethcathinone	C12H17NO		+
2-MeOPP / 1-(2-methoxyphenyl)piperazine	C11H16N2O	35386-24-4	+
2-Methylamino-5-chlorobenzophenone (Diazepam HY)	C14H12ClNO	1022-13-5	+
2-MMC / 2-Methoxymethcathinone	C11H15NO2		+
2-MMC / 2-Methylmethcathinone	C11H15NO	1246911-71-6	+
2-MPBP / 2-Methyl- α -pyrrolidinobutiophenone	C15H21NO		+
2-Phenyl-1,3-indandione	C15H10O2	83-12-5	+
2-Phenylphenol (Orthophenylphenol)	C12H10O	90-43-7	-
2-tert-Butyl-4-methoxyphenol	C11H16O2	25013-16-5	-

Compound Name	Formula	CAS	Polarity
3-(Acetylamino)-5-amino-2,4,6-triiodobenzoic acid	C9H7I3N2O3	1713-07-1	+
3,3',5,5'-Tetrabromobisphenol A	C15H12Br4O2	79-94-7	-
3,4,5,6-Tetrahydrophthalic acid anhydride	C8H8O3	2426-02-0	+
3,4-Dimethoxyphenylglyoxylic acid	C10H10O5	4732-70-1	-
3,4-DMMA / 3,4-Dimethoxymethamphetamine	C12H19NO2	33236-61-2	+
3,4-DMMC / 3,4-Dimethylmethcathinone	C12H17NO	1082110-00-6	+
3,5-Diiodotyrosine	C9H9I2NO3	66-02-4	+
3,5-Dimethoxyphenethylamine	C10H15NO2	3213-28-3	+
3,6-Diamino-10-methylacridinium	C14H14N3	86-40-8	+
3-EEC / 3-Ethylethcathinone	C13H19NO		+
3-EMC / 3-Ethylmethcathinone	C12H17NO		+
3-FA / 3-Fluoroamphetamine (3-Fluoroamfetamine)	C9H12FN	1626-71-7	+
3-FEC / 3-Fluoroethcathinone	C11H14FNO		+
3-FMA / 3-Fluoromethamphetamine	C10H14FN	1182818-14-9	+
3-FMC / 3-Fluoromethcathinone	C10H12FNO	1049677-77-1	+
3-Formylrifampicin SV	C38H47NO13	13292-22-3	-
3-Hydroxycotinine	C10H12N2O2	34834-67-8	+
3-Hydroxyethylflurazepam (Flurazepam-M (HO-ethyl-))	C17H14ClFN2O2	20971-53-3	+ -
3-Hydroxyflunitrazepam	C16H12FN3O4	67739-71-3	+
3-Hydroxylicocaine	C14H22N2O2	34604-55-2	+
3-Hydroxynitrazepam	C15H11N3O4	16442-74-3	-
3-Hydroxynorflurazepam	C15H10ClFN2O2	17617-60-6	+
3-Hydroxyphenylacetic acid	C8H8O3	621-37-4	+ -
3-MEC / 3-Methylethcathinone	C12H17NO		+
3-MeOMC / 3-Methoxymethcathinone	C11H15NO2	1435933-70-2	+
3-Methyl-2-oxopentanoic acid	C6H10O3	39748-49-7	-
3-MMC / 3-Methylmethcathinone	C11H15NO	1246816-62-5	+
3-MPBP / 3-Methyl-a-pyrrolidinobutiophenone	C15H21NO		+
4-Aminohippuric acid	C9H10N2O3	61-78-9	+ -
4-Aminosalicilyc acid	C7H7NO3	65-49-6	-
4-Benzamidosalicylic acid	C14H11NO4	13898-58-3	-
4-Biphenylacetic acid	C14H12O2	5728-52-9	-
4-Chlorophenol	C6H5ClO	106-48-9	-
4-Chlorosalicylic acid	C7H5ClO3	5106-98-9	-
4-CPA / 4-Chlorophenoxyacetic acid	C8H7ClO3	122-88-3	-
4-EEC / 4-Ethylethcathinone	C13H19NO		+
4-EMC / 4-Ethylmethcathinone	C12H17NO	1225622-14-9	+
4-Ethyl-N,N-Dimethylcathinone	C13H19NO		+
4-FA / 4-Fluoroamphetamine	C9H12FN	459-02-9	+
4-FEC / 4-Fluoroethcathinone	C11H14FNO		+
4-FIC / 4-Fluoroisocathinone	C9H10FNO		+
4-FMA / 4-Fluoromethamphetamine	C10H14FN	351-03-1	+
4-FPP / 1-(4-Fluorophenyl)piperazine	C10H13FN2	2252-63-3	+
4-HO-DMT (Psilocine)	C12H16N2O	520-53-6	+
4-HO-MA (Pholedrine)	C10H15NO	370-14-9	+

Compound Name	Formula	CAS	Polarity
4'-Hydroxy-3'-methoxynomifensine	C17H20N2O2	62080-80-2	+
4-Hydroxyalprazolam	C17H13ClN4O	30896-57-2	+
4-Hydroxybenzoic acid	C7H6O3	99-96-7	+ -
4-Hydroxyglibenclamide	C23H28ClN3O6S	23155-04-6	+
4-Hydroxymidazolam	C18H13ClFN3O	59468-85-8	+
4'-Hydroxynomifensine	C16H18N2O	55774-26-0	+
4'-Hydroxynordiazepam	C15H11ClN2O2	17270-12-1	+
4-Hydroxytriazolam	C17H12Cl2N4O	65686-11-5	+
4-MEC / 4-Methylethcathinone	C12H17NO	1225617-18-4	+
4-MeO-DMT / 4-Methoxy-DMT	C13H18N2O	3965-97-7	+ -
4-MeOPP / 1-(4-Methoxyphenyl)piperazine	C11H16N2O	38212-30-5	+
4'-MeOPPP / 4'-Methoxy- α -pyrrolidinopropiophenone	C14H19NO2	478243-09-3	+
4'-MePPP / 4'-Methyl- α -pyrrolidinopropiophenone (MPPP)	C14H19NO	28117-80-8	+
4-Methyl-2-oxopentanoic acid	C6H10O3	816-66-0	-
4-Methylaminorex	C10H12N2O	3568-94-3	+
4-Methylumbelliferyl acetate	C12H10O4	2747-05-9	+
4-MMC / 4-Methylmethcathinone (Mephedrone)	C11H15NO	1189805-46-6	+
4-MPBP / 4-Methyl- α -pyrrolidinobutiophenone	C15H21NO	732180-91-5	+
4-Nitroaniline	C6H6N2O2	100-01-6	+
4-Phenolsulfonic acid	C6H6O4S	98-67-9	-
4-Phenylbenzophenone	C19H14O	2128-93-0	+
4Q3C CB2 Ligand / 4-Quinolone-3-Carboxamide CB2 Ligand	C26H34N2O3	1314230-69-7	+
5-(4-methylphenyl)- 5-Phenylhydantoin	C16H14N2O2	51169-17-6	-
5,5-Dipropylbarbituric acid	C10H16N2O3	2217-08-5	-
5-Aminosalicylic acid	C7H7NO3	89-57-6	+ -
5-APB / 5-(2-Aminopropyl)Benzofuran	C11H13NO	286834-81-9	+
5-APDI (Indanylaminopropane)	C12H17N	152624-02-7	+
5-Bromo-4'-chlorosalicylanilide	C13H9BrClNO2	3679-64-9	-
5-Bromo-N-isopropylsalicylamide	C10H12BrNO2		+
5-Carboxybupranolol	C14H20ClNO4	42242-69-3	+
5-Ethyldeoxyuridine	C11H16N2O5	15176-29-1	+ -
5-HO-DMT (Bufotenine)	C12H16N2O	487-93-4	+
5-Hydroxyclethodim-sulfone	C17H26ClNO6S	111031-11-9	+
5-Hydroxydantrolene	C14H10N4O6	52130-25-3	+
5-Hydroxyomeprazole	C17H19N3O4S	92340-57-3	+
5-Hydroxypropafenone	C21H27NO4	86384-10-3	+
5-Hydroxy-Thiabendazole	C10H7N3OS	948-71-0	+
5-IAI /5-Iodo-2-Aminoindan	C9H10IN	132367-76-1	+
5-MeO-AMT / 5-Methoxy- α -methyltryptamine	C12H16N2O	1137-04-8	+
5-MeO-DALT / 5-methoxy DALT	C17H22N2O	928822-98-4	+
5-MeO-DiPT (FOXY)	C17H26N2O	4021-34-5	+
5-MeO-DMT / 5-methoxy DMT	C13H18N2O	1019-45-0	+
5-MeO-MiPT / 5-methoxy MiPT	C15H22N2O	96096-55-8	+
5-MeO-T / 5-Methoxytryptamine (Meksamin)	C11H14N2O	608-07-1	+
6-Acetylmorphine	C19H21NO4	2784-73-8	+

Compound Name	Formula	CAS	Polarity
6beta-Hydroxytestosterone	C19H28O3	62-99-7	+
6-Chlorothymol	C10H13ClO	89-68-9	-
6H-dibenzo[c,e][1,2]oxaphosphinine 6-oxide	C12H9O2P	35948-25-5	+
6-Hydroxybrotizolam	C15H10BrClN4OS	88883-43-6	+
6-Methoxytryptamine	C11H14N2O	3610-36-4	+
6-Methylcoumarin	C10H8O2	92-48-8	+
7-(2-chloroethyl)-Theophylline	C9H11ClN4O2	5878-61-5	+
7-Acetaminonitrazepam	C17H15N3O2	4928-03-4	+
7-Aminoflunitrazepam	C16H14FN3O	34084-50-9	+
7-Aminonitrazepam	C15H13N3O	4928-02-3	+
7-Aminonorflunitrazepam (Flunitrazepam-M (noramino-))	C15H12FN3O	894-76-8	+
7-Desoxycholic acid	C24H40O4	83-44-3	+ -
7-Hydroxyquetiapine	C21H25N3O3S	139079-39-3	+
8-Chlorotheophylline	C7H7ClN4O2	85-18-7	+ -
8-Hydroxychinolin (8-Hydroxyquinoline)	C9H7NO	148-24-3	+
8-Hydroxyefavirenz	C14H9ClF3NO3	205754-32-1	-
9-Aminoacridine	C13H10N2	90-45-9	-
Abacavir	C14H18N6O	136470-78-5	+
Acarbose	C25H43NO18	56180-94-0	+
Acebutolol	C18H28N2O4	37517-30-9	+
Acecaidine	C15H23N3O2	32795-44-1	+
Acecarbromal	C9H15BrN2O3	77-66-7	+
Aceclidine	C9H15NO2	827-61-2	+
Aceclofenac	C16H13Cl2NO4	89796-99-6	+
Acemetacin	C21H18ClNO6	53164-05-9	+ -
Acenocoumarol	C19H15NO6	152-72-7	+ -
Acephate	C4H10NO3PS	30560-19-1	+ -
Acepromazine	C19H22N2OS	61-00-7	+
Aceprometazine	C19H22N2OS	13461-01-3	+
Acetaminophen (Paracetamol)	C8H9NO2	103-90-2	+
Acetaminosalol	C15H13NO4	118-57-0	+
Acetamidiprid	C10H11ClN4	135410-20-7	+
Acetanilide	C8H9NO	103-84-4	+ -
Acetarsol	C8H10AsNO5	97-44-9	+ -
Acetazolamide	C4H6N4O3S2	59-66-5	+ -
Acetiamine	C16H22N4O4S	299-89-8	+
Acetochlor	C14H20ClNO2	34256-82-1	+
Acetohexamide	C15H20N2O4S	968-81-0	+ -
Acetrizoic acid	C9H6I3NO3	85-36-9	+
Acetyl andromedol	C22H36O7	4720-09-6	-
Acetylcodeine	C20H23NO4	6703-27-1	+
Acetylcysteine	C5H9NO3S	616-91-1	+ -
Acetylisoniazid	C8H9N3O2	1078-38-2	+ -
Acetylsalicylic acid	C9H8O4	530-75-6	-
Acetylsulfadiazine (N4-Acetylsulfadiazine)	C12H12N4O3S	127-74-2	+ -

Compound Name	Formula	CAS	Polarity
Acexamic acid	C8H15NO3	57-08-9	+ -
Aciclovir	C8H11N5O3	59277-89-3	+ -
Acifluorfen	C14H7ClF3NO5	50594-66-6	-
Acipimox	C6H6N2O3	51037-30-0	+
Acitretin	C21H26O3	55079-83-9	+
Aclarubicin	C42H53NO15	57576-44-0	+ -
Aclonifen	C12H9ClN2O3	74070-46-5	+
Actinoquinol	C11H11NO4S	15301-40-3	+
Adefovir	C8H12N5O4P	106941-25-7	+
Adenosine	C10H13N5O4	58-61-7	+ -
Adenosine phosphate	C10H14N5O7P	61-19-8	+ -
Adiphenine	C20H25NO2	64-95-9	+
Adrenone	C9H11NO3	99-45-6	+ -
AET / a-Ethyltryptamine (Etryptamine)	C12H16N2	2235-90-7	+
Agomelatine	C15H17NO2	138112-76-2	+ -
Ajmaline	C20H26N2O2	4360-12-7	+
AKB48 (APINACA)	C23H31N3O	1345973-53-6	+
Aklomide	C7H5ClN2O3	3011-89-0	-
Alachlor	C14H20ClNO2	15972-60-8	+
Alantolactone	C15H20O2	546-43-0	+ -
Alaproclate	C13H18ClNO2	60719-82-6	+
Albendazole	C12H15N3O2S	54965-21-8	+
Albendazole sulfone	C12H15N3O4S	75184-71-3	+
Albendazole-2-aminosulfone	C10H13N3O2S	80983-34-2	+
Alclofenac	C11H11ClO3	22131-79-9	-
Aldicarb	C7H14N2O2S	116-06-3	+
Aldicarb sulfoxide (Aldicarb sulphoxide)	C7H14N2O3S	1646-87-3	+
Aldimorph	C18H37NO	91315-15-0	+
Aldoxycarb (Aldicarb Sulfone)	C7H14N2O4S	1646-88-4	+
Alfentanil	C21H32N6O3	71195-58-9	+
Alfuzosin	C19H27N5O4	81403-80-7	+ -
Alimemazine	C18H22N2S	84-96-8	+
Alizapride	C16H21N5O2	59338-93-1	+
Allethrin	C19H26O3	584-79-2	+
Allobarbitol	C10H12N2O3	52-43-7	-
Allopurinol	C5H4N4O	315-30-0	+ -
Alloxydim	C17H25NO5	55634-91-8	+
Allylhydroxypropylbarbituric acid	C10H14N2O4	2537-29-3	+
Almitrine	C26H29F2N7	27469-53-0	+
Almotriptan	C17H25N3O2S	154323-57-6	-
Aloin	C21H22O9	1415-73-2	+ -
alpha-Hydroxyalprazolam	C17H13ClN4O	37115-43-8	+
alpha-Hydroxybrotizolam	C15H10BrClN4O5	62551-41-1	+
alpha-Hydroxymidazolam	C18H13ClFN3O	59468-90-5	+
alpha-Hydroxytriazolam	C17H12Cl2N4O	37115-45-0	+

Compound Name	Formula	CAS	Polarity
Alprazolam	C17H13ClN4	28981-97-7	+
Alprenolol	C15H23NO2	13655-52-2	+
Alprostadil	C20H34O5	745-65-3	-
Althiazide	C11H14ClN3O4S3	5588-16-9	-
Altrenogest	C21H26O2	850-52-2	+
Altretamine	C9H18N6	645-05-6	+
Alverine	C20H27N	150-59-4	+
AM-1172	C27H39NO2	251908-92-6	+ -
AM-1220	C26H26N2O	137642-54-7	+
AM-1235	C24H21FN2O3	335161-27-8	+
AM-1241	C22H22IN3O3	444912-48-5	+
AM-1248	C26H34N2O	335160-66-2	+
AM-2201	C24H22FNO	335161-24-5	+
AM-2201 2'-naphthyl isomer	C24H22FNO		+
AM-2201 6-hydroxyindole metabolite	C24H22FNO2		+
AM-2201 7-hydroxyindole metabolite	C24H22FNO2		+ -
AM-2201 N-(2-fluoropentyl) isomer	C24H22FNO		+
AM-2201 N-(3-fluoropentyl) isomer	C24H22FNO		+
AM-2201 N-(4-fluoropentyl) isomer	C24H22FNO		+
AM-2201 N-(4-hydroxypentyl) metabolite	C24H22FNO2		+ -
AM-2232	C24H20N2O	335161-19-8	+
AM-2233	C22H23IN2O	444912-75-8	+
AM-251	C22H21Cl2IN4O	183232-66-8	+
AM-3102	C21H41NO2	213182-22-0	+
AM-356	C23H39NO2	157182-49-5	+
AM-630 (Iodopravadoline)	C23H25IN2O3	164178-33-0	+
AM-679	C20H20INO	335160-91-3	+
AM-694	C20H19FINO	335161-03-0	+ -
AM-694 3-iodo isomer	C20H19FINO		+
AM-694 4-iodo isomer	C20H19FINO		+ -
Amantadine	C10H17N	768-94-5	+
Ambazone	C8H11N7S	539-21-9	+
Ambroxol	C13H18Br2N2O	18683-91-5	+ -
Ambucetamide	C17H28N2O2	519-88-0	+
Ambutonium	C20H27N2O	115-51-5	+
Amcinonide	C28H35FO7	51022-69-6	+
Ametoctradin	C15H25N5	865318-97-4	+
Ametryne (Ametrex)	C9H17N5S	834-12-8	+
Amezinium	C11H12N3O	41658-78-0	+
Amfepramone (N,N-Diethylcathinone)	C13H19NO	90-84-6	+
Amfomycin (Amphomycin)	C58H91N13O20	1402-82-0	+ -
Amidithion	C7H16NO4PS2	919-76-6	+
Amidosulfuron	C9H15N5O7S2	120923-37-7	+
Amidotrizoic acid	C11H9I3N2O4	117-96-4	+
Amikacin	C22H43N5O13	37517-28-5	+

Compound Name	Formula	CAS	Polarity
Amiloride	C6H8ClN7O	2609-46-3	+
Amineptine	C22H27NO2	57574-09-1	+
Aminitrozol	C5H5N3O3S	140-40-9	-
Aminocaproic acid	C6H13NO2	60-32-2	+ -
Aminocarb	C11H16N2O2	2032-59-9	+
Aminodantrolene	C14H12N4O3	14663-28-6	+
Aminoflubendazol	C14H10FN3O	82050-13-3	+
Amino-mebendazole	C14H11N3O	52329-60-9	+ -
Aminophenazone	C13H17N3O	58-15-1	+
Aminopromazine	C19H25N3S	58-37-7	+
Aminopterin	C19H20N8O5	54-62-6	+
Aminoquinuride	C21H20N6O	3811-56-1	+
Aminorex	C9H10N2O	2207-50-3	+
Amiodarone	C25H29I2NO3	1951-25-3	+
Amiphenazole	C9H9N3S	490-55-1	+
Amisulbrom	C13H13BrFN5O4S 2	348635-87-0	+
Amisulpride	C17H27N3O4S	71675-85-9	+
Amitraz	C19H23N3	33089-61-1	+
Amitriptyline	C20H23N	50-48-6	+
Amitriptylinoxide	C20H23NO	4317-14-0	+
Amlodipine	C20H25ClN2O5	88150-42-9	+
Ammeline (Atrazine-desethyl-desisopropyl-2-OH)	C3H5N5O	645-92-1	+ -
Ammoidin	C12H8O4	298-81-7	+
Amobarbital	C11H18N2O3	57-43-2	-
Amorolfine	C21H35NO	78613-35-1	+
Amoxapine	C17H16ClN3O	14028-44-5	+
Amoxicillin	C16H19N3O5S	26787-78-0	+
Amphetamine (Amfetamine)	C9H13N	300-62-9	+
Ampicillin	C16H19N3O4S	69-53-4	-
Amprenavir	C25H35N3O6S	161814-49-9	+
Amprolium	C14H19N4	121-25-5	+
Ampyrone	C11H13N3O	83-07-8	+
Amrinone	C10H9N3O	60719-84-8	+ -
Amsacrine	C21H19N3O3S	51264-14-3	+
Amydracaine	C16H26N2O2	963-07-5	+
Amylocaine	C14H21NO2	644-26-8	+
Anastrozole	C17H19N5	120511-73-1	+ -
Anatabine	C10H12N2	2743-90-0	+
Androstanolone	C19H30O2	521-18-6	+
Anetholtrithione	C10H8OS3	532-11-6	+
Angelicin	C11H6O3	523-50-2	+
Anhydroecgonine	C9H13NO2	74242-55-0	+
Anhydroecgonine methylester	C10H15NO2	43021-26-7	+
Anilazine	C9H5Cl3N4	101-05-3	+
Anilofos	C13H19ClNO3PS2	64249-01-0	+

Compound Name	Formula	CAS	Polarity
Aniracetam	C12H13NO3	72432-10-1	+
Anisomycin	C14H19NO4	22862-76-6	+
Antazoline	C17H19N3	91-75-8	+
Anthrabin	C14H10O3	577-33-3	+
Antimycin	C13H14O5	518-75-2	+
Antu (Naphthylthiourea)	C11H10N2S	86-88-4	+
Apalcillin	C25H23N5O6S	63469-19-2	+ -
Apomorphine	C17H17NO2	58-00-4	+
Apovincamine	C21H24N2O2	4880-92-6	+
Apraclonidine	C9H10Cl2N4	66711-21-5	+
Aprepitant	C23H21F7N4O3	170729-80-3	+
Aprindine	C22H30N2	37640-71-4	+
Aprobarbital	C10H14N2O3	77-02-1	-
Arbutin	C12H16O7	497-76-7	-
Arecoline	C8H13NO2	63-75-2	+
Aripiprazole	C23H27Cl2N3O2	129722-12-9	+
Arprinocid	C12H9ClFN5	55779-18-5	+
Artemisinin	C15H22O5	63968-64-9	+
Articaine	C13H20N2O3S	23964-58-1	+
Aspartame	C14H18N2O5	22839-47-0	+ -
Aspirin (Acetylsalicylic acid)	C9H8O4	50-78-2	-
Astemizole	C28H31FN4O	68844-77-9	+ -
Astragalin	C21H20O11	480-10-4	+
Asulam	C8H10N2O4S	3337-71-1	+
Atazanavir	C38H52N6O7	198904-31-3	+
Atenolol	C14H22N2O3	29122-68-7	+
Atorvastatin	C33H35FN2O5	134523-00-5	+
Atraton	C9H17N5O	1610-17-9	+
Atraton-desisopropyl	C6H11N5O	30360-56-6	+
Atrazine	C8H14ClN5	1912-24-9	+
Atrazine-2-hydroxy (Hydroxyatrazine)	C8H15N5O	2163-68-0	+
Atrazine-desethyl (Desethylatrazine)	C6H10ClN5	6190-65-4	+
Atrazine-desethyl-2-OH	C6H11N5O	19988-24-0	+
Atrazine-desisopropyl (Deisopropylatrazine)	C5H8ClN5	1007-28-9	+
Atropine	C17H23NO3	51-55-8	+
Atropine methyl	C18H26NO3	31610-87-4	+
Atropine-N-octyl	C25H40NO3	5843-82-3	+
Auranofin	C20H34AuO9PS	34031-32-8	+
Azacitidine	C8H12N4O5	320-67-2	+ -
Azaconazole	C12H11Cl2N3O2	60207-31-0	+
Azamethiphos	C9H10ClN2O5PS	35575-96-3	+
Azaperone	C19H22FN3O	1649-18-9	+
Azapropazone	C16H20N4O2	13539-59-8	+
Azatadine	C20H22N2	3964-81-6	+
Azathioprine	C9H7N7O2S	446-86-6	+

Compound Name	Formula	CAS	Polarity
Azelaic acid	C9H16O4	123-99-9	-
Azelastine	C22H24ClN3O	58581-89-8	+
Azimsulfuron (IN A8947)	C13H16N10O5S	120162-55-2	+
Azinphos-ethyl (Guthion ethyl)	C12H16N3O3PS2	2642-71-9	+
Azinphos-methyl (Guthion)	C10H12N3O3PS2	86-50-0	+
Azintamide	C10H14ClN3OS	1830-32-6	+
Aziprotryne	C7H11N7S	4658-28-0	+
Azithromycin	C38H72N2O12	83905-01-5	+ -
Azlocillin	C20H23N5O6S	37091-66-0	+ -
Azobenzene (Bumadizone artifact)	C12H10N2	103-33-3	+
Azoluron	C12H14N4O	4058-90-6	+
Azosemide	C12H11ClN6O2S2	27589-33-9	+
Azoxystrobin	C22H17N3O5	131860-33-8	+
Aztreonam	C13H17N5O8S2	78110-38-0	+ -
Bacampicillin	C21H27N3O7S	50972-17-3	+
Bacitracin	C66H103N17O16S	1405-87-4	+
Baclofen	C10H12ClNO2	1134-47-0	+
Baicalein	C15H10O5	491-67-8	+ -
BAM / Dichlorbenzamide	C7H5Cl2NO	2008-58-4	+
Bambuterol	C18H29N3O5	81732-65-2	+
Bamethan	C12H19NO2	3703-79-5	+
Bamifylline	C20H27N5O3	2016-63-9	+
Bamipine	C19H24N2	4945-47-5	+
Barbital	C8H12N2O3	57-44-3	-
Barverin	C29H43N5O3	1639-79-8	+
BDB / alpha-Ethyl-1,3-benzodioxole-5-ethanamine	C11H15NO2	107447-03-0	+
Beclamide	C10H12ClNO	501-68-8	+
Beclometasone (Beclomethasone)	C22H29ClO5	4419-39-0	+
Beflubutamid	C18H17F4NO2	113614-08-7	+
Befunolol	C16H21NO4	39552-01-7	+
Benactyzine	C20H25NO3	302-40-9	+
Benalaxyl	C20H23NO3	71626-11-4	+
Benazepril	C24H28N2O5	86541-75-5	+
Benazeprilat	C22H24N2O5	86541-78-8	+
Benazolin	C9H6ClNO3S	3813-05-6	+
Benazolin-ethyl	C11H10ClNO3S	25059-80-7	+
Bencyclane	C19H31NO	2179-37-5	+
Bendamustine	C16H21Cl2N3O2	16506-27-7	+
Bendiocarb	C11H13NO4	22781-23-3	+
Bendroflumethiazide	C15H14F3N3O4S2	73-48-3	-
Benfluorex	C19H20F3NO2	23602-78-0	+
Benfluralin	C13H16F3N3O4	1861-40-1	+
Benfotiamine	C19H23N4O6PS	22457-89-2	+ -
Benfuracarb	C20H30N2O5S	82560-54-1	+
Benodanil	C13H10INO	15310-01-7	+

Compound Name	Formula	CAS	Polarity
Benoxaprofen	C16H12ClNO3	51234-28-7	+
Benperidol	C22H24FN3O2	2062-84-2	+
Benproperine	C21H27NO	2156-27-6	+
Benserazide	C10H15N3O5	322-35-0	+
Bensulfuron-methyl (Bianmihuanglong)	C16H18N4O7S	83055-99-6	+
Bensulide	C14H24NO4PS3	741-58-2	+
Bensultap	C17H21NO4S4	17606-31-4	+
Bentazone	C10H12N2O3S	25057-89-0	-
Bentranil	C14H9NO2	1022-46-4	+
Benzarone	C17H14O3	1477-19-6	+
Benzatropine	C21H25NO	86-13-5	+
Benzethonium	C27H42NO2	121-54-0	+
Benzhydryloxyethyl-diethylamine	C19H25NO	642-58-0	+
Benzocaine	C9H11NO2	94-09-7	+
Benzoctamine	C18H19N	17243-39-9	+
Benzododecinium (Ajatin)	C21H38N	10328-35-5	+
Benzoximate	C18H18ClNO5	29104-30-1	+
Benzoxonium (Absonal) (Cohortan)	C23H42NO2	19379-90-9	+
Benzoylecgonine	C16H19NO4	519-09-5	+
Benzoylprop-ethyl	C18H17Cl2NO3	22212-55-1	+
Benzquinamide	C22H32N2O5	63-12-7	+
Benzthiazuron	C9H9N3OS	1929-88-0	+
Benzylamine	C19H23N3O	642-72-8	+
Benzylcinnamate	C16H14O2	103-41-3	+
Benzylhydrochlorothiazide	C14H14ClN3O4S2	1824-50-6	-
Benzylnicotinate	C13H11NO2	94-44-0	+
Benzylsalicylate	C14H12O3	16122-06-8	-
Berberine	C20H18NO4	2086-83-1	+
Betahistine	C8H12N2	5638-76-6	+
Betaine	C5H12NO2	107-43-7	+
Betamethasone	C22H29FO5	378-44-9	+ -
Betamethasone 17,21-dipropionate	C28H37FO7	5593-20-4	+
Betamethasone 21-phosphate	C22H30FO8P	360-63-4	-
Betamethasone acetate	C24H31FO6	987-24-6	+
Betamethasone benzoate	C29H33FO6	22298-29-9	+
Betamethasone valerate	C27H37FO6	2152-44-5	+
beta-Nicotyrine	C10H10N2	487-19-4	+
Betanidine	C10H15N3	55-73-2	+
Betaxolol	C18H29NO3	63659-18-7	+
Bethanechol (Amidopropyldimethylbetaine)	C7H17N2O2	674-38-4	+
Bezafibrate	C19H20ClNO4	41859-67-0	+ -
Bezitramide	C31H32N4O2	15301-48-1	+
Bicalutamide	C18H14F4N2O4S	90357-06-5	+ -
Bicyclophenamine	C20H27NO2	3570-06-7	+
Bifemelane	C18H23NO	90293-01-9	+

Compound Name	Formula	CAS	Polarity
Bifenazate (D 2341)	C17H20N2O3	149877-41-8	+
Bifonazole	C22H18N2	60628-96-8	+
Bimatoprost	C25H37NO4	155206-00-1	+ -
Bioallethrin (Esbiothrin)	C19H26O3	28434-00-6	+
Biperiden	C21H29NO	514-65-8	+
Bis(aminopropyl)laurylamine	C18H41N3	2372-82-9	+
Bisacodyl	C22H19NO4	603-50-9	+
Bisbentiamine	C38H42N8O6S2	2667-89-2	+
Bisnorcitalopram (Didesmethylocitalopram)	C18H17FN2O	62498-69-5	+
Bisoprolol	C18H31NO4	66722-44-9	+
Bispyribac	C19H18N4O8	125401-75-4	+
Bitertanol	C20H23N3O2	55179-31-2	+
Bithionol	C12H6Cl4O2S	97-18-7	-
bk-DMBDB (Dibutylone)	C13H17NO3	802286-83-5	+
bk-EBDB (Eutylone)	C13H17NO3	802855-66-9	+
bk-MBDB (Butylone)	C12H15NO3	802575-11-7	+
bk-MBDP / Pentylone	C13H17NO3	698963-77-8	+
bk-MDDMA (Dimethylone)	C12H15NO3	765231-58-1	+
bk-MDEA (Ethylone)	C12H15NO3		+
bk-MDMA / Methylone	C11H13NO3	186028-79-5	+
b-Naltrexol (beta-Naltrexol)	C20H25NO4	49625-89-0	+ -
Bolasterone	C21H32O2	1605-89-6	+
Boldenone (Dehydrotestosterone)	C19H26O2	846-48-0	+
Boldenone undecanoate	C30H44O3	13103-34-9	+
Boldine	C19H21NO4	476-70-0	+ -
Boldione	C19H24O2	897-06-3	+
Bopindolol	C23H28N2O3	62658-63-3	+
Bornaprine	C21H31NO2	20448-86-6	+
Boscalid (Nicobifen)	C18H12Cl2N2O	188425-85-6	+
Bosentan	C27H29N5O6S	147536-97-8	+
Brallobarbital	C10H11BrN2O3	561-86-4	-
Bretylum	C11H17BrN	59-41-6	+
Brimonidine	C11H10BrN5	59803-98-4	+
Brinzolamide	C12H21N3O5S3	138890-62-7	+
Brodifacoum	C31H23BrO3	56073-10-0	+
Bromacil	C9H13BrN2O2	314-40-9	+
Bromazepam	C14H10BrN3O	1812-30-2	+
Bromazine	C17H20BrNO	118-23-0	+
Brombuterol	C12H18Br2N2O	41937-02-4	+
Bromfenvinphos	C12H14BrCl2O4P	33399-00-7	+
Bromfenvinphos-methyl	C10H10BrCl2O4P	13104-21-7	+
Bromhexine	C14H20Br2N2	3572-43-8	+
Bromisoval	C6H11BrN2O2	496-67-3	+
Bromoallylmethylbutylbarbituric acid (Sigmodal)	C12H17BrN2O3	1216-40-6	-
Bromochlorophene	C13H8Br2Cl2O2	15435-29-7	-

Compound Name	Formula	CAS	Polarity
Bromocriptine	C32H40BrN5O5	25614-03-3	+
Bromo-DragonFLY	C13H12BrNO2	502759-67-3	+
Bromofenoxim	C13H7Br2N3O6	13181-17-4	-
Bromophos-ethyl	C10H12BrCl2O3PS	4824-78-6	+
Bromopride	C14H22BrN3O2	4093-35-0	+ -
Bromopyrazon (Brompyrazon)	C10H8BrN3O	3042-84-0	+
Bromothymol (Vermella)	C10H13BrO	15062-34-7	-
Bromoxynil	C7H3Br2NO	1689-84-5	-
Bromperidol	C21H23BrFNO2	10457-90-6	+
Brompheniramine	C16H19BrN2	86-22-6	+
Bromtripelennamin	C16H20BrN3	531-09-9	+
Bromuconazole(I)	C13H12BrCl2N3O	116255-48-2	+
Bromuconazole(II)	C13H12BrCl2N3O	116255-48-2	+
Bromuron	C9H11BrN2O	3408-97-7	+
Brotizolam	C15H10BrClN4S	57801-81-7	+
Broxuridine	C9H11BrN2O5	59-14-3	-
Broxyquinoline	C9H5Br2NO	521-74-4	-
Brucine	C23H26N2O4	357-57-3	+
BTS 27271	C10H14N2	33089-74-6	+
BTS 27919 (N-(2,4-dimethylphenyl)formamide)	C9H11NO	60397-77-5	+
Bucetin	C12H17NO3	1083-57-4	+
Bucladesin	C18H24N5O8P	362-74-3	+ -
Buclizine	C28H33ClN2	82-95-1	+
Buclosamide	C11H14ClNO2	575-74-6	+
Budesonide	C25H34O6	51333-22-3	+
Budipine	C21H27N	57982-78-2	+
Bufexamac	C12H17NO3	2438-72-4	+ -
Buflomedil	C17H25NO4	35543-24-9	+
Buformine	C6H15N5	692-13-7	+
Bulbocapnine	C19H19NO4	298-45-3	+
Bumadizone	C19H22N2O3	3583-64-0	+
Bumetanide	C17H20N2O5S	28395-03-1	+ -
Bunazosin	C19H27N5O3	80755-51-7	+
Bunitrolol	C14H20N2O2	34915-68-9	+
Buphedrone (MABP)	C11H15NO	408332-79-6	+
Buphenine	C19H25NO2	447-41-6	+ -
Bupirimate	C13H24N4O3S	41483-43-6	+
Bupivacaine	C18H28N2O	2180-92-9	+
Bupranolol	C14H22ClNO2	14556-46-8	+
Buprenorphine	C29H41NO4	52485-79-7	+ -
Buprenorphine glucuronide	C35H49NO10	101224-22-0	+
Buprofezin	C16H23N3OS	69327-76-0	+
Bupropion (Amfebutamone)	C13H18ClNO	34911-55-2	+
Buserelin (Profact)	C60H86N16O13	57982-77-1	+
Buspirone	C21H31N5O2	36505-84-7	+

Compound Name	Formula	CAS	Polarity
Busulfan	C6H14O6S2	55-98-1	+
Butabarbital (Secubarbital)	C10H16N2O3	125-40-6	-
Butacaine	C18H30N2O2	149-16-6	+ -
Butalamine	C18H28N4O	22131-35-7	+
Butalbital	C11H16N2O3	77-26-9	+ -
Butallylonal	C11H15BrN2O3	1142-70-7	-
Butanilicaine	C13H19CIN2O	3785-21-5	+
Butaperazine	C24H31N3OS	653-03-2	+
Butaprost	C24H40O5	69648-38-0	+ -
Butethamate	C16H25NO2	14007-64-8	+
Buthalital	C11H16N2O2S	468-65-5	-
Butinoline	C20H21NO	968-63-8	+
Butobarbital	C10H16N2O3	77-28-1	-
Butocarboxim-sulfoxide	C7H14N2O3S	34681-24-8	+
Butorphanol	C21H29NO2	42408-82-2	+
Butoxycaine	C17H27NO3	2350-32-5	+
Butoxycarboxim	C7H14N2O4S	34681-23-7	+
Butralin (Sutralin)	C14H21N3O4	33629-47-9	+
Buturon	C12H13CIN2O	3766-60-7	+
Butylate (Sutan)	C11H23NOS	2008-41-5	+
Butylbenzylphthalate	C19H20O4	85-68-7	+
Butylscopolaminium	C21H30NO4	149-64-4	+
BZP / Benzylpiperazine	C11H16N2	110475-31-5	+
Cabergoline	C26H37N5O2	81409-90-7	+
Cacodylic acid (Dimethylarsenic acid)	C2H7AsO2	75-60-5	+ -
Cadusafos	C10H23O2PS2	95465-99-9	+
Cafaminol	C11H17N5O3	30924-31-3	+
Cafedrine	C18H23N5O3	58166-83-9	+
Caffeine	C8H10N4O2	58-08-2	+
Calciferol (Ergocalciferol) (Vitamin D2)	C28H44O	50-14-6	+
Camazepam	C19H18CIN3O3	36104-80-0	+
Cambendazole	C14H14N4O2S	26097-80-3	+
Camylofine	C19H32N2O2	54-30-8	+
Candesartan	C24H20N6O3	139481-59-7	+
Candesartan Cilexetil	C33H34N6O6	145040-37-5	+ -
Cannabipiperidiethanone	C24H28N2O2	1345970-43-5	+
Canrenoic acid	C22H30O4	4138-96-9	+
Canrenone	C22H28O3	976-71-6	+
Cantharidin	C10H12O4	56-25-7	+
Capreomycin 1A (Capstat)	C25H44N14O8	37280-35-6	+
Caproylresorcinol	C12H16O3	3144-54-5	+
Caprylicacid octanoic acid	C8H16O2	124-07-2	-
Capsaicin	C18H27NO3	404-86-4	+ -
Captodiame	C21H29NS2	486-17-9	+
Captopril	C9H15NO3S	62571-86-2	+

Compound Name	Formula	CAS	Polarity
Carazolol	C18H22N2O2	57775-29-8	+
Carbachol	C6H15N2O2	462-58-8	+
Carbadox	C11H10N4O4	6804-07-5	+
Carbamazepine	C15H12N2O	298-46-4	+
Carbamazepine 10,11-epoxide	C15H12N2O2	36507-30-9	+
Carbamoylphenoxyacetic acid	C9H9NO4	25395-22-6	-
Carbaryl	C12H11NO2	63-25-2	+
Carbazochrome	C10H12N4O3	69-81-8	-
Carbendazim (Azole)	C9H9N3O2	10605-21-7	+
Carbenicillin	C17H18N2O6S	4697-36-3	+
Carbenoxolone	C34H50O7	5697-56-3	-
Carbetamide	C12H16N2O3	16118-49-3	+
Carbidopa	C10H14N2O4	28860-95-9	+ -
Carbimazole	C7H10N2O2S	22232-54-8	+
Carbinoxamine	C16H19CIN2O	486-16-8	+
Carbochromene	C20H27NO5	804-10-4	+
Carbofuran	C12H15NO3	1563-66-2	+
Carbofuran, - 3 hydroxy	C12H15NO4	16655-82-6	+
Carbofuran-3-keto	C12H13NO4	16709-30-1	+
Carbomycin	C42H67NO16	4564-87-8	+ -
Carbophenothion	C11H16ClO2PS3	786-19-6	+
Carboprost	C21H36O5	35700-23-3	-
Carbosulfan	C20H32N2O3S	55285-14-8	+
Carboxin	C12H13NO2S	5234-68-4	+
Carbromal	C7H13BrN2O2	77-65-6	+
Carbutamide	C11H17N3O3S	339-43-5	+
Carbuterol	C13H21N3O3	34866-47-2	+
Carindacillin	C26H26N2O6S	35531-88-5	+ -
Carisoprodol	C12H24N2O4	78-44-4	+
Carmustine	C5H9Cl2N3O2	154-93-8	+
Carnidazole	C8H12N4O3S	42116-76-7	+
Carnitine	C7H16NO3	461-06-3	+
Carphedone	C12H14N2O2	77472-70-9	+
Carprofen	C15H12ClNO2	53716-49-7	-
Cartap	C7H15N3O2S2	15263-53-3	+
Carteolol	C16H24N2O3	51781-06-7	+
Carvacrol (Isopropyl cresol)	C10H14O	499-75-2	-
Carvedilol	C24H26N2O4	72956-09-3	+ -
Carvone	C10H14O	99-49-0	+
Carzenide	C7H7NO4S	138-41-0	-
Catalin	C16H8N2O5	1043-21-6	+
Cathine (d-Norpseudoephedrine)	C9H13NO	492-39-7	+
Cathinone	C9H11NO	71031-15-7	+
CB-13 (CRA-13)	C26H24O2	432047-72-8	+
CB-25	C25H41NO3	869376-63-6	+ -

Compound Name	Formula	CAS	Polarity
CB-52	C26H43NO3	869376-90-9	+ -
CB-86	C26H43NO3	1150586-64-3	+ -
CBD / Cannabidiol	C21H30O2	13956-29-1	+ -
CBN / Cannabinol	C21H26O2	521-35-7	+ -
CDEC / Sulfallate	C8H14ClNS2	95-06-7	+
Cefaclor	C15H14ClN3O4S	53994-73-3	+
Cefadroxil	C16H17N3O5S	50370-12-2	+ -
Cefalexin	C16H17N3O4S	15686-71-2	+ -
Cefalotin	C16H16N2O6S2	153-61-7	-
Cefdinir	C14H13N5O5S2	91832-40-5	+ -
Cefepime	C19H25N6O5S2	88040-23-7	+
Cefixime	C16H15N5O7S2	79350-37-1	+
Cefmenoxime	C16H17N9O5S3	65085-01-0	+
Cefmetazole	C15H17N7O5S3	56796-20-4	+
Cefodizime	C20H20N6O7S4	69739-16-8	+
Cefoperazone	C25H27N9O8S2	62893-19-0	+ -
Cefotaxime	C16H17N5O7S2	63527-52-6	+ -
Cefotiam	C18H23N9O4S3	61622-34-2	+
Cefoxitin	C16H17N3O7S2	35607-66-0	-
Cefpodoxim	C21H27N5O9S2	87239-81-4	+
Cefradine	C16H19N3O4S	38821-53-3	+ -
Ceftazidime	C22H23N6O7S2	72558-82-8	+
Ceftibuten	C15H14N4O6S2	97519-39-6	+ -
Ceftiofur	C19H17N5O7S3	80370-57-6	+
Ceftriaxone	C18H18N8O7S3	73384-59-5	+ -
Cefuroxime	C16H16N4O8S	55268-75-2	-
Celecoxib	C17H14F3N3O2S	169590-42-5	+ -
Celiprolol	C20H33N3O4	56980-93-9	+
Cephalosporin C	C16H21N3O8S	61-24-5	+
Cerivastatin	C26H34FNO5	145599-86-6	+
Cerulenin	C12H17NO3	17397-89-6	-
Cetaben	C23H39NO2	55986-43-1	+ -
Cetirizine	C21H25ClN2O3	83881-51-0	+
Cetobemidone	C15H21NO2	469-79-4	+
Cetylpyridinium	C21H38N	7773-52-6	+
Cevadin	C32H49NO9	62-59-9	+ -
Chartreusin	C32H32O14	6377-18-0	+ -
Chelidonine	C20H19NO5	476-32-4	+
Chenodeoxycholic acid (Chenodiol)	C24H40O4	474-25-9	-
Chloralose	C8H11Cl3O6	15879-93-3	-
Chlorambucil	C14H19Cl2NO2	305-03-3	+
Chloraminophenamide	C6H8ClN3O4S2	121-30-2	-
Chloramphenicol	C11H12Cl2N2O5	56-75-7	+ -
Chloramphenicol palmitate	C27H42Cl2N2O6	530-43-8	-
Chlorantraniliprole	C18H14BrCl2N5O 2	500008-45-7	+

Compound Name	Formula	CAS	Polarity
Chlorazaniil	C9H8CIN5	500-42-5	+
Chlorbenzoxamine	C27H31CIN2O	522-18-9	+
Chlorbromuron	C9H10BrCIN2O2	13360-45-7	+
Chlorbufam	C11H10CINO2	1967-16-4	+
Chlorcarvacrol	C10H13CIO	5665-94-1	-
Chlorcyclizine	C18H21CIN2	82-93-9	+
Chlordiazepoxide	C16H14CIN3O	58-25-3	+ -
Chlordimeform	C10H13CIN2	6164-98-3	+
Chlorfenvinphos(I)	C12H14Cl3O4P	470-90-6	+
Chlorfenvinphos(II)	C12H14Cl3O4P	470-90-6	+
Chlorflurazurone (Chlorfluazurone)	C20H9Cl3F5N3O3	71422-67-8	+
Chlorhexidine	C22H30Cl2N10	55-56-1	+
Chloridazon (PAC)	C10H8CIN3O	1698-60-8	+
Chloridazon-desphenyl	C4H4CIN3O	6339-19-1	+
Chloridazon-desphenyl-methyl	C5H6CIN3O	17254-80-7	+
Chlorimuron-ethyl	C15H15CIN4O6S	90982-32-4	+
Chlormequat	C5H13CIN	7003-89-6	+
Chlormezanone	C11H12CINO3S	80-77-3	+ -
Chlormidazole	C15H13CIN2	3689-76-7	+
Chlorocresol	C7H7CIO	59-50-7	-
Chlorophacinone (Rozol)	C23H15ClO3	3691-35-8	+ -
Chloroprotham (Chlorprotham)	C10H12CINO2	101-21-3	-
Chloropyramine	C16H20CIN3	59-32-5	+
Chloroquine	C18H26CIN3	54-05-7	+ -
Chlorothiazide	C7H6CIN3O4S2	58-94-6	+ -
Chloroxuron	C15H15CIN2O2	1982-47-4	+
Chloroxylenol	C8H9CIO	88-04-0	-
Chlorphenethazine	C16H17CIN2S	2095-24-1	+
Chlorpheniramine	C16H19CIN2	132-22-9	+
Chlorphenoxamine	C18H22CINO	77-38-3	+
Chlorphentermine	C10H14CIN	461-78-9	+
Chlorphoxim	C12H14CIN2O3PS	14816-20-7	+
Chlorpromazine	C17H19CIN2S	50-53-3	+
Chlorpromazine-S-oxide	C17H19CIN2OS	969-99-3	+
Chlorpropamide	C10H13CIN2O3S	94-20-2	+ -
Chlorprothixene	C18H18CINS	113-59-7	+
Chlorpyrifos	C9H11Cl3NO3PS	2921-88-2	+
Chlorpyrifos-methyl	C7H7Cl3NO3PS	5598-13-0	+
Chlorquinaldol	C10H7Cl2NO	72-80-0	-
Chlorsulfuron	C12H12CIN5O4S	64902-72-3	+
Chlortalidone	C14H11CIN2O4S	77-36-1	+
Chlorthenoxazine	C10H10CINO2	132-89-8	+
Chlorthiamid	C7H5Cl2NS	1918-13-4	+
Chlorthiophos	C11H15Cl2O3PS2	60238-56-4	+
Chlortoluron (Chlorotoluron)	C10H13CIN2O	15545-48-9	+

Compound Name	Formula	CAS	Polarity
Chlorzoxazone	C7H4ClNO2	95-25-0	-
Cholic acid	C24H40O5	81-25-4	-
Cholotauric acid	C26H45NO7S	81-24-3	-
Cholyglycine (Glycocholic acid)	C26H43NO6	475-31-0	+ -
Chromafenozone	C24H30N2O3	143807-66-3	+
Ciclacillin	C15H23N3O4S	3485-14-1	+ -
Ciclesonide	C32H44O7	126544-47-6	+
Cicletanine	C14H12ClNO2	89943-82-8	+
Ciclonium	C22H34NO	29546-59-6	+
Ciclopirox	C12H17NO2	29342-05-0	+
Ciclopiroxolamin	C14H24N2O3	41621-49-2	+
Cilastatin	C16H26N2O5S	82009-34-5	+
Cilazapril	C22H31N3O5	88768-40-5	+
Cimbuterol	C13H19N3O	54239-39-3	+
Cimetidine	C10H16N6S	51481-61-9	+ -
Cinchocaine	C20H29N3O2	85-79-0	+
Cinchonidine	C19H22N2O	485-71-2	+
Cinchonine	C19H22N2O	118-10-5	+
Cinchophen	C16H11NO2	132-60-5	+
Cinchophen methyl ester	C17H13NO2	4546-48-9	+
Cinidon-ethyl	C19H17Cl2NO4	132057-06-8	+
Cinnarizine	C26H28N2	298-57-7	+
Cinosulfuron	C15H19N5O7S	94593-91-6	+
Cinoxacin	C12H10N2O5	28657-80-9	+
Ciprofloxacin	C17H18FN3O3	85721-33-1	+
Ciprostene	C22H36O4	81845-44-5	-
Cisapride	C23H29ClFN3O4	81098-60-4	+
Citalopram	C20H21FN2O	59729-33-8	+
Citolone	C6H9NO2S	1195-16-0	+
Cladribine	C10H12ClN5O3	4291-63-8	+
Clarithromycin	C38H69NO13	81103-11-9	+
Clavulanic acid	C8H9NO5	58001-44-8	-
Clebopride	C20H24ClN3O2	55905-53-8	+
Clemastine	C21H26ClNO	15686-51-8	+
Clemizole	C19H20ClN3	442-52-4	+
Clenbuterol	C12H18Cl2N2O	37148-27-9	+
Clencyclohexerol	C14H20Cl2N2O2	157877-79-7	+
Clenhexerol (Granisetron) (Kytril)	C18H24N4O	109889-09-0	+
Clenpenterol	C13H20Cl2N2O	38339-21-8	+
Clenproperol	C11H16Cl2N2O	38339-11-6	+
Clethodim	C17H26ClNO3S	99129-21-2	+ -
Clethodim-sulfone	C17H26ClNO5S	111031-17-5	+
Clethodim-sulfoxide	C17H26ClNO4S	111031-14-2	+
Clibucaine	C15H20Cl2N2O	15302-10-0	+
Clidinium	C22H26NO3	7020-55-5	+

Compound Name	Formula	CAS	Polarity
Climbazole	C15H17CIN2O2	38083-17-9	+
Clindamycin	C18H33CIN2O5S	18323-44-9	+ -
Clioquinol	C9H5ClINO	130-26-7	+
Clobazam (Urbadan)	C16H13CIN2O2	22316-47-8	+
Clobenzepam	C17H18CIN3O	1159-93-9	+
Clobenzorex	C16H18CIN	13364-32-4	+
Clobetasol propionate	C25H32CIFO5	25122-46-7	+ -
Clobetasone butyrate	C26H32CIFO5	25122-57-0	+
Clobutinol	C14H22CINO	14860-49-2	+
Clocortolone 21-caproate	C28H38CIFO5	4891-71-8	+
Clocortolone pivalate	C27H36CIFO5	34097-16-0	+
Clodantoin	C11H17Cl3N2O2S	5588-20-5	-
Clodinafop-propargyl	C17H13CIFNO4	105512-06-9	+
Clodronic acid	CH4Cl2O6P2	10596-23-3	-
Clofazimine	C27H22Cl2N4	2030-63-9	+
Clofedanol	C17H20CINO	791-35-5	+
Clofenamide	C6H7CIN2O4S2	671-95-4	-
Clofenciclan	C18H28CINO	5632-52-0	+
Clofenelamine	C20H26CINO	511-46-6	+
Clofentezin	C14H8Cl2N4	74115-24-5	+
Clofexamide	C14H21CIN2O2	1223-36-5	+
Clofibrate	C12H15ClO3	637-07-0	+
Clofibric acid	C10H11ClO3	882-09-7	-
Clofoctol	C21H26Cl2O	37693-01-9	-
Clomazone	C12H14CINO2	81777-89-1	+
Clomfene	C26H28CINO	911-45-5	+
Clomipramine	C19H23CIN2	303-49-1	+
Clonazepam	C15H10CIN3O3	1622-61-3	+
Clonidine	C9H9Cl2N3	4205-90-7	+
Clopamide	C14H20CIN3O3S	636-54-4	+ -
Clopendithiol (cis)	C22H25CIN2OS	53772-83-1	+
Clopendithiol (trans)	C22H25CIN2OS	982-24-1	+
Cloperastine	C20H24CINO	3703-76-2	+
Clopidogrel	C16H16CINO2S	113665-84-2	+
Clopidol	C7H7Cl2NO	2971-90-6	+ -
Cloprostenol	C22H29ClO6	40665-92-7	+ -
Clopyralid	C6H3Cl2NO2	1702-17-6	-
Cloquintocet-mexyl	C18H22CINO3	99607-70-2	+
Clorexolon	C14H17CIN2O3S	2127-01-7	+
Clorindanol	C9H9ClO	145-94-8	-
Clorindione	C15H9ClO2	1146-99-2	+
Clorphene	C13H11ClO	120-32-1	-
Clorsulon	C8H8Cl3N3O4S2	60200-06-8	-
Clostebol acetate	C21H29ClO3	855-19-6	+
Clothianidin	C6H8CIN5O2S	210880-92-5	+

Compound Name	Formula	CAS	Polarity
Clotiapine	C18H18CIN3S	2058-52-8	+
Clotiazepam	C16H15CIN2OS	33671-46-4	+
Clotrimazole	C22H17CIN2	23593-75-1	+
Clozapine	C18H19CIN4	5786-21-0	+ -
Clozapine N-oxide	C18H19CIN4O	34233-69-7	+ -
Cocaethylene	C18H23NO4	529-38-4	+
Cocaine	C17H21NO4	50-36-2	+
Codeine	C18H21NO3	76-57-3	+
Codeine glucuronide	C24H29NO9	20736-11-2	+ -
Colchiceine	C21H23NO6	477-27-0	+
Colchicine	C22H25NO6	64-86-8	+
Colforsin	C22H34O7	66575-29-9	+
Colistin	C52H98N16O13	1066-17-7	+
Convallotoxin	C29H42O10	508-75-8	+
Corbadrine	C9H13NO3	829-74-3	+
Cornecain (TM)	C15H24N2O3	3686-68-8	+
Corticosterone	C21H30O4	50-22-6	+
Corticosterone acetate	C23H32O5	1173-26-8	+
Cortisone	C21H28O5	53-06-5	+ -
Cortisone acetate	C23H30O6	50-04-4	-
Cotinine	C10H12N2O	486-56-6	+
Coumachlor	C19H15ClO4	81-82-3	+
Coumafuryl	C17H14O5	117-52-2	+
Coumaphos	C14H16ClO5PS	56-72-4	+
Coumarin	C9H6O2	91-64-5	+
Coumatetralyl	C19H16O3	5836-29-3	+
cPA / Cyclopiazonic acid	C20H20N2O3	18172-33-3	-
Cresyl diphenyl phosphate	C19H17O4P	26444-49-5	+
Crimidine	C7H10CIN3	535-89-7	+
Croconazole	C18H15CIN2O	77175-51-0	+
Cromoglicic acid	C23H16O11	16110-51-3	+ -
Cropropamide	C13H24N2O2	633-47-6	+
Crotamiton	C13H17NO	483-63-6	+
Crotetamide	C12H22N2O2	6168-76-9	+
Crotylbarbital	C10H14N2O3	1952-67-6	-
Crystal Violet (Methyl violet) (Basic Violet 3)	C25H30N3	14426-25-6	+
CTC / Chlortetracycline	C22H23CIN2O8	57-62-5	+ -
Curcumin	C21H20O6	458-37-7	+ -
Cyamemazine	C19H21N3S	3546-03-0	+
Cyanazine (Fortrol)	C9H13CIN6	21725-46-2	+
Cyanofenphos (Cyanophenphos)	C15H14NO2PS	13067-93-1	+
Cyclazodone	C12H12N2O2	14461-91-7	+
Cyclizine	C18H22N2	82-92-8	+
Cycloate	C11H21NOS	1134-23-2	+
Cyclobarbital	C12H16N2O3	52-31-3	-

Compound Name	Formula	CAS	Polarity
Cyclobenzaprine	C20H21N	303-53-7	+
Cyclodrin	C19H29NO3	52109-93-0	+
Cyclofenil	C23H24O4	2624-43-3	+
Cycloheximide	C15H23NO4	66-81-9	+ -
Cyclopentamine	C9H19N	102-45-4	+
Cyclopenthiiazide	C13H18CIN3O4S2	742-20-1	-
Cyclopentobarbital (Cyclopal)	C12H14N2O3	76-68-6	-
Cyclopentolate	C17H25NO3	512-15-2	+
Cyclophosphamide	C7H15Cl2N2O2P	50-18-0	+
Cycloserine	C3H6N2O2	68-41-7	+
Cyclosporin A (Ciclosporin)	C62H111N11O12	59865-13-3	+ -
Cyclothiazide	C14H16CIN3O4S2	2259-96-3	-
Cyclovalone	C22H22O5	579-23-7	+
Cycloxydim (Focus)	C17H27NO3S	101205-02-1	+ -
Cycluron	C11H22N2O	2163-69-1	+
Cyflée (Cythioate)	C8H12NO5PS2	115-93-5	+ -
Cyflufenamid	C20H17F5N2O2	180409-60-3	+
Cymarin	C30H44O9	508-77-0	+
Cymoxanil (Curzate)	C7H10N4O3	57966-95-7	+
Cyphenothrin	C24H25NO3	39515-40-7	+
Cyproconazole(I)	C15H18CIN3O	94361-06-5	+
Cyproconazole(II)	C15H18CIN3O	94361-06-5	+
Cyprodinil	C14H15N3	121552-61-2	+
Cyprofuram	C14H14CINO3	69581-33-5	+
Cyproheptadine	C21H21N	129-03-3	+
Cyproterone acetate	C24H29ClO4	427-51-0	+
Cyromazine	C6H10N6	66215-27-8	+
Cystamine	C4H12N2S2	51-85-4	+
Cytarabine	C9H13N3O5	147-94-4	+
Cytisine	C11H14N2O	485-35-8	+
D(+)-Norephedrine (d- Phenylpropanolamine)	C9H13NO	14838-15-4	+
D,L-beta-(fluorophenyl)-Alanine	C9H10FNO2	51-65-0	+ -
D2PM (Diphenylprolinol)	C17H19NO	112068-01-6	+
Dacarbazine	C6H10N6O	4342-03-4	+ -
Dactinomycin	C62H86N12O16	50-76-0	+
Dalfopristin	C34H50N4O9S	112362-50-2	+
Daminozide	C6H12N2O3	1596-84-5	+
Danazole	C22H27NO2	17230-88-5	+
Danofloxacin	C19H20FN3O3	112398-08-0	+
Dantrolene	C14H10N4O5	7261-97-4	+ -
Dantron (Laxapur)	C14H8O4	117-10-2	-
Daphnetin	C9H6O4	486-35-1	+
Dapiprazole	C19H27N5	72822-12-9	+
Dapson	C12H12N2O2S	80-08-0	+
Darifenacin	C28H30N2O2	133099-04-4	+

Compound Name	Formula	CAS	Polarity
Daunorubicin	C27H29NO10	20830-81-3	+
Dazomet	C5H10N2S2	533-74-4	+
DBZP / Dibenzylpiperazine	C18H22N2	1034-11-3	+
DCL / Diclazuril	C17H9Cl3N4O2	101831-37-2	-
DDM / Dichlorophen	C13H10Cl2O2	97-23-4	-
De(hydroxyethyl)opipramol (Opipramol)	C21H25N3	315-72-0	+
Debrisoquine	C10H13N3	1131-64-2	+
Dectaflur	C18H37N	1838-19-3	+
DEET / Diethyltoluamide	C12H17NO	134-62-3	+
Deferoxamine	C25H48N6O8	70-51-9	+
Deguelin	C23H22O6	522-17-8	+
Dehydro aripiprazole	C23H25Cl2N3O2	129722-25-4	+
Dehydroabietic acid	C20H28O2	1740-19-8	+ -
Dehydrocholic acid	C24H34O5	81-23-2	+ -
Delorazepam	C15H10Cl2N2O	2894-67-9	+
Dembroxol	C13H17Br2NO2	83200-09-3	+
Demeclocycline	C21H21ClN2O8	127-33-3	+
Demelverine	C17H21N	13977-33-8	+
Demeton-O	C8H19O3PS2	298-03-3	+
Demeton-O-methyl	C6H15O3PS2	867-27-6	+
Demeton-S-methyl	C6H15O3PS2	919-86-8	+
Demeton-S-methylsulfone	C6H15O5PS2	17040-19-6	+
Demeton-S-methylsulfoxide	C6H15O4PS2	301-12-2	+
Demoxepam	C15H11ClN2O2	963-39-3	+ -
Denatonium	C21H29N2O	47324-98-1	+
Denaverine	C24H33NO3	3579-62-2	+
Deoxycorticosterone acetate	C23H32O4	56-47-3	+
DEP / Diethyl phthalate	C12H14O4	84-66-2	+
Deptropine	C23H27NO	604-51-3	+
Desacetylmetipranolol	C15H25NO3	57193-14-3	+
Desalkyldisopyramide	C18H23N3O	38236-46-3	+
Desalkylflurazepam	C15H10ClFN2O	2886-65-9	+
Desethylamidarone	C23H25I2NO3	83409-32-9	+
Desethylsebutylazine (Sebutylazine-desethyl)	C7H12ClN5	37019-18-4	+
Desipramine	C18H22N2	50-47-5	+
Deslanoside	C47H74O19	17598-65-1	+
Desloratadine	C19H19ClN2	100643-71-8	+
Desmedipham	C16H16N2O4	13684-56-5	+
Desmeninol	C5H10O3S	120-91-2	-
Desmethyl trimipramine (Nortrimipramine)	C19H24N2	2293-21-2	+
Desmethylclomipramine	C18H21ClN2	303-48-0	+
Desmethyldiphenhydramine	C16H19NO	53499-40-4	+
Desmethylnortriptyline	C18H19N	4444-42-2	+
Desmethyl-pirimicarb	C10H16N4O2	30614-22-3	+
Desmetryn	C8H15N5S	1014-69-3	+

Compound Name	Formula	CAS	Polarity
Desomorphine	C17H21NO2	427-00-9	+
Desonide	C24H32O6	638-94-8	+
Desoximetasone	C22H29FO4	382-67-2	+ -
Desoxycortone (11-Deoxycorticosterone)	C21H30O3	64-85-7	+
Desoxycortone 21-(3-phenylpropionate)	C30H38O4	14007-50-2	+
Desoxy-D2PM / (S)-2-Diphenylmethylpyrrolidine	C17H19N	119237-64-8	+
Desoxyhydroxycorticosterone	C21H30O4	152-58-9	+ -
Desthio-Prothioconazole(I)	C14H15Cl2N3O	120983-64-4	+
Desthio-Prothioconazole(II)	C14H15Cl2N3O	120983-64-4	+
DET / N,N-Diethyltryptamine	C14H20N2	7558-72-7	+
Detajmium	C27H42N3O3	47719-70-0	+
Detlazacort	C25H31NO6	14484-47-0	+
Dexamethasone	C22H29FO5	50-02-2	+ -
Dexamethasone 21-acetate	C24H31FO6	1177-87-3	+
Dexamethasone 21-phosphate	C22H30FO8P	312-93-6	+
Dexamethasone 21-pivalate	C27H37FO6	1926-94-9	+
Dexamethasone isonicotinate	C28H32FNO6	2265-64-7	+
Dexbromopheniramine	C16H19BrN2	132-21-8	+
Dexchlorpheniramine	C16H19ClN2	25523-97-1	+
Dexfenfluramine	C12H16F3N	3239-44-9	+
Dexketoprofen	C16H14O3	22161-81-5	+
Dexpanthenol (Panthenol)	C9H19NO4	81-13-0	+ -
Dextromoramide	C25H32N2O2	357-56-2	+
Dextronorgestrel ((+)-Norgestrel)	C21H28O2	797-64-8	+
Dextrorphan (Levorphanol - d form)	C17H23NO	125-73-5	+ -
Dextrothyroxine (Thyroxine)	C15H11I4NO4	51-49-0	-
DHSM / Dihydrostreptomycin	C21H41N7O12	128-46-1	+
Diacerein	C19H12O8	13739-02-1	-
Diacetamate	C10H11NO3	2623-33-8	+
Diacetolol	C16H24N2O4	28197-69-5	+
Diafenthuron	C23H32N2O5	80060-09-9	+
Dialifos	C14H17ClNO4PS2	10311-84-9	+
Diaveridin	C13H16N4O2	5355-16-8	+
Diazepam	C16H13ClN2O	439-14-5	+
Diazinon (Dimpylate)	C12H21N2O3PS	333-41-5	+
Diazoxide	C8H7ClN2O2S	364-98-7	+
Dibenzepin	C18H21N3O	4498-32-2	+
Dibromodihydroxybenzil	C14H8Br2O4	523-88-6	-
Dibromophenol sulfonic acid	C6H4Br2O4S	4232-99-9	-
Dibunate	C18H24O3S	14992-58-6	-
Dicamba	C8H6Cl2O3	1918-00-9	-
Dichlobutrazol (Diclobutrazol)	C15H19Cl2N3O	75736-33-3	+
Dichlofenthion	C10H13Cl2O3PS	97-17-6	+
Dichloran	C6H4Cl2N2O2	99-30-9	-
Dichloroquinolinol	C9H5Cl2NO	773-76-2	+ -

Compound Name	Formula	CAS	Polarity
Diclofenac	C14H11Cl2NO2	15307-86-5	+ -
Diclofenamide	C6H6Cl2N2O4S2	120-97-8	-
Diclofop-methyl	C16H14Cl2O4	51338-27-3	+
Diclosulam	C13H10Cl2FN5O3S	145701-21-9	+
Dicloxacillin	C19H17Cl2N3O5S	3116-76-5	+ -
Dicoumarol	C19H12O6	66-76-2	-
Dicrotophos (Bidrin)	C8H16NO5P	141-66-2	+
Dicryl (Chloranocryl)	C10H9Cl2NO	2164-09-2	+
Dicyclanil	C8H10N6	112636-83-6	+
Dicycloverine (Dicyclomine)	C19H35NO2	77-19-0	+
Didanosine	C10H12N4O3	69655-05-6	+
Dienestrol diacetate	C22H22O4	84-19-5	+
Dienogest	C20H25NO2	65928-58-7	+
Diethazine	C18H22N2S	60-91-3	+
Diethofencarb	C14H21NO4	87130-20-9	+
Diethylcarbamazine	C10H21N3O	90-89-1	+
Diethylstilbestrol	C18H20O2	56-53-1	-
Difenacoum	C31H24O3	56073-07-5	+
Difenconazole(I)	C19H17Cl2N3O3	119446-68-3	+
Difenconazole(II)	C19H17Cl2N3O3	119446-68-3	+
Difenidol	C21H27NO	972-02-1	+
Difenoxuron	C16H18N2O3	14214-32-5	+
Difenzoquat	C17H17N2	49866-87-7	+
Difethialone	C31H23BrO2S	104653-34-1	-
Diflorasone diacetate	C26H32F2O7	33564-31-7	+ -
Difloxacin	C21H19F2N3O3	98106-17-3	+
Diflubenzuron	C14H9ClF2N2O2	35367-38-5	+
Diflufenican	C19H11F5N2O2	83164-33-4	+
Diflufenzopyr (BAS 65400H)	C15H12F2N4O3	109293-97-2	+
Digitonin	C56H92O29	11024-24-1	-
Digitoxin	C41H64O13	71-63-6	+
Digoxin	C41H64O14	20830-75-5	+ -
Dihexyverine	C20H35NO2	561-77-3	+
Dihydralazin	C8H10N6	484-23-1	+
Dihydrocodeine	C18H23NO3	125-28-0	+
Dihydroergocornine	C31H41N5O5	25447-65-8	+
Dihydroergocristine	C35H41N5O5	17479-19-5	+
Dihydroergocryptine	C32H43N5O5	25447-66-9	+
Dihydroergotamine	C33H37N5O5	511-12-6	+
Dihydromorphine	C17H21NO3	509-60-4	+
Dihydroxyphenylpropanolamine	C9H13NO3	6539-57-7	+ -
Dihyprylone	C9H15NO2	77-03-2	+
Diiodohydroxybenzolsulfonic acid	C6H4I2O4S	554-71-2	-
Diiodohydroxyquinoline	C9H5I2NO	83-73-8	-
Diisopromine	C21H29N	5966-41-6	+

Compound Name	Formula	CAS	Polarity
Dilazep	C31H44N2O10	35898-87-4	+
Diltiazem	C22H26N2O4S	42399-41-7	+
Dimefox	C4H12FN2OP	115-26-4	+
Dimefuron	C15H19CIN4O3	34205-21-5	+
Dimepiperate	C15H21NOS	61432-55-1	+
Dimetacrine	C20H26N2	4757-55-5	+
Dimetamphetamine (Dimetamfetamine)	C11H17N	17279-39-9	+
Dimethachlor	C13H18CINO2	50563-36-5	+
Dimethametryn	C11H21N5S	22936-75-0	+
Dimethenamid (SAN 582H)	C12H18CINO2S	87674-68-8	+
Dimethoate	C5H12NO3PS2	60-51-5	+
Dimethomorph(E)	C21H22CINO4	110488-70-5	+
Dimethomorph(Z)	C21H22CINO4	110488-70-5	+
Dimethyl-4-aminophenol	C8H11NO	619-60-3	+
Dimethylphenylthiazolanimin	C11H14N2S	14007-67-1	+
Dimetilan	C10H16N4O3	644-64-4	+
Dimetindene	C20H24N2	5636-83-9	+
Dimetotiazine	C19H25N3O2S2	7456-24-8	+
Dimetridazole	C5H7N3O2	551-92-8	+
Dimoxystrobin	C19H22N2O3	149961-52-4	+
Diniconazole(I)	C15H17Cl2N3O	76714-88-0	+
Diniconazole(II)	C15H17Cl2N3O	83657-18-5	+
Dinitramine	C11H13F3N4O4	29091-05-2	+
Dinoprost	C20H34O5	551-11-1	+ -
Dinoprostone	C20H32O5	363-24-6	-
Dinoseb (Subitex)	C10H12N2O5	88-85-7	-
Dinotefuran	C7H14N4O3	165252-70-0	+
Dinoterb	C10H12N2O5	1420-07-1	-
Dioxacarb	C11H13NO4	6988-21-2	+
Dioxethdrine	C11H17NO3	497-75-6	+
Dioxoprothazine	C17H20N2O2S	13754-56-8	+
Dioxybenzone	C14H12O4	131-53-3	-
Diphenadione (Diphacinone)	C23H16O3	82-66-6	+ -
Diphenamid	C16H17NO	957-51-7	+
Diphenhydramine	C17H21NO	58-73-1	+
Diphenoxylate	C30H32N2O2	915-30-0	+
Diphenyl octyl phosphate	C20H27O4P	115-88-8	+
Diphenylamine	C12H11N	122-39-4	+ -
Diphenylmethoxyacetic acid	C15H14O3	21409-25-6	-
Diphenylprolinol	C17H19NO	22348-32-9	+
Diphenylpyraline	C19H23NO	147-20-6	+
Dipiproverine	C20H30N2O2	117-30-6	+
Dipivefrine	C19H29NO5	52365-63-6	+
Diponium	C20H38NO2	58875-33-5	+
Diprafenone	C23H31NO3	81447-80-5	+

Compound Name	Formula	CAS	Polarity
Dipropetryn	C11H21N5S	4147-51-7	+
Diprophylline	C10H14N4O4	479-18-5	+
Dipyridamol	C24H40N8O4	58-32-2	+
Dipyrrone (Metamizolum)	C13H17N3O4S	68-89-3	-
Diquat (Deiquat)	C12H12N2	2764-72-9	+
Disopyramide	C21H29N3O	3737-09-5	+
Disulfiram	C10H20N2S4	97-77-8	+
Disulfoton (Ethylthiometon)	C8H19O2PS3	298-04-4	+
Ditalimfos (Plondrel)	C12H14NO4PS	5131-24-8	+
Ditazol	C19H20N2O3	18471-20-0	+
Dithranol	C14H10O3	1143-38-0	+
Diuron	C9H10Cl2N2O	330-54-1	+ -
Dixyrazine	C24H33N3O2S	2470-73-7	+
DMPEA (Dimethylmescaline)	C10H15NO2	120-20-7	+
DMST / N,N-Dimethyl-N'-p-tolylsulfonyldiamide	C9H14N2O2S	66840-71-9	+
DOB / Dimethoxybromoamphetamine	C11H16BrNO2	64638-07-9	+ -
Dobutamine	C18H23NO3	34368-04-2	+
DOC / 2,5-Dimethoxy-4-chloroamphetamine	C11H16ClNO2	123431-31-2	+
Docetaxel	C43H53NO14	114977-28-5	+
Dodemorph	C18H35NO	1593-77-7	+
Dodine	C13H29N3	2439-10-3	+
Dolasetron	C19H20N2O3	115956-12-2	+
DOM (STP)	C12H19NO2	18539-33-8	+
Domperidone	C22H24ClN5O2	57808-66-9	+
Donepezil	C24H29NO3	120014-06-4	+
Dopexamine	C22H32N2O2	86197-47-9	+
Dormovit	C12H14N2O4	1146-21-0	-
Dorzolamide	C10H16N2O4S3	120279-96-1	+
Dothiepin	C19H21NS	113-53-1	+
Doxapram	C24H30N2O2	309-29-5	+
Doxazosin	C23H25N5O5	74191-85-8	+
Doxepin	C19H21NO	1668-19-5	+
Doxorubicin	C27H29NO11	23214-92-8	+ -
Doxycycline	C22H24N2O8	564-25-0	+ -
Doxylamine	C17H22N2O	469-21-6	+
Drazoxolon	C10H8ClN3O2	5707-69-7	+
Drofenine	C20H31NO2	1679-76-1	+
Drometizole	C13H11N3O	2440-22-4	+
Droperidol	C22H22FN3O2	548-73-2	+
Dropropizine	C13H20N2O2	17692-31-8	+
Drospirenone	C24H30O3	67392-87-4	+
D-Tryptophan	C11H12N2O2	153-94-6	+ -
Duloxetine	C18H19NOS	116539-59-4	+
Dutasteride	C27H30F6N2O2	164656-23-9	+
DXM / Dextromethorphan (Methorphan)	C18H25NO	125-71-3	+

Compound Name	Formula	CAS	Polarity
Dyclonine	C18H27NO2	586-60-7	+
Dydrogesterone	C21H28O2	152-62-5	+
Ecgonine	C9H15NO3	481-37-8	+
Ecgonine methyl ester	C10H17NO3	7143-09-1	+
Echinomycin (Quinomycin A)	C51H64N12O12S2	512-64-1	+ -
Econazole	C18H15Cl3N2O	27220-47-9	+
EDPP / Edifenphos	C14H15O2PS2	17109-49-8	+
E-Ferulic acid	C10H10O4	537-98-4	-
Eletriptan	C22H26N2O2S	143322-58-1	+
Ellipticine	C17H14N2	519-23-3	+ -
EMA / Ethylamphetamine (Etilamfetamine)	C11H17N	457-87-4	+
Emamectin B1a	C49H75NO13	121124-29-6	+
Embelin	C17H26O4	550-24-3	-
Embutramide	C17H27NO3	15687-14-6	+
EMDP / 2-Ethyl-5-methyl-3,3-diphenylpyrrolone	C19H21N		+
Emedastine	C17H26N4O	87233-61-2	+
Emepronium	C20H28N	3614-30-0	+
Emetine	C29H40N2O4	483-18-1	+
Emodin	C15H10O5	518-82-1	+
Empenthrin	C18H26O2	54406-48-3	+
Emtricitabine	C8H10FN3O3S	143491-57-0	+
Enalapril	C20H28N2O5	75847-73-3	+ -
Enalaprilat	C18H24N2O5	76420-72-9	+ -
Endomide	C17H28N2O2	4582-18-7	+
Endothal	C8H10O5	145-73-3	+ -
Endothion	C9H13O6PS	2778-04-3	+
Enoxacin	C15H17FN4O3	74011-58-8	+
Enoximone	C12H12N2O2S	77671-31-9	+
Enoximone sulfoxide	C12H12N2O3S	83982-78-9	+
Enoxolone	C30H46O4	471-53-4	+
Enrofloxacin	C19H22FN3O3	93106-60-6	+
Entacapone	C14H15N3O5	130929-57-6	+ -
Ephedrine	C10H15NO	299-42-3	+
Epicillin	C16H21N3O4S	26774-90-3	+
Epiestriol	C18H24O3	547-81-9	-
Epinephrine	C9H13NO3	51-43-4	+
Epirubicin	C27H29NO11	56420-45-2	+
Epivincamine	C21H26N2O3	6835-99-0	+
Eplerenone	C24H30O6	107724-20-9	+
EPN / Tsumaphos	C14H14NO4PS	2104-64-5	+
Epoxiconazole (BAS 480F)	C17H13ClFN3O	133855-98-8	+
Eprazinone	C24H32N2O2	10402-90-1	+
Eprosartan	C23H24N2O4S	133040-01-4	+
EPTC / Epthame	C9H19NOS	759-94-4	+
Equilin sulfate	C18H20O5S	27540-07-4	-

Compound Name	Formula	CAS	Polarity
Ergocornine	C31H39N5O5	564-36-3	+
Ergometrine (Ergonovine)	C19H23N3O2	60-79-7	+
Ergotamine (Ergotamine I)	C33H35N5O5	113-15-5	+
Erythritol	C4H10O4	149-32-6	+ -
Erythromycin	C37H67NO13	114-07-8	+
Erythromycin ethyl succinate	C43H75NO16	1264-62-6	+
Esculetin	C9H6O4	305-01-1	+ -
Esculetin dinicotinate	C21H12N2O6		+
Esmolol	C16H25NO4	103598-03-4	+
Esomeprazole	C17H19N3O3S	119141-88-7	+
Estazolam	C16H11ClN4	29975-16-4	+
Estradiol benzoate	C25H28O3	50-50-0	+
Estradiol cypionate	C26H36O3	313-06-4	-
Estradiol valerate	C23H32O3	979-32-8	-
Estramustine	C23H31Cl2NO3	2998-57-4	+
Estrone	C18H22O2	53-16-7	-
Estrone hydrogen sulfate	C18H22O5S	481-97-0	-
Etaconazole	C14H15Cl2N3O2	60207-93-4	+
Etafedrine	C12H19NO	48141-64-6	+
Etafenone	C21H27NO2	90-54-0	+
Etamiphylline	C13H21N5O2	314-35-2	+
Etamivan	C12H17NO3	304-84-7	+
Etanidazole	C7H10N4O4	22668-01-5	+ -
Etaqualone	C17H16N2O	7432-25-9	+
Ethaboxam	C14H16N4OS2	162650-77-3	+
Ethacridine	C15H15N3O	442-16-0	+
Ethacrynic acid	C13H12Cl2O4	58-54-8	-
Ethambutol	C10H24N2O2	74-55-5	+
Ethametsulfuron-methyl	C15H18N6O6S	97780-06-8	+
Ethaverine	C24H29NO4	486-47-5	+
Ethephon	C2H6ClO3P	16672-87-0	+
Ethidimuron (Sulfadiazole)	C7H12N4O3S2	30043-49-3	+
Ethidium	C21H20N3	3546-21-2	+
Ethinodiol diacetate	C24H32O4	297-76-7	+ -
Ethinylestradiol	C20H24O2	57-63-6	+ -
Ethiofencarb	C11H15NO2S	29973-13-5	+
Ethiofencarb sulfone	C11H15NO4S	53380-23-7	+
Ethiofencarb sulfoxide	C11H15NO3S	53380-22-6	+
Ethiolate	C7H15NOS	2941-55-1	+
Ethion	C9H22O4P2S4	563-12-2	+
Ethionamide	C8H10N2S	536-33-4	+ -
Ethiprole	C13H9Cl2F3N4OS	181587-01-9	+
Ethirimol	C11H19N3O	23947-60-6	+
Ethisterone	C21H28O2	434-03-7	+
Ethofumesate	C13H18O5S	26225-79-6	+

Compound Name	Formula	CAS	Polarity
Ethoheptazine	C16H23NO2	77-15-6	+
Ethopabate	C12H15NO4	59-06-3	+
Ethoprop (Ethoprophos)	C8H19O2PS2	13194-48-4	+
Ethosuximide	C7H11NO2	77-67-8	-
Ethotoin	C11H12N2O2	86-35-1	+ -
Ethoxyquin	C14H19NO	91-53-2	+
Ethoxysulfuron	C15H18N4O7S	126801-58-9	+
Ethyl 4-hydroxybenzoate	C9H10O3	120-47-8	-
Ethyl glucuronide	C8H14O7	17685-04-0	-
Ethyl nicotinate	C8H9NO2	614-18-6	+
Ethylbiscoumacetate	C22H16O8	548-00-5	+
Ethylcathinone (Ethcathinone)	C11H15NO	51553-17-4	+
Ethylmorphine	C19H23NO3	76-58-4	+
Ethylnorepinephrine	C10H15NO3	536-24-3	+ -
Ethylpiperidylbarbituric acid	C11H17N3O3	509-87-5	+
Ethylvanillin	C9H10O3	121-32-4	+
Etidocaine	C17H28N2O	36637-18-0	+
Etilefrine	C10H15NO2	709-55-7	+
Etiracetam	C8H14N2O2	33996-58-6	+
Etiroxate	C18H17I4NO4	17365-01-4	+
Etisazole	C9H10N2S	7716-60-1	+
Etodolac	C17H21NO3	41340-25-4	-
Etodroxizine	C23H31ClN2O3	17692-34-1	+
Etofenamate	C18H18F3NO4	30544-47-9	+
Etofibrate	C18H18ClNO5	31637-97-5	+
Etofilline	C9H12N4O3	519-37-9	+
Etofilline clofibrate	C19H21ClN4O5	54504-70-0	+
Etoloxamine	C19H25NO	1157-87-5	+
Etomidate	C14H16N2O2	33125-97-2	+ -
Etonitazene	C22H28N4O3	911-65-9	+
Etonogestrel	C22H28O2	54048-10-1	+
Etoricoxib	C18H15ClN2O2S	202409-33-4	+
Etoxazole	C21H23F2NO2	153233-91-1	+
Etozolin	C13H20N2O3S	73-09-6	+
Etrimfos	C10H17N2O4PS	38260-54-7	+
ETU / Ethylene thiourea (Imidazolidinethione)	C3H6N2S	96-45-7	+
Eucatropine	C17H25NO3	100-91-4	+
Eugenol	C10H12O2	97-53-0	+
Exalamide	C13H19NO2	53370-90-4	+
Exemestane	C20H24O2	107868-30-4	+
Ezetimibe	C24H21F2NO3	163222-33-1	-
Famciclovir	C14H19N5O4	104227-87-4	+
Famotidine	C8H15N7O2S3	76824-35-6	+
Famphur (Famophos)	C10H16NO5PS2	52-85-7	+
Famprofazone	C24H31N3O	22881-35-2	+

Compound Name	Formula	CAS	Polarity
Febantel	C20H22N4O6S	58306-30-2	+
Febuprol	C13H20O3	3102-00-9	+
Fedrilate	C20H29NO4	23271-74-1	+
Felbamate	C11H14N2O4	25451-15-4	+
Felodipine	C18H19Cl2NO4	72509-76-3	+
Fenamidone	C17H17N3OS	161326-34-7	+
Fenaminoisulf (Dexon)	C8H11N3O3S	150-70-9	-
Fenamiphos	C13H22NO3PS	22224-92-6	+
Fenamiphos - sulfone	C13H22NO5PS	31972-44-8	+
Fenamiphos - sulfoxide	C13H22NO4PS	31972-43-7	+
Fenamisal	C13H11NO3	133-11-9	+
Fenarimol	C17H12Cl2N2O	60168-88-9	+
Fenazaflo	C15H7Cl2F3N2O2	14255-88-0	+
Fenazaquin	C20H22N2O	120928-09-8	+
Fenazepam (Phenazepam)	C15H10BrClN2O	51753-57-2	+
Fenazox (Azoxybenzene)	C12H10N2O	495-48-7	+
Fenbendazole	C15H13N3O2S	43210-67-9	+ -
Fenbendazol-sulfone (Oxfendazole sulfone)	C15H13N3O4S	54029-20-8	+
Fenbuconazole	C19H17ClN4	114369-43-6	+
Fenbufen	C16H14O3	36330-85-5	+ -
Fenbutrazate	C23H29NO3	4378-36-3	+
Fencamfamine (Norcamphane)	C15H21N	1209-98-9	+
Fencarbamide	C19H24N2OS	3735-90-8	+
Fenchlorazole-ethyl	C12H8Cl5N3O2	103112-35-2	+
Fenclonin	C9H10ClNO2	7424-00-2	+ -
Fendiline	C23H25N	13042-18-7	+
Fenetylline	C18H23N5O2	3736-08-1	+
Fenfluramine	C12H16F3N	458-24-2	+
Fenfuram	C12H11NO2	24691-80-3	+
Fenhexamid	C14H17Cl2NO2	126833-17-8	+
Fenitrothion	C9H12NO5PS	122-14-5	+
Fenobucarb (Baycarb)	C12H17NO2	3766-81-2	+
Fenofibrate	C20H21ClO4	49562-28-9	+
Fenoldopam	C16H16ClNO3	67227-56-9	+
Fenoprofen	C15H14O3	31879-05-7	-
Fenoterol (Th 1165a)	C17H21NO4	13392-18-2	+
Fenoxanil	C15H18Cl2N2O2	115852-48-7	+
Fenoxaprop-ethyl	C18H16ClNO5	66441-23-4	+
Fenoxazoline	C13H18N2O	4846-91-7	+
Fenoxycarb	C17H19NO4	79127-80-3	+
Fenpiclonil	C11H6Cl2N2	74738-17-3	+
Fenpipramide	C21H26N2O	77-01-0	+
Fenpiprane	C20H25N	3540-95-2	+
Fenpropathrin	C22H23NO3	39515-41-8	+
Fenpropidin	C19H31N	67306-00-7	+

Compound Name	Formula	CAS	Polarity
Fenpropimorph (Ro 14-3169)	C20H33NO	67564-91-4	+
Fenproporex	C12H16N2	15686-61-0	+
Fenpyroximate	C24H27N3O4	134098-61-6	+
Fenretinide	C26H33NO2	65646-68-6	+
Fenspiride	C15H20N2O2	5053-08-7	+
Fensulfothion	C11H17O4PS2	115-90-2	+
Fentanyl	C22H28N2O	437-38-7	+
Fenthion	C10H15O3PS2	55-38-9	+
Fenthion sulfoxide (Mesulfenfos)	C10H15O4PS2	3761-41-9	+
Fenthion-oxon	C10H15O4PS	6552-12-1	+
Fenthion-oxon-sulfoxide	C10H15O5PS	6552-13-2	+
Fenthion-sulfone	C10H15O5PS2	3761-42-0	+
Fenticlor (Fentichlor)	C12H8Cl2O2S	97-24-5	-
Fenticonazole	C24H20Cl2N2OS	72479-26-6	+
Fentrazamid (Innova)	C16H20ClN5O2	158237-07-1	+
Fenuron (N,N-Dimethyl-N-phenylurea)	C9H12N2O	101-42-8	+
Fenyramidol	C13H14N2O	553-69-5	+
Fexofenadine	C32H39NO4	83799-24-0	+ -
Finasteride	C23H36N2O2	98319-26-7	+
Fipexide	C20H21ClN2O4	34161-24-5	+
Fipronil	C12H4Cl2F6N4OS	120068-37-3	-
Fisetin	C15H10O6	528-48-3	+
Flamprop-isopropyl	C19H19ClFNO3	52756-22-6	+
Flamprop-methyl	C17H15ClFNO3	52756-25-9	+
Flazasulfuron	C13H12F3N5O5S	104040-78-0	+
Flecaïnide	C17H20F6N2O3	54143-55-4	+
Flephedrone (4-FMC)	C10H12FNO	7589-35-7	+
Fleroxacin	C17H18F3N3O3	79660-72-3	+
Flocoumafen	C33H25F3O4	90035-08-8	-
Floctafenine	C20H17F3N2O4	23779-99-9	+
Flonicamid	C9H6F3N3O	158062-67-0	+
Flopropion	C9H10O4	2295-58-1	+
Florasulam	C12H8F3N5O3S	145701-23-1	+
Floxuridine	C9H11FN2O5	50-91-9	-
Fluacrypyrim	C20H21F3N2O5	229977-93-9	+
Fluanisone	C21H25FN2O2	1480-19-9	+
Fluazifop	C15H12F3NO4	69335-91-7	+
Fluazifop-butyl	C19H20F3NO4	69806-50-4	+
Fluazinam (Shirlan)	C13H4Cl2F6N4O4	79622-59-6	-
Fluazuron	C20H10Cl2F5N3O3	86811-58-7	+
Flubendazole	C16H12FN3O3	31430-15-6	+
Flubenzimine	C17H10F6N4S	37893-02-0	+
Fluchloralin	C12H13ClF3N3O4	33245-39-5	+
Flucloxacillin	C19H17ClFN3O5S	5250-39-5	+
Fluconazole(l) (Diflucan)	C13H12F2N6O	86386-73-4	+ -

Compound Name	Formula	CAS	Polarity
Fluconazole(II) (Diflucan)	C13H12F2N6O	86386-73-4	+ -
Flucytosine	C4H4FN3O	2022-85-7	+
Fludarabine phosphate	C10H13FN5O7P	75607-67-9	+ -
Fludiazepam	C16H12ClFN2O	3900-31-0	+
Fludioxonil	C12H6F2N2O2	131341-86-1	-
Fludrocortisone	C21H29FO5	127-31-1	+ -
Fludrocortisone acetate	C23H31FO6	514-36-3	+ -
Flufenacet (Fluthiamide) (BAY FOE 5043)	C14H13F4N3O2S	142459-58-3	+
Flufenamic acid	C14H10F3NO2	530-78-9	+ -
Flufenoxuron	C21H11ClF6N2O3	101463-69-8	+
Flugestone	C21H29FO4	337-03-1	+
Flumazenil	C15H14FN3O3	78755-81-4	+
Flumequine	C14H12FNO3	42835-25-6	+
Flumethasone (Flumetasone)	C22H28F2O5	2135-17-3	+ -
Flumethasone pivalate	C27H36F2O6	2002-29-1	+
Flumetralin	C16H12ClF4N3O4	62924-70-3	+
Flumetsulam	C12H9F2N5O2S	98967-40-9	+
Flunarizine	C26H26F2N2	52468-60-7	+
Flunisolide	C24H31FO6	3385-03-3	+
Flunitrazepam	C16H12FN3O3	1622-62-4	+
Flunixin	C14H11F3N2O2	38677-85-9	+
Fluocinolone acetonide	C24H30F2O6	67-73-2	+
Fluocinonide	C26H32F2O7	356-12-7	+ -
Fluocortin butyl	C26H35FO5	41767-29-7	+
Fluocortolone	C22H29FO4	152-97-6	+
Fluocortolone pivalate	C27H37FO5	29205-06-9	+
Fluometuron	C10H11F3N2O	2164-17-2	+
Fluopicolid	C14H8Cl3F3N2O	239110-15-7	+
Fluorandrenolone	C24H33FO6	1524-88-5	+ -
Fluorescein	C20H12O5	2321-07-5	+
Fluoromethalone	C22H29FO4	426-13-1	+
Fluorotyrosine	C9H10FNO3	139-26-4	+
Fluorouracil	C4H3FN2O2	51-21-8	-
Fluoxastrobin	C21H16ClFN4O5	193740-76-0	+
Fluoxetine	C17H18F3NO	54910-89-3	+
Fluoxymesterone	C20H29FO3	76-43-7	+
Flupentixol	C23H25F3N2OS	2709-56-0	+
Fluphenazine	C22H26F3N3OS	69-23-8	+
Fluphenazine decanoate	C32H44F3N3O2S	5002-47-1	+
Flupirtine	C15H17FN4O2	56995-20-1	+
Fluprednidene acetate	C24H29FO6	1255-35-2	+
Fluquinconazole(I)	C16H8Cl2FN5O	136426-54-5	+
Fluquinconazole(II)	C16H8Cl2FN5O	136426-54-5	+
Flurazepam	C21H23ClFN3O	17617-23-1	+
Flurbiprofen	C15H13FO2	5104-49-4	-

Compound Name	Formula	CAS	Polarity
Fluridone	C19H14F3NO	59756-60-4	+
Flurochloridone	C12H10Cl2F3NO	61213-25-0	+
Fluroxypyr	C7H5Cl2FN2O3	69377-81-7	+ -
Fluroxypyr 1-methylheptyl ester (Starane)	C15H21Cl2FN2O3	81406-37-3	+
Flurtamone	C18H14F3NO2	96525-23-4	+
Flusilazol	C16H15F2N3Si	85509-19-9	+
Flutamide	C11H11F3N2O3	13311-84-7	-
Fluthiacet-methyl	C15H15ClFN3O3S 2	117337-19-6	+
Fluticasone 17-propionate	C25H31F3O5S	80474-14-2	+
Flutolanil	C17H16F3NO2	66332-96-5	+
Flutriafol	C16H13F2N3O	76674-21-0	+
Fluvalinate	C26H22ClF3N2O3	69409-94-5	+
Fluvastatin	C24H26FNO4	93957-54-1	-
Fluvoxamine	C15H21F3N2O2	54739-18-3	+
Folic acid	C19H19N7O6	59-30-3	+ -
Folinic acid	C20H23N7O7	58-05-9	+
Fomesafen	C15H10ClF3N2O6 S	72178-02-0	-
Fominoben	C21H24ClN3O3	18053-31-1	+
Fomocaine	C20H25NO2	17692-39-6	+
Fonofos (Dyfonate)	C10H15OPS2	944-22-9	+
Foramsulfuron	C17H20N6O7S	173159-57-4	+
Forchlorfenuron	C12H10ClN3O	68157-60-8	+
Formestane	C19H26O3	566-48-3	+
Formetanate	C11H15N3O2	22259-30-9	+
Formocortal	C29H38ClFO8	2825-60-7	+
Formononetin	C16H12O4	485-72-3	+ -
Formoterol	C19H24N2O4	73573-87-2	+
Formothion	C6H12NO4PS2	2540-82-1	+ -
Formylsulfisomidine	C13H14N4O3S	795-13-1	+
Fosazepam	C18H18ClN2O2P	35322-07-7	+
Fosfomicin	C3H7O4P	23155-02-4	-
Fosfosal	C7H7O6P	6064-83-1	+ -
Fosthiazate	C9H18NO3PS2	98886-44-3	+
Frovatriptan	C14H17N3O	158747-02-5	+
Fuberidazole	C11H8N2O	3878-19-1	+
Fumonisin B1	C34H59NO15	116355-83-0	-
Fumonisin B2	C34H59NO14	116355-84-1	+ -
Furafylline	C12H12N4O3	80288-49-9	+ -
Furalaxyl	C17H19NO4	57646-30-7	+
Furaltadone	C13H16N4O6	139-91-3	+
Furathiocarb	C18H26N2O5S	65907-30-4	+
Furazolidon	C8H7N3O5	67-45-8	+
Furegrelate	C15H11NO3	85666-24-6	+ -
Furmecyclox	C14H21NO3	60568-05-0	+
Furosemide	C12H11ClN2O5S	54-31-9	-

Compound Name	Formula	CAS	Polarity
Fusidic acid	C31H48O6	6990-06-3	-
GABA / gamma-Aminobutyric acid	C4H9NO2	56-12-2	+ -
Gabapentin	C9H17NO2	60142-96-3	+
Gaboxadol	C6H8N2O2	64603-91-4	+ -
Galantamine	C17H21NO3	357-70-0	+
Gallopamil	C28H40N2O5	16662-47-8	+
gamma-Tocopherol	C28H48O2	7616-22-0	+
Gamolenic acid	C18H30O2	506-26-3	-
Ganciclovir	C9H13N5O4	107910-75-8	+
Gemcitabine	C9H11F2N3O4	95058-81-4	+ -
Gemfibrozil	C15H22O3	25812-30-0	-
Gentamicin (Gentamycin C1)	C21H43N5O7	1403-66-3	+
Gentisic acid	C7H6O4	490-79-9	-
Gepefrine	C9H13NO	18840-47-6	+
Gestodene	C21H26O2	60282-87-3	+
Gestonorone	C20H28O3	2137-18-0	+
Gestonorone acetate	C22H30O4	31981-44-9	+
Gestonorone caproate	C26H38O4	1253-28-7	+
Gestrinone	C21H24O2	16320-04-0	+ -
Glafenin	C19H17ClN2O4	3820-67-5	+ -
Glaucine	C21H25NO4	475-81-0	+
Glibenclamide	C23H28ClN3O5S	10238-21-8	+ -
Gliclazide	C15H21N3O3S	21187-98-4	+ -
Glimepiride	C24H34N4O5S	93479-97-1	+
Glipizide	C21H27N5O4S	29094-61-9	+ -
Gliquidone	C27H33N3O6S	33342-05-1	+
Glisoxepid	C20H27N5O5S	25046-79-1	+
Glucuro lactone	C6H8O6	32449-92-6	-
Glufosinate	C5H12NO4P	35597-44-5	+
Glutethimide	C13H15NO2	77-21-4	+
Glutril (Glibornuride)	C18H26N2O4S	26944-48-9	+
Glycerol	C3H8O3	56-81-5	+
Glycocylamine	C3H7N3O2	352-97-6	+
Glycopyrrolate	C19H28NO3	596-51-0	+
Glycyrrhizinic acid	C42H62O16	1405-86-3	+ -
Glymidine	C13H15N3O4S	339-44-6	+
Glyphosate	C3H8NO5P	1071-83-6	-
Gossypol	C30H30O8	303-45-7	+ -
Grepafloxacin	C19H22FN3O3	119914-60-2	+
Griseofulvin	C17H17ClO6	126-07-8	+
Guafecainol	C16H27NO4	36199-78-7	+
Guaiacol phenylacetate	C15H14O3	4112-89-4	+
Guaifenesin	C10H14O4	93-14-1	+
Guanabenz	C8H8Cl2N4	5051-62-7	+
Guanacline	C9H18N4	1463-28-1	+

Compound Name	Formula	CAS	Polarity
Guanethidine	C10H22N4	55-65-2	+
Guanfacine	C9H9Cl2N3O	29110-47-2	+
Guanine	C5H5N5O	73-40-5	+
Guazatine (Iminoctadine)	C18H41N7	13516-27-3	+
Halazepam	C17H12ClF3N2O	23092-17-3	+
Halcinonide	C24H32ClFO5	3093-35-4	+ -
Halofantrine	C26H30Cl2F3NO	69756-53-2	+
Halofenozone	C18H19ClN2O2	112226-61-6	+
Halofuginone	C16H17BrClN3O3	55837-20-2	+
Halopemide	C21H22ClFN4O2	59831-65-1	+ -
Haloperidol	C21H23ClFNO2	52-86-8	+
Haloperidol decanoate	C31H41ClFNO3	74050-97-8	+
Halosulfuron-methyl	C13H15ClN6O7S	100784-20-1	+
Haloxyfop	C15H11ClF3NO4	69806-34-4	+
Haloxyfop ethoxyethyl	C19H19ClF3NO5	87237-48-7	+
Harmaline	C13H14N2O	304-21-2	+
Harmine	C13H12N2O	442-51-3	-
Harmol	C12H10N2O	487-03-6	+ -
Hematoporphyrin	C34H38N4O6	14459-29-1	+
Heptabarbital	C13H18N2O3	509-86-4	-
Heptaminol	C8H19NO	543-15-7	+
Heptenophos	C9H12ClO4P	23560-59-0	+
Heroin	C21H23NO5	561-27-3	+
Hetacillin	C19H23N3O4S	3511-16-8	+ -
Hexachlorophene	C13H6Cl6O2	70-30-4	-
Hexaconazole(I)	C14H17Cl2N3O	79983-71-4	+
Hexaconazole(II)	C14H17Cl2N3O	79983-71-4	+
Hexaflumuron	C16H8Cl2F6N2O3	86479-06-3	+ -
Hexamidine	C20H26N4O2	3811-75-4	+
Hexazinone	C12H20N4O2	51235-04-2	+
Hexetidine	C21H45N3	141-94-6	+
Hexethylamine	C16H31NO2	20145-18-0	+
Hexobarbital	C12H16N2O3	56-29-1	-
Hexobendine	C30H44N2O10	54-03-5	+
Hexocyclium	C20H33N2O	6004-98-4	+
Hexoprenaline	C22H32N2O6	3215-70-1	+
Hexylnicotinate	C12H17NO2	23597-82-2	+
Hexylresorcinol	C12H18O2	136-77-6	-
Hexythiazox	C17H21ClN2O2S	78587-05-0	+
Histapyrrodine	C19H24N2	493-80-1	+
HMMNI / Hydroxydimetridazole (Dimetridazol-OH)	C5H7N3O3	936-05-0	+
Homarylamine	C10H13NO2	451-77-4	+
Homatropine	C16H21NO3	87-00-3	+
Homofenazine	C23H28F3N3OS	3833-99-6	+
Hordenine	C10H15NO	539-15-1	+

Compound Name	Formula	CAS	Polarity
HU-210	C25H38O3	112830-95-2	+ -
HU-211 (Dexanabinol)	C25H38O3	112924-45-5	+ -
HU-308	C27H42O3	256934-39-1	+
HU-331	C21H28O3	137252-25-6	+ -
Hycanthone	C20H24N2O2S	3105-97-3	+ -
Hydralazin	C8H8N4	86-54-4	+
Hydramethylnon	C25H24F6N4	67485-29-4	+
Hydrochlorothiazide	C7H8ClN3O4S2	58-93-5	-
Hydrocodone	C18H21NO3	125-29-1	+
Hydrocortisone (Cortisol)	C21H30O5	50-23-7	+ -
Hydrocortisone 17-butyrate	C25H36O6	13609-67-1	+
Hydrocortisone 21-phosphate (Cortisol 21-phosphate) (Cleiton)	C21H31O8P	6000-74-4	-
Hydrocortisone aceponate	C26H36O7	74050-20-7	+
Hydrocortisone acetate	C23H32O6	50-03-3	+ -
Hydrocortisone buteprate	C28H40O7	72590-77-3	+
Hydrocortisone succinate	C25H34O8	2203-97-6	+ -
Hydrocotarnine	C12H15NO3	550-10-7	+
Hydroflumethiazide	C8H8F3N3O4S2	135-09-1	-
Hydromorphone	C17H19NO3	466-99-9	+
Hydroquinine	C20H26N2O2	522-66-7	-
Hydroquinone	C6H6O2	123-31-9	-
Hydroxybupropion	C13H18ClNO2	357399-43-0	+
Hydroxychloroquine	C18H26ClN3O	118-42-3	+
Hydroxy-Ipronidazole	C7H11N3O3	35175-14-5	+
Hydroxymetoprolol	C15H25NO4	56392-16-6	+
Hydroxyprocaine	C13H20N2O3	487-53-6	+
Hydroxyprogesterone acetate	C23H32O4	302-23-8	+
Hydroxyprogesterone caproate	C27H40O4	630-56-8	+
Hydroxysimazine	C7H13N5O	2599-11-3	+
Hydroxyzine	C21H27ClN2O2	68-88-2	+
Hygromycin b (Simazine-2-OH)	C20H37N3O13	31282-04-9	+
Hymecromone	C10H8O3	90-33-5	+
Ibafloxacin	C15H14FNO3	91618-36-9	+
Ibandronic acid	C9H23NO7P2	114084-78-5	-
Ibogaine	C20H26N2O	83-74-9	+
Idarubicin	C26H27NO9	58957-92-9	+
Ifosfamide	C7H15Cl2N2O2P	3778-73-2	+
Iloprost	C22H32O4	78919-13-8	-
Imatinib	C29H31N7O	152459-95-5	+
Imazalil (Enilconazole)	C14H14Cl2N2O	35554-44-0	+
Imazapyr	C13H15N3O3	81334-34-1	+
Imazaquin	C17H17N3O3	81335-37-7	+
Imazethapyr	C15H19N3O3	81335-77-5	+
Imibenconazole	C17H13Cl3N4S	86598-92-7	+
Imiclopazine	C25H32ClN5O5	7414-95-1	+

Compound Name	Formula	CAS	Polarity
Imidacloprid	C9H10ClN5O2	138261-41-3	+
Imidapril	C20H27N3O6	89371-37-9	+
Iminostilbene	C14H11N	256-96-2	+
Imipramine	C19H24N2	50-49-7	+
Imiquimod	C14H16N4	99011-02-6	+
IMMA / Indomethacin Morpholinylamide	C23H23ClN2O4	2854-32-2	+
Imolamine	C14H20N4O	318-23-0	+
Indanazoline	C12H15N3	40507-78-6	+
Indapamide	C16H16ClN3O3S	26807-65-8	+ -
Indinavir	C36H47N5O4	150378-17-9	+
Indole	C8H7N	120-72-9	+
Indometacin	C19H16ClNO4	53-86-1	+ -
Indoprofen	C17H15NO3	31842-01-0	+ -
Indoramine	C22H25N3O	26844-12-2	+
Indoxacarb	C22H17ClF3N3O7	173584-44-6	+
Inosine	C10H12N4O5	58-63-9	+ -
Inositol nicotinate	C42H30N6O12	6556-11-2	+
lobenzamic acid	C16H13I3N2O3	3115-05-7	+
locetamic acid	C12H13I3N2O3	16034-77-8	+
Iodipamide	C20H14I6N2O6	606-17-7	+ -
Iodosulfuron-methyl	C14H14IN5O6S	144550-36-7	+
loglicic acid	C13H12I3N3O5	49755-67-1	+
Iohexol	C19H26I3N3O9	66108-95-0	+
Iomeprol	C17H22I3N3O8	78649-41-9	+
Ionomycin	C41H72O9	56092-81-0	+ -
Iopanoic acid	C11H12I3NO2	96-83-3	-
Iopentol	C20H28I3N3O9	89797-00-2	+
Iopodic acid	C12H13I3N2O2	5587-89-3	+
Iopromide	C18H24I3N3O8	73334-07-3	+
Iosarcol	C21H29I3N4O9	97702-82-4	+
Iotalaminic acid	C11H9I3N2O4	2276-90-6	+
Ioversol	C18H24I3N3O9	87771-40-2	+
Ioxaglic acid	C24H21I6N5O8	59017-64-0	-
Ioxitalamic acid	C12H11I3N2O5	28179-44-4	+
Ioxynil	C7H3I2NO	1689-83-4	-
IPC / Propham	C10H13NO2	122-42-9	+
Ipconazole(I)	C18H24ClN3O	125225-28-7	+
Ipconazole(II)	C18H24ClN3O	125225-28-7	+
Ipratropium	C20H30NO3	60205-81-4	+
Iprazochrome	C12H16N4O3	7248-21-7	+
Ipriflavone	C18H16O3	35212-22-7	+
Iprindole	C19H28N2	5560-72-5	+
Iprobenfos	C13H21O3PS	26087-47-8	+
Iprodione (Glycophen)	C13H13Cl2N3O3	36734-19-7	-
Iproniazid	C9H13N3O	54-92-2	+

Compound Name	Formula	CAS	Polarity
Iprnidazole	C7H11N3O2	14885-29-1	+
Iprovalicarb	C18H28N2O3	140923-17-7	+
Irbesartan	C25H28N6O	138402-11-6	+ -
Irgarol (Cybutryne)	C11H19N5S	28159-98-0	+
Irinotecan	C33H38N4O6	97682-44-5	+
Isazofos (Miral)	C9H17ClN3O3PS	42509-80-8	+
Isoaminile	C16H24N2	77-51-0	+
Iso carbamide	C8H15N3O2	30979-48-7	+
Iso carbamazid	C12H13N3O2	59-63-2	+
Isoconazole	C18H14Cl4N2O	27523-40-6	+
Isoetarine	C13H21NO3	530-08-5	+
Isofenphos	C15H24NO4PS	25311-71-1	+
Isofenphos methyl	C14H22NO4PS	99675-03-3	+
Isofenphos oxon	C15H24NO5P	31120-85-1	+
Isometheptene	C9H19N	503-01-5	+
Isomethiozin	C12H20N4OS	57052-04-7	+
Isoniazid	C6H7N3O	54-85-3	+
Isonicotinic acid	C6H5NO2	55-22-1	+ -
Isorenaline	C11H17NO3	7683-59-2	+
Isoprocarb	C11H15NO2	2631-40-5	+
Isopropalin (Bifenthrin)	C15H23N3O4	33820-53-0	+
Isopropamide	C23H33N2O	7492-32-2	+
Isopropyl 4-hydroxybenzoate	C10H12O3	4191-73-5	+
Isoprothiolane	C12H18O4S2	50512-35-1	+
Isoproturon	C12H18N2O	34123-59-6	+ -
Isopyrin	C14H19N3O	3615-24-5	+
Isoquercitrin	C21H20O12	21637-25-2	+
Isosteviol	C20H30O3	27975-19-5	+ -
Isothipendyl	C16H19N3S	482-15-5	+
Isotretinoin	C20H28O2	4759-48-2	+
Isoxaben	C18H24N2O4	82558-50-7	+
Isoxadifen-ethyl (AE F122006)	C18H17NO3	163520-33-0	+
Isoxaflutole	C15H12F3NO4S	141112-29-0	-
Isoxathion	C13H16NO4PS	18854-01-8	+
Isoxicam	C14H13N3O5S	34552-84-6	+ -
Isoxsuprine (Isolait)	C18H23NO3	395-28-8	+ -
Isradipine	C19H21N3O5	75695-93-1	+ -
Itraconazole	C35H38Cl2N8O4	84625-61-6	+
Ivabradine	C27H36N2O5	155974-00-8	+
Jasmolin I	C21H30O3	4466-14-2	+
Josamycin propionate	C45H73NO16	40922-77-8	+
JP-104	C25H30N2O3		+
JWH-007	C25H25NO	155471-10-6	+
JWH-011 (JWH-004 1-methylhexyl analog)	C27H29NO	155471-13-9	+ -
JWH-015	C23H21NO	155471-08-2	+

Compound Name	Formula	CAS	Polarity
JWH-016	C24H23NO	155471-09-3	+
JWH-018 (AM-678)	C24H23NO	209414-07-3	+
JWH-018 2'-naphthyl isomer	C24H23NO	1131605-25-8	+
JWH-018 2'-naphthyl-N-(1,1-dimethylpropyl) isomer	C24H23NO		+
JWH-018 2'-naphthyl-N-(1,2-dimethylpropyl) isomer	C24H23NO		+ -
JWH-018 2'-naphthyl-N-(1-ethylpropyl)	C24H23NO		+
JWH-018 2'-naphthyl-N-(1-methylbutyl) isomer	C24H23NO		+ -
JWH-018 2'-naphthyl-N-(2,2-dimethylpropyl) isomer	C24H23NO		+
JWH-018 2'-naphthyl-N-(2-methylbutyl) isomer	C24H23NO		+
JWH-018 2'-naphthyl-N-(3-methylbutyl) isomer	C24H23NO		+ -
JWH-018 6-methoxyindole analog	C25H25NO2		+
JWH-018 adamantyl analog (AB-001)	C24H31NO	1345973-49-0	+
JWH-018 adamantyl carboxamide (2NE1)	C24H32N2O	1345973-50-3	+
JWH-018 N-(1,1-dimethylpropyl) isomer	C24H23NO	1358118-35-0	+
JWH-018 N-(1,2-dimethylpropyl) isomer	C24H23NO		+
JWH-018 N-(1-ethylpropyl) isomer	C24H23NO		+
JWH-018 N-(1-methylbutyl) isomer	C24H23NO		+
JWH-018 N-(2,2-dimethylpropyl) isomer	C24H23NO		+ -
JWH-018 N-(2-methylbutyl) isomer	C24H23NO		+
JWH-018 N-(3-methylbutyl) isomer	C24H23NO	1346604-93-0	+ -
JWH-018 N-(4,5-epoxypentyl) analog	C24H21NO2		+ -
JWH-018 N-(5-bromopentyl) analog	C24H22BrNO		+
JWH-018 N-(5-chloropentyl) analog	C24H22ClNO		+
JWH-018 N-(5-hydroxypentyl) β -D-Glucuronide	C30H31NO8	1307803-55-9	+ -
JWH-018 N-pentanoic acid metabolite	C24H21NO3	1254475-87-0	+
JWH-019	C25H25NO	209414-08-4	+
JWH-019 N-(6-hydroxyhexyl) metabolite	C25H25NO2		+
JWH-020	C26H27NO	209414-09-5	+
JWH-022 (AM-2201 N-(4-pentenyl) analog)	C24H21NO	209414-16-4	+
JWH-030	C20H21NO	162934-73-8	+
JWH-031	C21H23NO	162934-74-9	+
JWH-072 (N-Propyl-3-(1-naphthoyl)indole)	C22H19NO	209414-06-2	+
JWH-073	C23H21NO	208987-48-8	+
JWH-073 2-methylnaphthyl analog	C24H23NO		+ -
JWH-073 2'-naphthyl isomer	C23H21NO		+
JWH-073 2'-naphthyl-N-(1,1-dimethylethyl) isomer	C23H21NO		+
JWH-073 2'-naphthyl-N-(1-methylpropyl) isomer	C23H21NO		+
JWH-073 2'-naphthyl-N-(2-methylpropyl) isomer	C23H21NO		+ -
JWH-073 4-methylnaphthyl analog	C24H23NO	1354631-21-2	+ -
JWH-073 N-(1,1-dimethylethyl) isomer	C23H21NO		+
JWH-073 N-(1-methylpropyl) isomer	C23H21NO		+
JWH-073 N-(2-methylpropyl) isomer	C23H21NO		+
JWH-081	C25H25NO2	210179-46-7	+
JWH-081 2-methoxynaphthyl isomer (JWH-267)	C25H25NO2	824960-76-1	+
JWH-081 3-methoxynaphthyl isomer	C25H25NO2		+

Compound Name	Formula	CAS	Polarity
JWH-081 5-methoxynaphthyl isomer	C25H25NO2		+
JWH-081 6-methoxynaphthyl isomer (JWH-166)	C25H25NO2	824961-41-3	+
JWH-081 7-methoxynaphthyl isomer (JWH-164)	C25H25NO2	824961-61-7	+
JWH-081 8-methoxynaphthyl isomer	C25H25NO2	1349837-48-4	+
JWH-098	C26H27NO2	316189-74-9	+
JWH-122	C25H25NO	619294-47-2	+
JWH-122 2-methylnaphthyl isomer	C25H25NO		+ -
JWH-122 3-methylnaphthyl isomer	C25H25NO	1391052-25-7	+
JWH-122 5-methylnaphthyl isomer	C25H25NO	1391052-02-0	+
JWH-122 6-methylnaphthyl isomer	C25H25NO		+
JWH-122 7-methylnaphthyl isomer	C25H25NO	824960-56-7	+
JWH-122 8-methylnaphthyl isomer	C25H25NO		+
JWH-122 N-(4-pentenyl) Analog	C25H23NO		+
JWH-122 N-(5-hydroxypentyl) metabolite	C25H25NO2	1379604-68-8	+ -
JWH-145	C26H25NO	914458-19-8	+
JWH-147	C27H27NO	914458-20-1	+
JWH-175	C24H25N	619294-35-8	+
JWH-180	C25H25NO	824959-87-7	+
JWH-182	C27H29NO	824960-02-3	+ -
JWH-200 (WIN-55225)	C25H24N2O2	103610-04-4	+
JWH-200 2'-naphthyl isomer	C25H24N2O2	133438-66-1	+ -
JWH-200 4-hydroxyindole metabolite	C25H24N2O3		+ -
JWH-200 7-hydroxyindole metabolite	C25H24N2O3		+ -
JWH-201	C22H25NO2	864445-47-6	+
JWH-203	C21H22CINO	864445-54-5	+
JWH-203 3-chlorophenyl isomer (JWH-237)	C21H22CINO	864445-56-7	+
JWH-203 4-chlorophenyl isomer (JWH-206)	C21H22CINO	864445-58-9	+ -
JWH-210	C26H27NO	824959-81-1	+
JWH-210 2-ethylnaphthyl isomer	C26H27NO		+
JWH-210 3-ethylnaphthyl isomer	C26H27NO		+
JWH-210 5-ethylnaphthyl isomer	C26H27NO		+
JWH-210 6-ethylnaphthyl isomer	C26H27NO		+
JWH-210 7-ethylnaphthyl isomer (JWH-234)	C26H27NO	824960-64-7	+
JWH-210 8-ethylnaphthyl isomer	C26H27NO		+
JWH-210 N-(4-hydroxypentyl) metabolite	C26H27NO2		+ -
JWH-210 N-(5-carboxypentyl) metabolite	C26H25NO3		+ -
JWH-249	C21H22BrNO	864445-60-3	+
JWH-250	C22H25NO2	864445-43-2	+
JWH-250 5-hydroxyindole metabolite	C22H25NO3	1379604-67-7	+ -
JWH-250 N-(5-hydroxypentyl) metabolite	C22H25NO3		+ -
JWH-251	C22H25NO	864445-39-6	+
JWH-251 3-methylphenyl isomer	C22H25NO		+ -
JWH-251 4-methylphenyl isomer (JWH-208)	C22H25NO	864445-41-0	+ -
JWH-302	C22H25NO2	864445-45-4	+
JWH-307	C26H24FNO	914458-26-7	+

Compound Name	Formula	CAS	Polarity
JWH-309	C30H27NO	914458-42-7	+
JWH-368	C26H24FNO	914458-31-4	+
JWH-369	C26H24ClNO	914458-27-8	+
JWH-370	C27H27NO	914458-22-3	+
JWH-398	C24H22ClNO	1292765-18-4	+
JWH-398 2-chloronaphthyl isomer	C24H22ClNO	1391054-25-3	+
JWH-398 3-chloronaphthyl isomer	C24H22ClNO		+
JWH-398 5-chloronaphthyl isomer	C24H22ClNO		+
JWH-398 6-chloronaphthyl isomer	C24H22ClNO		+
JWH-398 7-chloronaphthyl isomer	C24H22ClNO	1391051-95-8	+
JWH-398 8-chloronaphthyl isomer	C24H22ClNO	1366067-88-0	+
JWH-424	C24H22BrNO	1366068-04-3	+
JZL 195	C24H23N3O5	1210004-12-8	+
Kadethrin	C23H24O4S	58769-20-3	+
Kainic acid	C10H15NO4	487-79-6	+ -
Karbutilate	C14H21N3O3	4849-32-5	+
Kavain	C14H14O3	500-64-1	+
Kebuzone	C19H18N2O3	853-34-9	+
Kelevan	C17H12Cl10O4	4234-79-1	-
Ketamine	C13H16ClNO	6740-88-1	+
Ketanserin	C22H22FN3O3	74050-98-9	+ -
Ketazolam (Loftran) (Anseren)	C20H17ClN2O3	27223-35-4	+
Ketoconazole	C26H28Cl2N4O4	65277-42-1	+
Ketoprofen	C16H14O3	22071-15-4	+
Ketorolac	C15H13NO3	74103-06-3	+
Ketotifen	C19H19NOS	34580-13-7	+
Ketotriclabendazole	C13H7Cl3N2O2	1201920-88-8	+
Khellin	C14H12O5	82-02-0	+
Khellinoacetic acid	C15H12O7	15114-43-9	+
Kresoxim-methyl	C18H19NO4	143390-89-0	+
Labetalol (Laberalol)	C19H24N2O3	36894-69-6	+
Lacididine	C26H33NO6	103890-78-4	+
Lactitol	C12H24O11	585-86-4	-
Lamivudine	C8H11N3O3S	134678-17-4	+ -
Lamotrigine	C9H7Cl2N5	84057-84-1	+
Lanatoside C	C49H76O20	17575-22-3	+
Lansoprazole	C16H14F3N3O2S	103577-45-3	+ -
Lasalacid A	C34H54O8	25999-31-9	+ -
Latanoprost	C26H40O5	130209-82-4	+
Laudanosine	C21H27NO4	2688-77-9	+
Lauroguadine	C20H36N6O	135-43-3	+
Lawsone	C10H6O3	83-72-7	-
Leflunomide	C12H9F3N2O2	75706-12-6	-
Leflunomide metabolite A 771726	C12H9F3N2O2	108605-62-5	-
Lenacil	C13H18N2O2	2164-08-1	+

Compound Name	Formula	CAS	Polarity
Lercanidipine	C36H41N3O6	100427-26-7	+
Letrozole	C17H11N5	112809-51-5	+ -
Levallorphan	C19H25NO	152-02-3	+
Levamisole	C11H12N2S	14769-73-4	+
Levetiracetam	C8H14N2O2	102767-28-2	+
Levobunolol	C17H25NO3	47141-42-4	+
Levofloxacin	C18H20FN3O4	100986-85-4	+
Levomepromazine	C19H24N2OS	60-99-1	+
Levomethadone	C21H27NO	125-58-6	+
Levonorgestrel ((-)-Norgestrel)	C21H28O2	797-63-7	+
Levopropoxyphene	C22H29NO2	2338-37-6	+
Levopropylhexedrine	C10H21N	6192-97-8	+
Levorphanol	C17H23NO	77-07-6	+
Lidocaine (Diocaine)	C14H22N2O	137-58-6	+
Limaprost	C22H36O5	74397-12-9	+ -
Lincomycin	C18H34N2O6S	154-21-2	+
Linuron	C9H10Cl2N2O2	330-55-2	+
Liothyronin	C15H12I3NO4	5817-39-0	-
Lisinopril	C21H31N3O5	83915-83-7	+ -
Lisuride	C20H26N4O	18016-80-3	+
Lobeline	C22H27NO2	90-69-7	+ -
Lodoxamide	C11H6ClN3O6	53882-12-5	-
Lofepramine	C26H27ClN2O	23047-25-8	+
Lofexidine	C11H12Cl2N2O	31036-80-3	+
Lomefloxacin	C17H19F2N3O3	98079-51-7	+
Lonazolac	C17H13ClN2O2	53808-88-1	+ -
Loperamide	C29H33ClN2O2	53179-11-6	+
Loprazolam	C23H21ClN6O3	61197-73-7	+
Loracarbef	C16H16ClN3O4	76470-66-1	+
Loratadine	C22H23ClN2O2	79794-75-5	+
Lorazepam	C15H10Cl2N2O2	846-49-1	+ -
Lormetazepam	C16H12Cl2N2O2	848-75-9	+
Lornoxicam	C13H10ClN3O4S2	70374-39-9	+
Losartan	C22H23ClN6O	114798-26-4	+ -
Lovastatin	C24H36O5	75330-75-5	+
Loxapine	C18H18ClN3O	1977-10-2	+
LSD / Lysergide	C20H25N3O	50-37-3	+
Lufenuron	C17H8Cl2F8N2O3	103055-07-8	+
Lumefantrine	C30H32Cl3NO	82186-77-4	+
Lupanine	C15H24N2O	550-90-3	+
Lysergic acid	C16H16N2O2	82-58-6	+
Mafenide (component of Sulfatolamide)	C7H10N2O2S	138-39-6	+
Maitansine	C34H46ClN3O10	35846-53-8	+ -
Malaoxon	C10H19O7PS	1634-78-2	+
Malathion	C10H19O6PS2	121-75-5	+

Compound Name	Formula	CAS	Polarity
Maleic acid	C4H4O4	110-16-7	-
Malonoben	C18H22N2O	10537-47-0	+ -
MAM-2201	C25H24FNO	1354631-24-5	+
Mandelic acid	C8H8O3	90-64-2	-
Mandipropamid	C23H22CINO4	374726-62-2	+
Mannitol	C6H14O6	69-65-8	+
Maprotiline	C20H23N	10262-69-8	+
Marbofloxacin	C17H19FN4O4	115550-35-1	+
Mazindol	C16H13CIN2O	22232-71-9	+
MBC / Benomyl	C14H18N4O3	17804-35-2	+
MBDB / Methylbenzodioxolylbutanamine	C12H17NO2	103818-46-8	+
MCC (Swep)	C8H7Cl2NO2	1918-18-9	-
MCPA (MCP)	C9H9ClO3	94-74-6	-
MCPB (4-(MCB))	C11H13ClO3	94-81-5	-
mCPP	C10H13CIN2	6640-24-0	+
MCPP / Mecoprop	C10H11ClO3	7085-19-0	-
MDA / Methylenedioxyamphetamine	C10H13NO2	4764-17-4	+
MDA-19	C21H23N3O2	1048973-47-2	+
MDA-77	C21H23N3O3	1103774-21-5	+
MDAI / 5,6-Methylenedioxy-2-aminoindane	C10H11NO2	132741-81-2	+
MDEA (MDE)	C12H17NO2	82801-81-8	+
MDMA / Methylenedioxymethamphetamine	C11H15NO2	42542-10-9	+
MDMA methylene homolog	C12H17NO2		+
MDPBP / 3',4'-Methylenedioxy-a-pyrrolidinobutiophenone	C15H19NO3	784985-33-7	+
MDPPP / 3',4'-methylenedioxy-a-pyrrolidinopropiophenone	C14H17NO3	783241-66-7	+
MDPR (N-Propyl-3,4-methylenedioxyamphetamine)	C13H19NO2	74698-36-5	+
MDPV / Methylenedioxyprovalerone	C16H21NO3	687603-66-3	+
Mebendazole	C16H13N3O3	31431-39-7	+ -
Mebeverine	C25H35NO5	3625-06-7	+
Mecamylamine	C11H21N	60-40-2	+
Mecarbam	C10H20NO5PS2	2595-54-2	+
Mecetronium	C20H44N	3006-10-8	+
Meclocycline	C22H21CIN2O8	2013-58-3	+ -
Meclofenamic acid	C14H11Cl2NO2	644-62-2	+ -
Meclofenoxate	C12H16CINO3	51-68-3	+
Mecloxamine	C19H24CINO	5668-06-4	+
Meclozine	C25H27CIN2	569-65-3	+
Medazepam	C16H15CIN2	2898-12-6	+
Medrogestone	C23H32O2	977-79-7	+
Medroxyprogesterone	C22H32O3	520-85-4	+
Medroxyprogesterone acetate	C24H34O4	71-58-9	+
Medrysone	C22H32O3	2668-66-8	+
Mefenacet (Rancho)	C16H14N2O2S	73250-68-7	+
Mefenamic acid	C15H15NO2	61-68-7	+ -
Mefenorex	C12H18CIN	17243-57-1	+

Compound Name	Formula	CAS	Polarity
Mefenpyr-diethyl	C16H18Cl2N2O4	135590-91-9	+
Mefexamide	C15H24N2O3	1227-61-8	+ -
Mefloquine	C17H16F6N2O	53230-10-7	+ -
Mefluidide	C11H13F3N2O3S	53780-34-0	+
Mefruside	C13H19ClN2O5S2	7195-27-9	+
Megestrol acetate	C24H32O4	595-33-5	+
Meglutol	C6H10O5	503-49-1	-
Melamine	C3H6N6	108-78-1	+
Melengestrol acetate	C25H32O4	2919-66-6	+
Melitracene	C21H25N	5118-29-6	+
Meloxicam	C14H13N3O4S2	71125-38-7	+ -
Melperone	C16H22FNO	3575-80-2	+
Melphalan	C13H18Cl2N2O2	148-82-3	+
Memantine	C12H21N	19982-08-2	+
Menadiol diphosphate	C11H12O8P2	84-98-0	-
Menbutone	C15H14O4	3562-99-0	+
Mepacrine	C23H30ClN3O	83-89-6	+
Mepaniprym	C14H13N3	110235-47-7	+
Mepenzolate	C21H26NO3	25990-43-6	+
Meperidine (Pethidine)	C15H21NO2	57-42-1	+
Mephesisin	C10H14O3	59-47-2	-
Mephentermine	C11H17N	100-92-5	+
Mephenytoin	C12H14N2O2	50-12-4	+ -
Mephosfolan	C8H16NO3PS2	950-10-7	+
Mepindolol	C15H22N2O2	23694-81-7	+
Mepivacaine	C15H22N2O	22801-44-1	+
Meprobamate	C9H18N2O4	57-53-4	+
Mepronil	C17H19NO2	55814-41-0	+
Meproscillarlin	C31H44O8	33396-37-1	+
Meptazinol	C15H23NO	54340-58-8	+
Mequitazine	C20H22N2S	29216-28-2	+
Mercaptopurine	C5H4N4S	50-44-2	+ -
Mesna	C2H6O3S2	3375-50-6	-
Mesoridazine	C21H26N2O5S2	5588-33-0	+
Mesosulfuron-methyl	C17H21N5O9S2	208465-21-8	+
Mesterolone	C20H32O2	1424-00-6	+
Mestranol	C21H26O2	72-33-3	+
Metaclazepam	C18H18BrClN2O	84031-17-4	+
Metacycline	C22H22N2O8	914-00-1	+
Metaflumizone	C24H16F6N4O2	139968-49-3	+
Metalaxyl	C15H21NO4	57837-19-1	+
Metamfepramone (N,N-Dimethylcathinone)	C11H15NO	15351-09-4	+
Metamitron	C10H10N4O	41394-05-2	+
Metampicillin	C17H19N3O4S	6489-97-0	+ -
Metaproterenol (Orciprenaline)	C11H17NO3	586-06-1	+

Compound Name	Formula	CAS	Polarity
Metaraminol	C9H13NO2	54-49-9	+
Metaxalone	C12H15NO3	1665-48-1	+ -
Metazachlor	C14H16ClN3O	67129-08-2	+
Metconazole(I)	C17H22ClN3O	125116-23-6	+
Metconazole(II)	C17H22ClN3O	125116-23-6	+
Meteneprost	C23H38O4	61263-35-2	+ -
Metenolone enantate	C27H42O3	303-42-4	+
Metergoline	C25H29N3O2	17692-51-2	+
Metformin	C4H11N5	657-24-9	+
Methabenzthiazuron	C10H11N3OS	18691-97-9	+
Methacholine	C8H18NO2	55-92-5	+
Methacrifos	C7H13O5PS	62610-77-9	+
Methadone	C21H27NO	76-99-3	+
Methamidophos (Metamidophos)	C2H8NO2PS	10265-92-6	+
Methamphetamine	C10H15N	537-46-2	+
Methanthelinium (Methantheline)	C21H26NO3	5818-17-7	+
Methaphenilene	C15H20N2S	493-78-7	+
Methapyrilene	C14H19N3S	91-80-5	+
Methaqualone	C16H14N2O	72-44-6	+
Metharbital	C9H14N2O3	50-11-3	-
Methazolamide	C5H8N4O3S2	554-57-4	+ -
Methcathinone (Ephedrone)	C10H13NO	5650-44-2	+
Methedrone (Methoxyphedrine)	C11H15NO2	530-54-1	+
Methenamine	C6H12N4	100-97-0	+
Methenolone acetate	C22H32O3	434-05-9	+
Methfuroxam	C14H15NO2	28730-17-8	+
Methidathion	C6H11N2O4PS3	950-37-8	+
Methiocarb sulfone	C11H15NO4S	2179-25-1	+
Methiocarb sulfoxide	C11H15NO3S	2635-10-1	+
Methiomeprazine	C19H24N2S2	7009-43-0	+
Methocarbamol	C11H15NO5	532-03-6	+
Methohexital	C14H18N2O3	151-83-7	-
Methomyl	C5H10N2O2S	16752-77-5	+
Methoprene	C19H34O3	40596-69-8	+
Methoprotryne	C11H21N5OS	841-06-5	+
Methotrexate	C20H22N8O5	59-05-2	+
Methoxamine	C11H17NO3	390-28-3	+
Methoxyfenozide (Intrepid)	C22H28N2O3	161050-58-4	+
Methoxyharmalan	C13H14N2O	3589-73-9	+
Methoxy-pyridinyl-sulfanil,1-acetamide	C13H14N4O4S	3568-43-2	+
Methyl 4-hydroxybenzoate	C8H8O3	99-76-3	-
Methyl lysergate	C17H18N2O2	4579-64-0	+
Methyl nicotinate	C7H7NO2	93-60-7	+
Methylcodeine	C19H23NO3	2859-16-7	+
Methylidopa	C10H13NO4	555-30-6	+

Compound Name	Formula	CAS	Polarity
Methylephedrine	C11H17NO	552-79-4	+
Methylergometrin	C20H25N3O2	113-42-8	+
Methylhexanamine (DMAA)	C7H17N	105-41-9	+
Methylphenidate (Ritalin)	C14H19NO2	113-45-1	+
Methylphenobarbital	C13H14N2O3	115-38-8	-
Methylprednisolone	C22H30O5	83-43-2	+ -
Methylprednisolone 21-cipionate	C30H42O6	3545-59-3	+
Methylprednisolone acetate	C24H32O6	53-36-1	+
Methylprednisolone succinate	C26H34O8	2921-57-5	+
Methylpromethazinium (Thiazinamium)	C18H23N2S	2338-21-8	+
Methylsalicylate	C8H8O3	119-36-8	-
Methylscopolamine	C18H24NO4	13265-10-6	+
Methyltestosterone	C20H30O2	58-18-4	+
Methylthiouracil	C5H6N2OS	56-04-2	+ -
Methysergide	C21H27N3O2	361-37-5	+
Metildigoxin	C42H66O14	30685-43-9	+
Metipranolol	C17H27NO4	22664-55-7	+
Metitepine	C20H24N2S2	20229-30-5	+
Metixene	C20H23NS	4969-02-2	+
Metobromuron	C9H11BrN2O2	3060-89-7	+
Metoclopramide	C14H22ClN3O2	364-62-5	+
Metofenazate	C31H36ClN3O5S	388-51-2	+
Metolachlor	C15H22ClNO2	51218-45-2	+
Metolachlor CGA 37735	C11H15NO2	97055-05-5	+
Metolachlor CGA 50267	C12H17NO2		+
Metolachloric acid	C15H21NO4	152019-73-3	+
Metolazone	C16H16ClN3O3S	17560-51-9	+ -
Metolcarb	C9H11NO2	1129-41-5	+
Metominostrobin, E- (SSF-126)	C16H16N2O3	133408-50-1	+
Metominostrobin, Z- (SSF-126)	C16H16N2O3	133408-51-2	+
Metoprolol	C15H25NO3	37350-58-6	+
Metosulam	C14H13Cl2N5O4S	139528-85-1	+
Metoxuron	C10H13ClN2O2	19937-59-8	+
Metrafenone	C19H21BrO5	220899-03-6	+
Metribuzin	C8H14N4OS	21087-64-9	+
Metrizamide	C18H22I3N3O8	31112-62-6	+
Metrizoic acid	C12H11I3N2O4	1949-45-7	+
Metronidazole	C6H9N3O3	443-48-1	+
Metsulfuron-methyl	C14H15N5O6S	74223-64-6	+ -
Mevastatin	C23H34O5	73573-88-3	+
Mevinphos (Phosdrin)	C7H13O6P	7786-34-7	+
Mexacarbate (Zectran)	C12H18N2O2	315-18-4	+
Mexiletine	C11H17NO	31828-71-4	+
Mezlocillin	C21H25N5O8S2	51481-65-3	+ -
m-Hydroxybenzoyllecgonine	C16H19NO5	129944-99-6	+

Compound Name	Formula	CAS	Polarity
Mianserin	C18H20N2	24219-97-4	+
Mibefradil	C29H38FN3O3	116644-53-2	+
Miconazole	C18H14Cl4N2O	22916-47-8	+
Midazolam	C18H13ClFN3	59467-70-8	+
Midodrine	C12H18N2O4	42794-76-3	+ -
Mifepristone	C29H35NO2	84371-65-3	+
Miglitol	C8H17NO5	72432-03-2	+ -
Miglustat (Miglustatum)	C10H21NO4	72599-27-0	+
Milrinone	C12H9N3O	78415-72-2	+
Miltefosine	C21H47NO4P	58066-85-6	+
Minaprine	C17H22N4O	25905-77-5	+
Minocyclin	C23H27N3O7	10118-90-8	+
Minoxidil	C9H15N5O	38304-91-5	+
Mirtazapine	C17H19N3	61337-67-5	+
Misoprostol	C22H38O5	59122-46-2	+
Mithracin (Plicamycin)	C52H76O24	18378-89-7	-
Mitobronitol	C6H12Br2O4	488-41-5	-
Mitomycine	C15H18N4O5	50-07-7	+ -
Mitoxantrone	C22H28N4O6	65271-80-9	+
Mitragynine (9-methoxy Corynantheidine)	C23H30N2O4	4098-40-2	+ -
Mizolastine	C24H25FN6O	108612-45-9	+
Moclobemide	C13H17ClN2O2	71320-77-9	+
Modafinil	C15H15NO2S	68693-11-8	+ -
Moexipril	C27H34N2O7	103775-10-6	+
Moisidomine	C9H15N4O4	25717-80-0	+
Molinate	C9H17NOS	2212-67-1	+
Mometasone furoate	C27H30Cl2O6	83919-23-7	+
Monalazone	C7H6ClNO4S	61477-95-0	-
Monalide	C13H18ClNO	7287-36-7	+
Monensin	C36H62O11	17090-79-8	+ -
Monocrotophos (Azodrin)	C7H14NO5P	6923-22-4	+
Monolinuron	C9H11ClN2O2	1746-81-2	+
Montelukast	C35H36ClNO3S	158966-92-8	+
Monuron	C9H11ClN2O	150-68-5	+
Moperone	C22H26FNO2	1050-79-9	+
Mopidamol	C19H31N7O4	13665-88-8	+
Morantel	C12H16N2S	20574-50-9	+
Morazone	C23H27N3O2	6536-18-1	+
Morfamquat	C26H36N4O4	7411-47-4	+
Moroxydine	C6H13N5O	3731-59-7	+
Morphine	C17H19NO3	57-27-2	+
Morphine-3-beta-D-glucuronide	C23H27NO9	20290-09-9	+
Morphine-6-beta-D-glucuronide	C23H27NO9	20290-10-2	+
Morpholine	C4H9NO	110-91-8	+
Moxaverine	C20H21NO2	10539-19-2	+

Compound Name	Formula	CAS	Polarity
Moxifloxacin	C21H24FN3O4	151096-09-2	+
Moxisylyt	C16H25NO3	54-32-0	+
Moxonidine	C9H12ClN5O	75438-57-2	+
MPHP / 4'-Methyl-a-pyrrolidinohexanophenone	C17H25NO	34138-58-4	+
MQD / Quinomethionate	C10H6N2OS2	2439-01-2	+
Mupirocin	C26H44O9	12650-69-0	+ -
Muscimol	C4H6N2O2	2763-96-4	+
Muzolimine	C11H11Cl2N3O	55294-15-0	+
MXE / Methoxetamine	C15H21NO2	1239908-48-5	+
Myclobutanil	C15H17ClN4	88671-89-0	+
Mycophenolate mofetil	C23H31NO7	128794-94-5	-
Mycophenolic acid	C17H20O6	24280-93-1	+
Myosmine	C9H10N2	532-12-7	+
N-(2-Hydroxyphenyl)piperazine	C10H14N2O	1011-17-2	+
N-(4-Tolyl)piperazine	C11H16N2	39593-08-3	+
N-(hydroxymethyl)-Nicotinamide (Bidbilan)	C7H8N2O2	3569-99-1	+ -
N,N-DMT / N,N-Dimethyltryptamine	C12H16N2	61-50-7	+
Nabumetone	C15H16O2	42924-53-8	+ -
N-Acetyl-5-hydroxytryptamine	C12H14N2O2	1210-83-9	+
N-Acetyl-DL-methionine	C7H13NO3S	1115-47-5	+ -
N-Acetyl-L-aspartic acid	C6H9NO5	997-55-7	-
N-Acetylneuramic acid (Sialic acid)	C11H19NO9	131-48-6	-
Nadolol	C17H27NO4	42200-33-9	+
Nafcillin	C21H22N2O5S	147-52-4	+ -
Naftidrofuryl	C24H33NO3	31329-57-4	+
Naftidrofurylic acid	C18H20O3	25379-26-4	+
Naftifine	C21H21N	65472-88-0	+
Nalbuphine	C21H27NO4	20594-83-6	+
Nalidixic acid	C12H12N2O3	389-08-2	+ -
Nalmefene	C21H25NO3	55096-26-9	+
Nalorphine	C19H21NO3	62-67-9	+
Naloxone	C19H21NO4	465-65-6	+
Naltrexone	C20H23NO4	16590-41-3	+
Nanafrocine (Nanaomycin)	C16H14O6	52934-83-5	+
Nandrolone	C18H26O2	434-22-0	+
Nandrolone decaonate	C28H44O3	360-70-3	+
Nandrolone hexyloxyphenylpropionate	C33H46O4	52279-57-9	+
Nandrolone phenpropionate	C27H34O3	62-90-8	+
Nandrolone propionate	C21H30O3	7207-92-3	+
Naphazoline	C14H14N2	835-31-4	+
Naphyrone	C19H23NO	850352-53-3	+
Naphyrone 1-naphthyl isomer	C19H23NO	1349245-31-3	+
Napropamide	C17H21NO2	15299-99-7	+
Naproxen	C14H14O3	22204-53-1	+ -
Naratriptan	C17H25N3O2S	121679-13-8	+

Compound Name	Formula	CAS	Polarity
Narcein	C23H27NO8	131-28-2	+
Narcobarbital	C11H15BrN2O3	125-55-3	-
Nateglinide	C19H27NO3	105816-04-4	+ -
N-Bis(desalkyl)verapamil (D 620)	C16H24N2O2	27487-66-7	+
N-Desalkylverapamil (D 617)	C17H26N2O2	34245-14-2	+
N-Desmethylclozapine	C17H17ClN4	6104-71-8	+ -
N-Desmethyldoxepin (Desmethyl-doxepine)	C18H19NO	1225-56-5	+
N-Desmethylflunitrazepam (Flunitrazepam-M (nor))	C15H10FN3O3	2558-30-7	+
N-Desmethylprochlorperazine	C19H22ClN3S	49780-18-9	+
N-Desmethylpropafenone	C18H21NO3	86383-21-3	+
N-Desmethylselegiline	C12H15N	18913-84-3	+
N-Desmethylzopiclone	C16H15ClN6O3	59878-63-6	+
Nebivolol	C22H25F2NO4	99200-09-6	+
Neburon (Phosphoramidothioic acid)	C12H16Cl2N2O	555-37-3	+
Nedoeromil	C19H17NO7	69049-73-6	-
Nefazodone	C25H32ClN5O2	83366-66-9	+
Nefopam	C17H19NO	13669-70-0	+
Nelfinavir	C32H45N3O4S	159989-64-7	+
Neohesperidin DHC	C28H36O15	20702-77-6	+
Neopine	C18H21NO3	467-14-1	+
Neostigmine	C12H19N2O2	59-99-4	+
N-Ethyl Nordazepam	C17H15ClN2O	5571-65-3	+
Nevirapine	C15H14N4O	129618-40-2	+
Nialamide	C16H18N4O2	51-12-7	+
Nicardipine	C26H29N3O6	55985-32-5	+
Nicergoline	C24H26BrN3O3	27848-84-6	+
Nicethamide	C10H14N2O	59-26-7	+
Niclosamide	C13H8Cl2N2O4	50-65-7	+ -
Nicoboxil	C12H17NO3	13912-80-6	+
Nicorandil	C8H9N3O4	65141-46-0	+
Nicosulfuron	C15H18N6O6S	111991-09-4	+
Nicothiazone	C7H8N4S	555-90-8	-
Nicotine	C10H14N2	54-11-5	+
Nicotinic acid propylester	C9H11NO2	7681-15-4	+
Nicotinic acid	C6H5NO2	59-67-6	+ -
Nicotinyl alcohol	C6H7NO	100-55-0	+
Nifedipine	C17H18N2O6	21829-25-4	+ -
Nifenalol	C11H16N2O3	7413-36-7	+
Nifenazone	C17H16N4O2	2139-47-1	+
Niflumic acid	C13H9F3N2O2	4394-00-7	+ -
Nifuratel	C10H11N3O5S	4936-47-4	+
Nifuroxazide	C12H9N3O5	965-52-6	-
Nifurprazine	C10H8N4O3	1614-20-6	+
Nilutamide	C12H10F3N3O4	63612-50-0	-
Nilvadipine	C19H19N3O6	75530-68-6	+

Compound Name	Formula	CAS	Polarity
Nimesulide	C13H12N2O5S	51803-78-2	-
Nimodipine	C21H26N2O7	66085-59-4	+ -
Nimorazole	C9H14N4O3	6506-37-2	+
Nimustine	C9H13ClN6O2	42471-28-3	+ -
Nisoldipine	C20H24N2O6	63675-72-9	+
Nitenpyram	C11H15ClN4O2	150824-47-8	+
Nitisinone	C14H10F3NO5	104206-65-7	+
Nitralin (Planavin)	C13H19N3O6S	4726-14-1	+
Nitrazepam	C15H11N3O3	146-22-5	+ -
Nitrendipine	C18H20N2O6	39562-70-4	+ -
Nitrobenzene	C6H5NO2	98-95-3	+
Nitrofurantoin	C8H6N4O5	67-20-9	-
Nitrofurazone (Nitrofurazone)	C6H6N4O4	59-87-0	+ -
Nitromide	C7H5N3O5	121-81-3	-
Nitrophenol, 4-	C6H5NO3	100-02-7	-
Nitro-propoxyacetanilide	C11H14N2O4	553-20-8	+
Nitroscanate	C13H8N2O3S	19881-18-6	-
Nitroxoline	C9H6N2O3	4008-48-4	-
Nizatidine	C12H21N5O2S2	76963-41-2	+
N-Methylpyrithylidione	C10H15NO2		+
N-Nicotinoylprocaine	C19H23N3O3	13424-56-1	+
Nomelidine	C15H15BrN2	60324-59-6	+
Nomifensine	C16H18N2	24526-64-5	+
Nonivamide	C17H27NO3	2444-46-4	+ -
Noramidopyrine	C12H15N3O	519-98-2	+
Norbuprenorphine	C25H35NO4	78715-23-8	+ -
Norcitalopram	C19H19FN2O	62498-67-3	+
Norclobazam	C15H11ClN2O2	22316-55-8	+ -
Norcocaine	C16H19NO4	18717-72-1	+
Norcyclizine	C17H20N2	841-77-0	+
Nordiazepam	C15H11ClN2O	1088-11-5	+
Norelgestromin	C21H29NO2	53016-31-2	+
Norethindrone acetate	C22H28O3	51-98-9	+ -
Norethisterone	C20H26O2	68-22-4	+
Norethisterone enantate	C27H38O3	3836-23-5	+
Norethynodrel	C20H26O2	68-23-5	+
Norfefrine	C8H11NO2	536-21-0	+
Norfentanyl	C14H20N2O	1609-66-1	+
Norfloracin	C16H18FN3O3	70458-96-7	+
Norfluoxetine	C16H16F3NO	56161-73-0	+
Norflurazon	C12H9ClF3N3O	27314-13-2	+
Norgestimate	C23H31NO3	35189-28-7	+
Norhydrocodone	C17H19NO3	71968-04-2	+
Norketamine	C12H14ClNO	35211-10-0	+
Nor-LAAM / Norlevacetylmethadol	C22H29NO2	43033-71-2	+

Compound Name	Formula	CAS	Polarity
Normeperidine (Norpethidine)	C14H19NO2	77-17-8	+
nor-Mephedrone	C10H13NO	31952-47-3	+
Normethadone	C20H25NO	467-85-6	+
Normorphine	C16H17NO3	466-97-7	+
Nornicotine	C9H12N2	494-97-3	+
Noroxycodone	C17H19NO4	57664-96-7	+
Norsertaline	C16H15Cl2N	87857-41-8	+
Norsufentanil	C16H24N2O2	61086-18-8	+
Northiaden	C18H19NS	1154-09-2	+
Northiaden S-oxide	C18H19NOS	54262-54-3	+
Northioridazine	C20H24N2S2	10538-32-6	+
Northioridazine-2-sulfoxide	C20H24N2OS2	14471-95-5	+
Nortilidine	C16H21NO2	38677-94-0	+
Nortriptyline	C19H21N	72-69-5	+
Norverapamil	C26H36N2O4	67018-85-3	+
Noscapine	C22H23NO7	128-62-1	+
Novaluron	C17H9ClF8N2O4	116714-46-6	+ -
Novobiocin	C31H36N2O11	303-81-1	+ -
Noxiptyline	C19H22N2O	3362-45-6	+
NPP (Phenylpiperazine)	C10H14N2	92-54-6	+
Nuarimol	C17H12ClFN2O	63284-71-9	+
Nystatin	C47H75NO17	34786-70-4	+
O-1602	C17H22O2	317321-41-8	+ -
O-1821	C17H22O2	35482-50-9	+ -
O-1918	C19H26O2	536697-79-7	+
Octacaine	C14H22N2O	13912-77-1	+
Octamylamine	C13H29N	502-59-0	+
Octenidine	C36H62N4	71251-02-0	+
Octhilinone	C11H19NOS	26530-20-1	+
Octopamine	C8H11NO2	104-14-3	+
Octotiamine	C23H36N4O5S3	137-86-0	+
Octyl gallate	C15H22O5	1034-01-1	-
O-Desmethylvenlafaxine (Desvenlafaxine)	C16H25NO2	93413-62-8	+
O-DT / O-Desmethyltramadol	C15H23NO2	73986-53-5	+
Ofloxacin	C18H20FN3O4	82419-36-1	+
Ofurace	C14H16ClNO3	58810-48-3	+
o-Hydroxyhippuric acid	C9H9NO4	487-54-7	+ -
Olaflur (Amine fluoride 297)	C27H58N2O3	6818-37-7	+
Olanzapine	C17H20N4S	132539-06-1	+
Olaquinox	C12H13N3O4	23696-28-8	+
Oleandomycin	C35H61NO12	3922-90-5	+
Oleandrin	C32H48O9	465-16-7	+
Olmesartan medoxomil	C29H30N6O6	144689-63-4	-
Olopatadine	C21H23NO3	113806-05-6	+
Olsalazine	C14H10N2O6	15722-48-2	-

Compound Name	Formula	CAS	Polarity
Omeprazole	C17H19N3O3S	73590-58-6	+
Omeprazole sulfone	C17H19N3O4S	88546-55-8	+
Omethoate	C5H12NO4PS	1113-02-6	+
Omoconazole	C20H17Cl3N2O2	105102-19-0	+
Ondansetron	C18H19N3O	99614-02-5	+
Opi Pramol	C23H29N3O	315-72-0	+
Orbencarb	C12H16ClNOS	34622-58-7	+
Orbifloxacin	C19H20F3N3O3	113617-63-3	+
Ornidazole	C7H10ClN3O3	16773-42-5	+
Orotic acid	C5H4N2O4	65-86-1	-
Orphenadrine	C18H23NO	83-98-7	+
Orthosulfamuron	C16H20N6O6S	213464-77-8	+
Oryzalin	C12H18N4O6S	19044-88-3	+
OTC / Oxytetracycline	C22H24N2O9	79-57-2	+ -
Oxabetrinil	C12H12N2O3	74782-23-3	+
Oxabolone cypionate	C26H38O4	1254-35-9	+
Oxacillin	C19H19N3O5S	66-79-5	-
Oxadiargyl	C15H14Cl2N2O3	39807-15-3	+
Oxadiazon	C15H18Cl2N2O3	19666-30-9	+
Oxadixyl	C14H18N2O4	77732-09-3	+
Oxamyl	C7H13N3O3S	23135-22-0	+
Oxapadol	C17H14N2O2	56969-22-3	+
Oxaprozin	C18H15NO3	21256-18-8	+ -
Oxasulfuron	C17H18N4O6S	144651-06-9	+
Oxatomide	C27H30N4O	60607-34-3	+
Oxazepam	C15H11ClN2O2	604-75-1	+ -
Oxazepam glucuronide	C21H19ClN2O8	28472-99-3	+ -
Oxazolam	C18H17ClN2O2	24143-17-7	+
Oxcarbazepine	C15H12N2O2	28721-07-5	+
Oxeladin	C20H33NO3	468-61-1	+
Oxetacaine	C28H41N3O3	126-27-2	+
Oxetorone	C21H21NO2	26020-55-3	+
Oxfendazole	C15H13N3O3S	53716-50-0	+ -
Oxibendazole	C12H15N3O3	20559-55-1	+ -
Oxiconazole	C18H13Cl4N3O	64211-45-6	+
Oxilofrine	C10H15NO2	52671-39-3	+
Oxitriptan	C11H12N2O3	4350-09-8	+
Oxitropium	C19H26NO4	30286-75-0	+
Oxolinic acid	C13H11NO5	14698-29-4	+
Oxomemazine	C18H22N2O2S	3689-50-7	+
Oxotremorine	C12H18N2O	70-22-4	+
Oxprenolol	C15H23NO3	6452-71-7	+
Oxybenzone	C14H12O3	131-57-7	+
Oxybuprocaine	C17H28N2O3	99-43-4	+
Oxybutynine	C22H31NO3	5633-20-5	+

Compound Name	Formula	CAS	Polarity
Oxycarboxin	C12H13NO4S	5259-88-1	+
Oxycodone	C18H21NO4	76-42-6	+
Oxyfedrine	C19H23NO3	15687-41-9	+
Oxyfluorofen	C15H11ClF3NO4	42874-03-3	+
Oxymesterone	C20H30O3	145-12-0	+
Oxymetazoline	C16H24N2O	1491-59-4	+
Oxymetholone	C21H32O3	434-07-1	+
Oxymorphone	C17H19NO4	76-41-5	+
Oxypendyl	C20H26N4OS	5585-93-3	+
Oxypertine	C23H29N3O2	153-87-7	+
Oxyphenbutazone	C19H20N2O3	129-20-4	+ -
Oxyphencyclimine	C20H28N2O3	125-53-1	+
Oxyphenisatin	C20H15NO3	125-13-3	+
Oxyphenisatin diacetate	C24H19NO5	115-33-3	+
Oxyphenonium	C21H34NO3	14214-84-7	+
Ozagrel	C13H12N2O2	82571-53-7	+ -
p-(Aminomethyl)benzoic acid (Aminomethylbenzoic acid)	C8H9NO2	56-91-7	+
PABA / para-aminobenzoic acid (4-Aminobenzoesaure)	C7H7NO2	150-13-0	+ -
Paclbutrazol	C15H20ClN3O	76738-62-0	+
Paliperidone (9-Hydroxyrisperidone)	C23H27FN4O3	144598-75-4	+ -
Palmidrol	C18H37NO2	544-31-0	+
Pantoprazole	C16H15F2N3O4S	102625-70-7	+
Papaverine	C20H21NO4	58-74-2	+
Paramethasone acetate	C24H31FO6	1597-82-6	+
Paraoxon	C10H14NO6P	311-45-5	+
Paraoxon-methyl	C8H10NO6P	950-35-6	+
Parathion	C10H14NO5PS	56-38-2	+
Paraxanthine	C7H8N4O2	611-59-6	+ -
Parecoxib	C19H18N2O4S	198470-84-7	+
Paromomycin	C23H45N5O14	7542-37-2	+
Paroxetine	C19H20FNO3	61869-08-7	+
PAS-hydrazide	C7H9N3O2	6946-29-8	+
p-Butylaminobenzoic acid	C11H15NO2	4740-24-3	+ -
PCP / Pentachlorophenol	C6HCl5O	87-86-5	-
PCP / Phencyclidine	C17H25N	77-10-1	+
PEA / Phenethylamine	C8H11N	64-04-0	+
Pebulate	C10H21NOS	1114-71-2	+
Pecazine	C19H22N2S	60-89-9	+
Pemetrexed	C20H21N5O6	137281-23-3	+
Pemoline	C9H8N2O2	2152-34-3	+
Pempidine	C10H21N	79-55-0	+
Penbutolol	C18H29NO2	38363-40-5	+
Penciclovir	C10H15N5O3	39809-25-1	+
Penconazole	C13H15Cl2N3	66246-88-6	+
Pencycuron	C19H21ClN2O	66063-05-6	+

Compound Name	Formula	CAS	Polarity
Pendimethalin (Penoxalin)	C13H19N3O4	40487-42-1	+
Penfluridol	C28H27CIF5NO	26864-56-2	+
Penflutizide	C13H18F3N3O4S2	1766-91-2	-
Penicillamin	C5H11NO2S	52-67-5	+
Penicillin G (Benzylpenicillin)	C16H18N2O4S	61-33-6	+ -
Penoxsulam (Penoxalim)	C16H14F5N5O5S	219714-96-2	+
Pentamidine	C19H24N4O2	100-33-4	+
Pentanochlor (Sloan)	C13H18ClNO	2307-68-8	+
Pentazocine	C19H27NO	359-83-1	+
Pentedrone	C12H17NO	879722-57-3	+
Pentetrazole	C6H10N4	54-95-5	+
Pentifylline	C13H20N4O2	1028-33-7	+
Pentobarbital	C11H18N2O3	76-74-4	-
Pentorex	C11H17N	434-43-5	+
Pentostatin	C11H16N4O4	53910-25-1	+
Pentoxifylline	C13H18N4O3	6493-05-6	+ -
Pentoxifylline (dihydro-)	C13H20N4O3	100324-81-0	+
Pentoxyverine	C20H31NO3	77-23-6	+
Perazine	C20H25N3S	84-97-9	+
Pergolide	C19H26N2S	66104-22-1	+
Perhexiline	C19H35N	6621-47-2	+
Periciazine	C21H23N3OS	2622-26-6	+
Perindopril	C19H32N2O5	82834-16-0	+ -
Perlapine	C19H21N3	1977-11-3	+
Perphenazine	C21H26ClN3OS	58-39-9	+
Peruvoside	C30H44O9	1182-87-2	+
Pethoxamid	C16H22ClNO2	106700-29-2	+
Peucedanin	C15H14O4	133-26-6	+
Phanquinone	C12H6N2O2	84-12-8	+
Phenacemide	C9H10N2O2	63-98-9	-
Phenacetin	C10H13NO2	62-44-2	+
Phenallymal	C13H12N2O3	115-43-5	-
Phenamazide	C13H19NO2	84580-27-8	+
Phenazocine	C22H27NO	127-35-5	+
Phenazone	C11H12N2O	60-80-0	+
Phenazopyridine	C11H11N5	94-78-0	+
Phendimetrazine	C12H17NO	634-03-7	+
Phenelzine	C8H12N2	51-71-8	+
Pheneticillin	C17H20N2O5S	147-55-7	+ -
Phenformin	C10H15N5	114-86-3	+
Phenglutarimide	C17H24N2O2	1156-05-4	+
Phenindamine	C19H19N	82-88-2	+
Pheniramine	C16H20N2	86-21-5	+
Phenkaptan	C11H15Cl2O2PS3	2275-14-1	+
Phenmedipham	C16H16N2O4	13684-63-4	+

Compound Name	Formula	CAS	Polarity
Phenmetrazine	C11H15NO	134-49-6	+
Phenobarbital	C12H12N2O3	50-06-6	-
Phenolphthalein	C20H14O4	77-09-8	+ -
Phenopyrazone	C15H12N2O2	3426-01-5	+
Phenothrin	C23H26O3	26002-80-2	+
Phenoxybenzamine	C18H22CINO	59-96-1	+
Phenprobamate	C10H13NO2	673-31-4	+
Phenprocoumon	C18H16O3	435-97-2	+
Phenpromethamine	C10H15N	93-88-9	+
Phentermine	C10H15N	122-09-8	+
Phenthoate (Fenthoate)	C12H17O4PS2	2597-03-7	+
Phentolamine	C17H19N3O	50-60-2	+
Phenylacrylic acid (Cinnamic acid)	C9H8O2	621-82-9	-
Phenylbutazone	C19H20N2O2	50-33-9	+ -
Phenylephrine	C9H13NO2	1477-63-0	+
Phenylpyruvic acid	C9H8O3	156-06-9	-
Phenyltoloxamine	C17H21NO	92-12-6	+
Phenytol	C15H12N2O2	57-41-0	+ -
Phloroglucin	C6H6O3	108-73-6	-
Pholcodine	C23H30N2O4	509-67-1	+
Phorate (Isothioate)	C7H17O2PS3	298-02-2	+
Phorate-sulfoxide	C7H17O3PS3	2588-03-6	+
Phosalone	C12H15CINO4PS2	2310-17-0	+
Phosmet (Imidan)	C11H12NO4PS2	732-11-6	+
Phosphamidon	C10H19CINO5P	13171-21-6	+
Phoxim	C12H15N2O3PS	14816-18-3	+
Phthalylsulfacetamide	C16H14N2O6S	131-69-1	-
Phthalylsulfathiazole	C17H13N3O5S2	85-73-4	+
p-Hydroxyphenytoin	C15H12N2O3	2784-27-2	+
Physcion	C16H12O5	521-61-9	-
Physostigmine	C15H21N3O2	57-47-6	+
Picaridin (Bayrepel)	C12H23NO3	119515-38-7	+
Picloram	C6H3Cl3N2O2	1918-02-1	+ -
Picolinafen	C19H12F4N2O2	137641-05-5	+
Picosulfate	C18H15NO8S2	10040-45-6	+ -
Picoxystrobin	C18H16F3NO4	117428-22-5	+
Picrotoxinin	C15H16O6	17617-45-7	-
Pilocarpine	C11H16N2O2	92-13-7	+
Pimaricin (Natamycin)	C33H47NO13	7681-93-8	+
Pimetremide	C16H18N2O2	578-89-2	+
Pimobendan	C19H18N4O2	74150-27-9	+
Pimozide	C28H29F2N3O	2062-78-4	+
Pindolol	C14H20N2O2	13523-86-9	+
Pindone (Pival)	C14H14O3	83-26-1	+ -
Pinoxaden	C23H32N2O4	243973-20-8	+

Compound Name	Formula	CAS	Polarity
Pioglitazone	C19H20N2O3S	111025-46-8	+ -
Pipamperone	C21H30FN3O2	1893-33-0	+
Pipazethate	C21H25N3O3S	2167-85-3	+
Pipemidic acid	C14H17N5O3	51940-44-4	+
Pipenzolate	C22H28NO3	13473-38-6	+
Piperazine	C4H10N2	110-85-0	+
Piperidolate	C21H25NO2	82-98-4	+
Piperine	C17H19NO3	94-62-2	+
Piperophos	C14H28NO3PS2	24151-93-7	+
Pipradrol	C18H21NO	467-60-7	+
Piprozolin	C14H22N2O3S	17243-64-0	+
Piracetam	C6H10N2O2	7491-74-9	+
Pirbuterol	C12H20N2O3	38677-81-5	+
Pirenperone	C23H24FN3O2	75444-65-4	+
Pirenzepine	C19H21N5O2	28797-61-7	+ -
Piretanide	C17H18N2O5S	55837-27-9	+
Piribedil	C16H18N4O2	3605-01-4	+
Piridoxilate	C10H13NO6	17692-44-3	-
Pirimicarb	C11H18N4O2	23103-98-2	+
Pirimicarb-desmethyl-formamido	C11H16N4O3	27218-04-8	+
Pirimiphos-ethyl (Pirimifos-ethyl)	C13H24N3O3PS	23505-41-1	+
Pirimiphos-methyl (Pirimifos-methyl)	C11H20N3O3PS	29232-93-7	+
Pirisudanol	C16H24N2O6	33605-94-6	+
Piritramide	C27H34N4O	302-41-0	+
Pirlimycin	C17H31ClN2O5S	79548-73-5	+
Pirlindole	C15H18N2	60762-57-4	+
Piromidic acid	C14H16N4O3	19562-30-2	+
Piroxicam	C15H13N3O4S	36322-90-4	+
Pirprofen	C13H14ClNO2	31793-07-4	+
Pitofenone	C22H25NO4	54063-52-4	+
Pivampicillin	C22H29N3O6S	33817-20-8	+
Pivmecillinam	C21H33N3O5S	32886-97-8	+
Pizotifen	C19H21NS	15574-96-6	+
PMA / 4-Methoxyamphetamine (4-Methoxyamfetamine)	C10H15NO	64-13-1	+
p-Nonylphenol (4-Nonylphenol)	C15H24O	104-40-5	-
Podophyllotoxin (Podophyllum)	C22H22O8	518-28-5	+ -
Polythiazide	C11H13ClF3N3O4S3	346-18-9	-
p-Phenetidine	C8H11NO	156-43-4	+ -
Practolol	C14H22N2O3	6673-35-4	+
Pralidoxime	C7H9N2O	6735-59-7	+
Pramipexole	C10H17N3S	104632-26-0	+
Pramiverine	C21H27N	14334-40-8	+
Pramocaine	C17H27NO3	140-65-8	+
Prasterone enantate	C26H40O3	23983-43-9	+ -
Pravastatin	C23H36O7	81093-37-0	+ -

Compound Name	Formula	CAS	Polarity
Prazepam	C19H17CIN2O	2955-38-6	+
Praziquantel	C19H24N2O2	55268-74-1	+
Prazosin	C19H21N5O4	19216-56-9	+
Prednicarbate	C27H36O8	73771-04-7	+
Prednimustine	C35H45Cl2NO6	29069-24-7	+
Prednisolone	C21H28O5	50-24-8	+ -
Prednisolone 21-hexanoate	C27H38O6	69164-69-8	+
Prednisolone acetate	C23H30O6	52-21-1	+ -
Prednisolone trimethylacetate	C26H36O6	1107-99-9	+
Prednisone	C21H26O5	53-03-2	+ -
Prednylidene	C22H28O5	599-33-7	+
Pregabalin	C8H17NO2	148553-50-8	+ -
Pregnenolone	C21H32O2	145-13-1	+
Premethadone (Methadone intermediate)	C19H22N2	125-79-1	+
Prenalterol	C12H19NO3	57526-81-5	+
Prenoxdiazine	C23H27N3O	47543-65-7	+
Prenylamine	C24H27N	390-64-7	+
Presinol	C10H13NO4	133161-54-3	+
Pretilachlor	C17H26ClNO2	51218-49-6	+
Pridinol	C20H25NO	511-45-5	+
Prilocaine	C13H20N2O	721-50-6	+
Primaquine	C15H21N3O	90-34-6	+
Primidone	C12H14N2O2	125-33-7	+ -
Primisulfuron-methyl	C15H12F4N4O7S	86209-51-0	+
Proadifen	C23H31NO2	302-33-0	+
Probenecid	C13H19NO4S	57-66-9	+ -
Probucol	C31H48O2S2	23288-49-5	-
Procainamide	C13H21N3O	51-06-9	+
Procaine (Novocaine)	C13H20N2O2	59-46-1	+
Procarbazine	C12H19N3O	671-16-9	+
Procaterol	C16H22N2O3	60443-17-6	+ -
Prochloraz	C15H16Cl3N3O2	67747-09-5	+
Prochlorperazine	C20H24ClN3S	58-38-8	+
Prochlorperazine S-oxide (5-Oxoprochlorperazine)	C20H24ClN3OS	10078-27-0	+
Procyclidine	C19H29NO	77-37-2	+
Procymidone	C13H11Cl2NO2	32809-16-8	+
Profenamine	C19H24N2S	522-00-9	+
Profenofos	C11H15BrClO3PS	41198-08-7	+
Profoxydim	C24H32ClNO4S	139001-49-3	+
Progesterone	C21H30O2	57-83-0	+
Proglumetacin	C46H58ClN5O8	57132-53-3	+
Proglumide	C18H26N2O4	6620-60-6	+ -
Proguanil	C11H16ClN5	500-92-5	+
Prolintane (Phenylpyrrolidinopentane)	C15H23N	493-92-5	+
Promazine	C17H20N2S	58-40-2	+

Compound Name	Formula	CAS	Polarity
Promazine S-oxide	C17H20N2OS	146-21-4	+
Promecarb	C12H17NO2	2631-37-0	+
Promethazine	C17H20N2S	60-87-7	+
Prometon	C10H19N5O	1610-18-0	+
Prometryn	C10H19N5S	7287-19-6	+
Propachlor	C11H14ClNO	1918-16-7	+
Propafenone	C21H27NO3	54063-53-5	+
Propallylonal	C10H13BrN2O3	545-93-7	-
Propamocarb	C9H20N2O2	24579-73-5	+
Propanil	C9H9Cl2NO	709-98-8	+ -
Propantheline	C23H30NO3	298-50-0	+
Propaphos	C13H21O4PS	7292-16-2	+
Propaquizafop	C22H22ClN3O5	111479-05-1	+
Propazine	C9H16ClN5	139-40-2	+
Propentofylline	C15H22N4O3	55242-55-2	+
Propetamphos (Tsar)	C10H20NO4PS	31218-83-4	+
Propicillin	C18H22N2O5S	551-27-9	+
Propiconazole(I)	C15H17Cl2N3O2	60207-90-1	+
Propiconazole(II)	C15H17Cl2N3O2	60207-90-1	+
Propiomazine	C20H24N2OS	362-29-8	+
Propionylpromazine	C20H24N2OS	3568-24-9	+
Propipocaine	C17H25NO2	3670-68-6	+
Propiram	C16H25N3O	15686-91-6	+
Propisochlor	C15H22ClNO2	86763-47-5	+
Propiverine	C23H29NO3	60569-19-9	+
Propofol	C12H18O	2078-54-8	-
Propoxur	C11H15NO3	114-26-1	+
Propoxyphene (Dextropropoxyphene)	C22H29NO2	469-62-5	+
Propranolol	C16H21NO2	525-66-6	+
Propyl 3,4,5-trihydroxybenzoate	C10H12O5	121-79-9	-
Propyl cresol (Thymol)	C10H14O	89-83-8	+ -
Propylhexedrine	C10H21N	101-40-6	+
Propylidone	C10H11I2NO3	587-61-1	+
Propylthiouracil	C7H10N2OS	51-52-5	+ -
Propyphenazone	C14H18N2O	479-92-5	+
Propyzamide (Pronamide)	C12H11Cl2NO	23950-58-5	+
Proquazone	C18H18N2O	22760-18-5	+
Proquinazid	C14H17IN2O2	189278-12-4	+
Proscillaridin	C30H42O8	466-06-8	+
Prosulfocarb	C14H21NOS	52888-80-9	+
Protheobromine	C10H14N4O3	50-39-5	+
Prothioconazole(I)	C14H15Cl2N3OS	178928-70-6	+
Prothioconazole(II)	C14H15Cl2N3OS	178928-70-6	+
Prothiofos	C11H15Cl2O2PS2	34643-46-4	+
Prothipendyl	C16H19N3S	303-69-5	+

Compound Name	Formula	CAS	Polarity
Prothoate	C9H20NO3PS2	2275-18-5	+
Protionamide	C9H12N2S	14222-60-7	+ -
Protirelin	C16H22N6O4	24305-27-9	+
Protokylol	C18H21NO5	136-70-9	+
Protopine	C20H19NO5	130-86-9	+
Protoveratrine B	C41H63NO15	124-97-0	-
Protriptyline	C19H21N	438-60-8	+
Proximpham	C10H12N2O2	2828-42-4	+
Proxymetacaine	C16H26N2O3	499-67-2	+
Proxiphylline	C10H14N4O3	603-00-9	+
Pseudococaine	C17H21NO4	478-73-9	+
Pseudoephedrine	C10H15NO	90-82-4	+
Psoralene	C11H6O3	66-97-7	+ -
Puromycin	C22H29N7O5	53-79-2	-
Pymetrozine	C10H11N5O	123312-89-0	+
Pyracarbolid	C13H15NO2	24691-76-7	+
Pyraclufos	C14H18CIN2O3PS	77458-01-6	+
Pyraclostrobin	C19H18CIN3O4	175013-18-0	+
Pyraflufen-ethyl	C15H13Cl2F3N2O 4	129630-19-9	+
Pyranocumarin (Cyclocoumarol)	C20H18O4	518-20-7	+
Pyrantel	C11H14N2S	15686-83-6	+
Pyrazinamide	C5H5N3O	98-96-4	+
Pyrazophos	C14H20N3O5PS	13457-18-6	+
Pyrazosulfuron ethyl	C14H18N6O7S	93697-74-6	+
Pyrethrin I	C21H28O3	121-21-1	+
Pyridaben	C19H25CIN2OS	96489-71-3	+
Pyridafenthion	C14H17N2O4PS	119-12-0	+
Pyridate	C19H23CIN2O2S	55512-33-9	+
Pyridostigmine	C9H13N2O2	155-97-5	+
Pyrifenoxy	C14H12Cl2N2O	88283-41-4	+
Pyrifthalid	C15H14N2O4S	135186-78-6	+
Pyrimethamine	C12H13CIN4	58-14-0	+
Pyrimethanil	C12H13N3	53112-28-0	+
Pyrimidifen	C20H28CIN3O2	105779-78-0	+
Pyriproxyfen (Pyriproxifen)	C20H19NO3	95737-68-1	+
Pyripyridone	C9H13NO2	77-04-3	+ -
Pyritinol	C16H20N2O4S2	1098-97-1	+
Pyrocatechol	C6H6O2	120-80-9	+ -
Pyrogallol	C6H6O3	87-66-1	-
Pyroquilon	C11H11NO	57369-32-1	+
Pyrovalerone	C16H23NO	3563-49-3	+
Pyroxsulam	C14H13F3N6O5S	422556-08-9	+
Pyrrbutamine	C20H22CIN	91-82-7	+
Quazepam	C17H11ClF4N2S	36735-22-5	+
Quetiapine	C21H25N3O2S	111974-69-7	+ -

Compound Name	Formula	CAS	Polarity
Quinagolide	C20H33N3O3S	87056-78-8	+
Quinalphos (Diethquinalphione)	C12H15N2O3PS	13593-03-8	+
Quinapril	C25H30N2O5	85441-61-8	+ -
Quinaprilat	C23H26N2O5	82768-85-2	+
Quinclorac	C10H5Cl2NO2	84087-01-4	+
Quinethazone	C10H12ClN3O3S	73-49-4	+
Quinidine	C20H24N2O2	56-54-2	+
Quinine	C20H24N2O2	130-95-0	+
Quinine ethylcarbonate	C23H28N2O4	83-75-0	+
Quinisocain	C17H24N2O	86-80-6	+
Quinmerac	C11H8ClNO2	90717-03-6	+
Quinoclamine (ACN)	C10H6ClNO2	2797-51-5	+
Quinoxyfen	C15H8Cl2FNO	124495-18-7	+
Quinupristin	C53H67N9O10S	120138-50-3	+
Quizalofop-ethyl	C19H17ClN2O4	76578-14-8	+
Quizalofop-p-ethyl	C19H17ClN2O4	100646-51-3	+
Rabenzazole	C12H12N4	40341-04-6	+
Rabeprazole	C18H21N3O3S	117976-89-3	+
Racecadotril	C21H23NO4S	81110-73-8	+
Raclopride	C15H20Cl2N2O3	84225-95-6	+ -
Ractopamine	C18H23NO3	97825-25-7	+
Raloxifene	C28H27NO4S	84449-90-1	+ -
Ramipril	C23H32N2O5	87333-19-5	+ -
Ranitidine	C13H22N4O3S	66357-35-5	+ -
Rasagiline	C12H13N	136236-51-6	+
Raubasin (Ajmalicine)	C21H24N2O3	483-04-5	+ -
Raupin	C19H22N2O2	482-68-8	+
RCS-4	C21H23NO2	1345966-78-0	+
RCS-4 2-methoxy isomer	C21H23NO2		+
RCS-4 3-methoxy isomer	C21H23NO2		+ -
RCS-4 N-(4-hydroxypentyl) metabolite	C21H23NO3		+
RCS-4 N-(5-carboxypentyl) metabolite	C21H21NO4		+ -
RCS-4-C4 homolog	C20H21NO2		+ -
RCS-8 (BTM-8)	C25H29NO2	1345970-42-4	+
RCS-8 3-methoxy isomer	C25H29NO2		+
RCS-8 4-methoxy isomer	C25H29NO2		+
Reboxetine	C19H23NO3	98769-81-4	+
Remoxipride	C16H23BrN2O3	80125-14-0	+
Repaglinide	C27H36N2O4	135062-02-1	+ -
Reproterol	C18H23N5O5	54063-54-6	+
Reserpine	C33H40N2O9	50-55-5	+ -
Resmethrin(I)	C22H26O3	10453-86-8	+
Resmethrin(II)	C22H26O3	10453-86-8	+
Resorcinol bis(diphenyl phosphate)	C30H24O8P2	57583-54-7	+
Resveratrol	C14H12O3	501-36-0	-

Compound Name	Formula	CAS	Polarity
Rhapontigenin	C15H14O4	500-65-2	-
Rhapontin	C21H24O9	155-58-8	+ -
Rhein	C15H8O6	478-43-3	-
Riboflavin	C17H20N4O6	83-88-5	+
Riboflavin phosphate	C17H21N4O9P	146-17-8	+
Rifabutin	C46H62N4O11	72559-06-9	+
Rifampicin	C43H58N4O12	13292-46-1	+
Rifampicin quinone	C43H56N4O12	13983-13-6	+
Rifaximin	C43H51N3O11	80621-81-4	+
Riluzole	C8H5F3N2OS	1744-22-5	+ -
Rimsulfuron	C14H17N5O7S2	122931-48-0	+
Risperidone	C23H27FN4O2	106266-06-2	+
Ritalinic acid	C13H17NO2	19395-41-6	+ -
Ritanserin	C27H25F2N3OS	87051-43-2	+
Ritodrine	C17H21NO3	26652-09-5	+
Ritonavir	C37H48N6O5S2	155213-67-5	+
Rizatriptan	C15H19N5	144034-80-0	+
Robenidine	C15H13Cl2N5	25875-51-8	+
Rocuronium	C32H53N2O4	143558-00-3	+
Rofecoxib	C17H14O4S	162011-90-7	+ -
Romifidine	C9H9BrFN3	65896-16-4	+
Ronidazole	C6H8N4O4	7681-76-7	+
Ropinirole	C16H24N2O	91374-21-9	+
Rosiglitazone	C18H19N3O3S	122320-73-4	+ -
Rosoxacin	C17H14N2O3	40034-42-2	+
Rotenone	C23H22O6	83-79-4	+ -
Roxarsone	C6H6AsNO6	121-19-7	-
Roxatidine acetate	C19H28N2O4	78628-28-1	+
Roxithromycin	C41H76N2O15	80214-83-1	+
Rufocromomycin (Streptonigrin)	C25H22N4O8	3930-19-6	+ -
Saccharin	C7H5NO3S	81-07-2	+ -
Salacetamide	C9H9NO3	487-48-9	+
Salazosulfapyridine	C18H14N4O5S	599-79-1	+ -
Salbutamol (Albuterol)	C13H21NO3	18559-94-9	+ -
Salicin	C13H18O7	138-52-3	+
Salicylamide	C7H7NO2	65-45-2	+ -
Salicylamide,N-isopropyl-	C10H13NO2	551-35-9	+
Salicylaminophenazone	C18H17N3O3	5712-95-8	+
Salicylanilide	C13H11NO2	87-17-2	+
Salicylic acid	C7H6O3	69-72-7	-
Salinomycin	C42H70O11	53003-10-4	-
Salmeterol	C25H37NO4	89365-50-4	+ -
Salsalate	C14H10O5	552-94-3	-
Salsoline	C11H15NO2	89-31-6	+
Salsolinol	C10H13NO2	525-72-4	+

Compound Name	Formula	CAS	Polarity
Salverine	C19H24N2O2	6376-26-7	+
Salvinorin A	C23H28O8	83729-01-5	+
Salvinorin B (Divinorin B)	C21H26O7	92545-30-7	+
Sanguinarine	C20H14NO4	2447-54-3	+
Santonin	C15H18O3	481-06-1	+
Saquinavir	C38H50N6O5	127779-20-8	+
Sarafloxacin	C20H17F2N3O3	98105-99-8	+
Scopolamine	C17H21NO4	51-34-3	+
Sebuthylazine	C9H16ClN5	7286-69-3	+
Secbumeton	C10H19N5O	26259-45-0	+
Secobarbital	C12H18N2O3	76-73-3	-
Selamectine	C43H63NO11	165108-07-6	+ -
Selegiline	C13H17N	14611-51-9	+
Sennoside	C42H38O20	517-43-1	-
Sennoside B	C42H38O20	128-57-4	-
Sertaconazole	C20H15Cl3N2OS	99592-32-2	+
Sertindole	C24H26ClFN4O	106516-24-9	+
Sertraline	C17H17Cl2N	79617-96-2	+
Sethoxydim	C17H29NO3S	74051-80-2	+
Sibutramine	C17H26ClN	106650-56-0	+
Siduron	C14H20N2O	1982-49-6	+
Sildenafil	C22H30N6O4S	139755-83-2	+ -
Silibinin	C25H22O10	22888-70-6	+ -
Silicristine	C25H22O10	33889-69-9	+
Silthiofam	C13H21NOSSi	175217-20-6	+
Simazine	C7H12ClN5	122-34-9	+
Simeconazole(I)	C14H20FN3OSi	149508-90-7	+
Simeconazole(II)	C14H20FN3OSi	149508-90-7	+
Simetryn	C8H15N5S	1014-70-6	+
Simvastatin	C25H38O5	79902-63-9	+
Sitagliptin	C16H15F6N5O	486460-32-6	+
Solanine	C45H73NO15	20562-02-1	+ -
Solifenacin	C23H26N2O2	242478-37-1	+
Sorbitol	C6H14O6	50-70-4	+ -
Sotalol	C12H20N2O3S	3930-20-9	+ -
Spaglumic acid	C11H16N2O8	3106-85-2	+ -
Sparfloxacin	C19H22F2N4O3	110871-86-8	+
Sparteine	C15H26N2	90-39-1	+
Spectinomycin	C14H24N2O7	1695-77-8	+
Spinosyn A	C41H65NO10	131929-60-7	+
Spinosyn D	C42H67NO10	131929-63-0	+
Spiperone	C23H26FN3O2	749-02-0	+ -
Spiramycin I	C43H74N2O14	24916-50-5	+
Spirapril	C22H30N2O5S2	83647-97-6	+
Spirodiclofen	C21H24Cl2O4	148477-71-8	+

Compound Name	Formula	CAS	Polarity
Spiromesifen	C23H30O4	283594-90-1	+
Spironolactone	C24H32O4S	52-01-7	-
Spirotetramat	C21H27NO5	203313-25-1	+
Spiroxamine	C18H35NO2	118134-30-8	+
Squalene	C30H50	7683-64-9	+
Stanozolol	C21H32N2O	10418-03-8	+
Stavudine	C10H12N2O4	3056-17-5	+ -
Streptomycin	C21H39N7O12	57-92-1	+
Streptozocin	C8H15N3O7	18883-66-4	-
Strychnine	C21H22N2O2	57-24-9	+
Strychnine N6-oxide	C21H22N2O3	7248-28-4	+ -
STS-135	C24H31FN2O	1354631-26-7	+
Styphnic acid	C6H3N3O8	82-71-3	-
Succinylsulfathiazole	C13H13N3O5S2	116-43-8	+ -
Sucralose	C12H19Cl3O8	56038-13-2	-
Sufentanil	C22H30N2O2S	56030-54-7	+
Sulazepam	C16H13ClN2S	2898-13-7	+
Sulbentin	C17H18N2S2	350-12-9	+
Sulcofuron	C19H12Cl4N2O5S	24019-05-4	+
Sulconazole	C18H15Cl3N2S	61318-90-9	+
Sulcotrione	C14H13ClO5S	99105-77-8	+
Sulfabenzamide	C13H12N2O3S	127-71-9	+ -
Sulfacarbamide	C7H9N3O3S	547-44-4	+
Sulfacetamide	C8H10N2O3S	144-80-9	+ -
Sulfachloropyridazine	C10H9ClN4O2S	80-32-0	+ -
Sulfacloimid	C12H13ClN4O2S	4015-18-3	+
Sulfadiazine (Silvadene)	C10H10N4O2S	68-35-9	+
Sulfadicramide	C11H14N2O3S	115-68-4	+
Sulfadimethoxine	C12H14N4O4S	122-11-2	+
Sulfadimidine (Sulfamethazine)	C12H14N4O2S	57-68-1	+ -
Sulfadoxine	C12H14N4O4S	2447-57-6	+ -
Sulfaethidole	C10H12N4O2S2	94-19-9	+
Sulfaguanidine	C7H10N4O2S	57-67-0	+
Sulfaguanole	C12H15N5O3S	27031-08-9	+
Sulfalene	C11H12N4O3S	152-47-6	+
Sulfamerazine	C11H12N4O2S	127-79-7	+ -
Sulfamethizole	C9H10N4O2S2	144-82-1	+ -
Sulfamethoxazole	C10H11N3O3S	723-46-6	+
Sulfamethoxypyridazine (Midicel)	C11H12N4O3S	80-35-3	+ -
Sulfamethylthiazole	C10H11N3O2S2	515-59-3	+
Sulfametoxydiazine	C11H12N4O3S	651-06-9	+ -
Sulfametrole	C9H10N4O3S2	32909-92-5	+
Sulfamonomethoxin	C11H12N4O3S	1220-83-3	+ -
Sulfamoxole	C11H13N3O3S	729-99-7	+
Sulfanilamide	C6H8N2O2S	63-74-1	+ -

Compound Name	Formula	CAS	Polarity
Sulfanitran	C14H13N3O5S	122-16-7	-
Sulfaperin	C11H12N4O2S	599-88-2	+
Sulfaphenazole	C15H14N4O2S	526-08-9	+ -
Sulfapyridine	C11H11N3O2S	144-83-2	+
Sulfaquinoxaline	C14H12N4O2S	59-40-5	+ -
Sulfathiazole	C9H9N3O2S2	72-14-0	+
Sulfathiourea (component of Sulfatolamide)	C7H9N3O2S2	515-49-1	+
Sulfentrazone	C11H10Cl2F2N4O3S	122836-35-5	+
Sulfinpyrazone	C23H20N2O3S	57-96-5	+ -
Sulfisomidine (Sulfamethin)	C12H14N4O2S	515-64-0	+
Sulfonal	C7H16O4S2	115-24-2	+
Sulforidazine	C21H26N2O2S2	14759-06-9	+
Sulfosulfuron	C16H18N6O7S2	141776-32-1	+
Sulfotep	C8H20O5P2S2	3689-24-5	+
Sulindac	C20H17FO3S	38194-50-2	+
Suloctidil	C20H35NOS	54063-56-8	+ -
Sulphisoazole	C11H13N3O3S	127-69-5	+ -
Sulpiride	C15H23N3O4S	15676-16-1	+
Sulprofos	C12H19O2PS3	35400-43-2	+
Sulprostone	C23H31NO7S	60325-46-4	+ -
Sultiame	C10H14N2O4S2	61-56-3	+
Sumatriptan	C14H21N3O2S	103628-46-2	+
Suprofen	C14H12O3S	40828-46-4	+ -
Suxibuzone	C24H26N2O6	27470-51-5	+ -
Synephrine	C9H13NO2	94-07-5	+
Syringaldehyde	C9H10O4	134-96-3	+
Syrosingopine	C35H42N2O11	84-36-6	+
Tacrine	C13H14N2	321-64-2	+ -
Tacrolimus	C44H69NO12	104987-11-3	-
Tadalafil	C22H19N3O4	171596-29-5	+
Talastine	C19H21N3O	16188-61-7	+
Talbutal	C11H16N2O3	115-44-6	-
Talinolol	C20H33N3O3	57460-41-0	+
Tamoxifen	C26H29NO	10540-29-1	+
Tamsulosin	C20H28N2O5S	106133-20-4	+ -
Tapentadol	C14H23NO	175591-23-8	+ -
Tau-fluvalinate	C26H22ClF3N2O3	102851-06-9	+
Taurolidine	C7H16N4O4S2	19388-87-5	-
Taxol (Paclitaxel)	C47H51NO14	33069-62-4	+
Taxuyunnanine A (Taxol C)	C46H57NO14	153415-45-3	+ -
Tazarotene	C21H21NO2S	118292-40-3	+
Tazobactam	C10H12N4O5S	89786-04-9	+
TC / Tetracycline	C22H24N2O8	60-54-8	+ -
TCA (Trichloroacetic acid)	C2HCl3O2	76-03-9	-
TCP / Tenocyclidine	C15H23NS	21500-98-1	+

Compound Name	Formula	CAS	Polarity
TDCP / Tris(1,3-dichloroisopropyl)phosphate	C9H15Cl6O4P	13674-87-8	+
Tebuconazole(I) (Terbuconazole)	C16H22ClN3O	107534-96-3	+
Tebuconazole(II) (Terbuconazole)	C16H22ClN3O	107534-96-3	+
Tebufenozide	C22H28N2O2	112410-23-8	+
Tebufenpyrad	C18H24ClN3O	119168-77-3	+
Tebupirimfos	C13H23N2O3PS	96182-53-5	+
Tebutam	C15H23NO	35256-85-0	+
Tebuthiuron	C9H16N4OS	34014-18-1	+
Teflubenzuron	C14H6Cl2F4N2O2	83121-18-0	+
Telmisartan	C33H30N4O2	144701-48-4	-
Temazepam	C16H13ClN2O2	846-50-4	+ -
Temephos (Abate)	C16H20O6P2S3	3383-96-8	+
Temozolomide	C6H6N6O2	85622-93-1	+
Teniposide	C32H32O13S	29767-20-2	+
Tenofovir	C9H14N5O4P	147127-20-6	+
Tenoxicam	C13H11N3O4S2	59804-37-4	+ -
Tepraloxymid (BAS 620H)	C17H24ClNO4	149979-41-9	+
Terazosin	C19H25N5O4	63590-64-7	+
Terbacil	C9H13ClN2O2	5902-51-2	-
Terbinafine	C21H25N	91161-71-6	+
Terbufos	C9H21O2PS3	13071-79-9	+
Terbumeton	C10H19N5O	33693-04-8	+
Terbumeton-desethyl	C8H15N5O	33124-62-8	+
Terbutaline	C12H19NO3	23031-25-6	+
Terbuthylazine (TERBA)	C9H16ClN5	5915-41-3	+
Terbuthylazine-2-hydroxy (Terbutmenton-desethyl)	C9H17N5O	66753-07-9	+
Terbutryn	C10H19N5S	886-50-0	+
Terconazole	C26H31Cl2N5O3	67915-31-5	+
Terfenadine	C32H41NO2	50679-08-8	+
Ternidazole	C7H11N3O3	1077-93-6	+
Terodiline	C20H27N	15793-40-5	+
Testolactone	C19H24O3	968-93-4	+
Testosterone	C19H28O2	58-22-0	+
Testosterone acetate	C21H30O3	1045-69-8	+
Testosterone benzoate	C26H32O3	2088-71-3	+
Testosterone caprylate	C29H46O3	5721-91-5	+
Testosterone enantate	C26H40O3	315-37-7	+
Testosterone isocaproate	C25H38O3	15262-86-9	+
Testosterone-17-propionate	C22H32O3	57-85-2	+
Testosteronephenylpropionate	C28H36O3	1255-49-8	+
Tetrabromo-o-cresol	C7H4Br4O	576-55-6	-
Tetracaine	C15H24N2O2	94-24-6	+
Tetrachlorophenol	C6H2Cl4O	25167-83-3	-
Tetrachlorvinphos (Dietreen T)	C10H9Cl4O4P	22248-79-9	+
Tetraconazole	C13H11Cl2F4N3O	112281-77-3	+

Compound Name	Formula	CAS	Polarity
Tetraethyl 1,2-ethanediybis(phosphonate)	C10H24O6P2		+
Tetrahydrocortisone	C21H32O5	53-05-4	+
Tetramethrin	C19H25NO4	7696-12-0	+
Tetramethylpyrazine	C8H12N2	1124-11-4	+
Tetramisole	C11H12N2S	1124-11-4	+
Tetrandrine	C38H42N2O6	518-34-3	+
Tetrazepam	C16H17CIN2O	10379-14-3	+
Tetrekis(2-chloroethyl)dichloroisopentyl diphosphate	C13H24Cl6O8P2	38051-10-4	+
Tetroxoprim	C16H22N4O4	53808-87-0	+
Tetryzoline	C13H16N2	84-22-0	+
TFMPP / 1-(3-Trifluoromethylphenyl)piperazine	C11H13F3N2	15532-75-9	+
Thalidomide	C13H10N2O4	50-35-1	+
THC / delta9-Tetrahydrocannabinol	C21H30O2	1972-08-3	+ -
THCA-A / delta9-Tetrahydrocannabinol-2-carboxylic acid	C22H30O4	23978-85-0	+
THC-COOH / 11-Nor-9-Carboxy-tetrahydrocannabinol	C21H28O4	64280-14-4	+ -
THC-OH / 11-Hydroxy-tetrahydrocannabinol	C21H30O3	36557-05-8	+ -
Thebacone	C20H23NO4	466-90-0	+
Thebaine	C19H21NO3	115-37-7	+
Thebaol	C16H14O3	481-81-2	+ -
Thenalidine	C17H22N2S	86-12-4	+
Thenyldiamine	C14H19N3S	91-79-2	+
Theobromine	C7H8N4O2	83-67-0	+
Theodrenaline	C17H21N5O5	13460-98-5	+
Theophylline	C7H8N4O2	58-55-9	+ -
Thiabendazole	C10H7N3S	148-79-8	-
Thiacloprid	C10H9CIN4S	111988-49-9	+
Thiamazole	C4H6N2S	60-56-0	+
Thiamethoxam	C8H10CIN5O3S	153719-23-4	+
Thiamine disulfide	C24H34N8O4S2	67-16-3	+
Thiamphenicol	C12H15Cl2NO5S	15318-45-3	+ -
Thiamylal (Barbituric acid)	C12H18N2O2S	77-27-0	-
Thiazafluron	C6H7F3N4OS	25366-23-8	+
Thidiazuron	C9H8N4OS	51707-55-2	+
Thiethylperazine	C22H29N3S2	1420-55-9	+
Thifensulfuron-methyl (DPX-M6316)	C12H13N5O6S2	79277-27-3	+
Thioacetazone	C10H12N4OS	104-06-3	+
Thiobencarb	C12H16CINOS	28249-77-6	+
Thioctic acid	C8H14O2S2	62-46-4	-
Thiodicarb	C10H18N4O4S3	59669-26-0	+
Thiofanox-sulfone	C9H18N2O4S	39184-59-3	+
Thiofanox-sulfoxide	C9H18N2O3S	39184-27-5	+
Thiolutin	C8H8N2O2S2	87-11-6	+
Thiometon	C6H15O2PS3	640-15-3	+
Thiopental	C11H18N2O2S	76-75-5	-
Thiophanate	C14H18N4O4S2	23564-06-9	+

Compound Name	Formula	CAS	Polarity
Thiophanate-methyl	C12H14N4O4S2	23564-05-8	+
Thiopropazate	C23H28ClN3O2S	84-06-0	+
Thiopropazine	C22H30N4O2S2	316-81-4	+
Thioquinox	C9H4N2S3	93-75-4	+
Thioridazine	C21H26N2S2	50-52-2	+
Thioridazine-2,5-disulfoxide	C21H26N2O2S2	53926-89-9	+
Thiosalicylic acid	C7H6O2S	147-93-3	-
Thiotepa	C6H12N3PS	52-24-4	+
Thiram	C6H12N2S4	137-26-8	+
Thymopentin	C30H49N9O9	69558-55-0	+ -
Thymotic acid	C11H14O3	548-51-6	-
Tiagabine	C20H25NO2S2	115103-54-3	+
Tiamenidine	C8H10ClN3S	31428-61-2	+
Tiamulin	C28H47NO4S	55297-95-5	+
Tiapride	C15H24N2O4S	51012-32-9	+ -
Tiaprofenic acid	C14H12O3S	33005-95-7	+
Tibolone	C21H28O2	5630-53-5	+ -
Ticlopidine	C14H14ClNS	55142-85-3	+
Tiemonium	C18H24NO2S	6252-92-2	+
Tienilic acid	C13H8Cl2O4S	40180-04-9	+ -
Tifatol (Cymiazole)	C12H14N2S	61676-87-7	+
Tiletamine	C12H17NOS	14176-49-9	+
Tilidine	C17H23NO2	20380-58-9	+
Tilmicosin	C46H80N2O13	108050-54-0	+
Tilorone	C25H34N2O3	27591-97-5	+
Timolol	C13H24N4O3S	26839-75-8	+
Timonacic	C4H7NO2S	444-27-9	+ -
Tinidazole	C8H13N3O4S	19387-91-8	+
Tiocarlide	C23H32N2O2S	910-86-1	+
Tioconazole	C16H13Cl3N2OS	65899-73-2	+
Tioguanine (Thioguanine)	C5H5N5S	154-42-7	+ -
Tiopronine	C5H9NO3S	1953-02-2	+
Tiotixene	C23H29N3O2S2	5591-45-7	+
Tiotropium	C19H22NO4S2	186691-13-4	+
Tioxolone	C7H4O3S	4991-65-5	-
Tipranavir	C31H33F3N2O5S	174484-41-4	+
Tiracizine	C21H25N3O3	83275-56-3	+
Tirofiban	C22H36N2O5S	144494-65-5	+
Tiropamide	C28H41N3O3	55837-29-1	+
Tixocortol 21-pivalate	C26H38O5S	55560-96-8	+
Tizanidine	C9H8ClN5S	51322-75-9	+
TMA / Trimethoxyamphetamine	C12H19NO3	1082-88-8	+
TMA-2 / 2,4,5-Trimethoxyamphetamine	C12H19NO3	1083-09-6	+
Tobramycin	C18H37N5O9	32986-56-4	+
Tocainide	C11H16N2O	41708-72-9	+

Compound Name	Formula	CAS	Polarity
Tocopherol	C29H50O2	59-02-9	+ -
Tolazamide	C14H21N3O3S	1156-19-0	+
Tolazoline	C10H12N2	59-98-3	+
Tolbutamide	C12H18N2O3S	64-77-7	+ -
Tolcapone	C14H11NO5	134308-13-7	-
Tolciclate	C20H21NOS	50838-36-3	+
Tolclofos-methyl	C9H11Cl2O3PS	57018-04-9	+
Tolfenamic acid	C14H12ClNO2	13710-19-5	+ -
Tolfenamic Acid-13C(6)	C8[13C]6H12ClNO2	1420043-61-3	+
Toliprolol	C13H21NO2	2933-94-0	+
Tolmetin	C15H15NO3	26171-23-3	+
Tolnaftate	C19H17NOS	2398-96-1	+
Toloxatone	C11H13NO3	29218-27-7	+
Tolperisone	C16H23NO	728-88-1	+
Tolpropamine	C18H23N	5632-44-0	+
Tolterodine	C22H31NO	124936-74-9	-
Toluene-2-sulfonamide	C7H9NO2S	88-19-7	+ -
Toluidine Blue (Tolonium)	C15H16N3S	22239-28-7	+
Tolycaine	C15H22N2O3	3686-58-6	+
Tolyfluanide	C10H13Cl2FN2O2S2	731-27-1	+
Tonzonium (Thonzonium)	C32H55N4O	25466-36-8	+
Topiramate	C12H21NO8S	97240-79-4	+ -
Topotecan	C23H23N3O5	123948-87-8	+
Topramezone	C16H17N3O5S	210631-68-8	+
Torasemide	C16H20N4O3S	56211-40-6	+ -
Toremifene	C26H28ClNO	89778-26-7	+
TPPA / Triphenyl phosphate	C18H15O4P	115-86-6	+
Tralkoxydim	C20H27NO3	87820-88-0	+
Tramadol	C16H25NO2	27203-92-5	+
Tramazoline	C13H17N3	1082-57-1	+
Trandolapril (Indoapril)	C24H34N2O5	80876-01-3	+
Trandolaprilat	C22H30N2O5	87679-71-8	+
trans-10,11-Dihydroxy-10,11-dihydrocarbazepine	C15H14N2O3	58955-93-4	+
trans-Calcifediol	C27H44O2	19356-17-3	+ -
Tranlycypromine	C9H11N	155-09-9	+
Trapidil	C10H15N5	15421-84-8	+
Trazodone	C19H22ClN5O	19794-93-5	+
Trenbolone	C18H22O2	10161-33-8	+
Trenbolone acetate	C20H24O3	10161-34-9	+
Tretinoin	C20H28O2	302-79-4	+
Triacetin	C9H14O6	102-76-1	+
Triadimefon	C14H16ClN3O2	43121-43-3	+ -
Triadimenol	C14H18ClN3O2	55219-65-3	+
Triallate	C10H16Cl3NOS	2303-17-5	+
Triamcinolone	C21H27FO6	124-94-7	+ -

Compound Name	Formula	CAS	Polarity
Triamcinolone acetonide	C24H31FO6	76-25-5	+
Triamcinolone diacetate	C25H31FO8	67-78-7	+
Triamcinolone hexacetonide	C30H41FO7	5611-51-8	+
Triamiphos	C12H19N6OP	1031-47-6	+
Triamterene	C12H11N7	396-01-0	+
Triasulfuron (Logran)	C14H16ClN5O5S	82097-50-5	+
Triazamate	C13H22N4O3S	112143-82-5	+
Triaziquon	C12H13N3O2	68-76-8	+
Triazolam	C17H12Cl2N4	28911-01-5	+
Triazophos	C12H16N3O3PS	24017-47-8	+
Tribenoside	C29H34O6	10310-32-4	+
Tribenuron-methyl	C15H17N5O6S	101200-48-0	+
Tribufos	C12H27OPS3	78-48-8	+
Trichlorfon (Dylox) (DEP)	C4H8Cl3O4P	52-68-6	+
Trichlormethiazide	C8H8Cl3N3O4S2	133-67-5	-
Trichlormethine	C6H12Cl3N	555-77-1	+
Triclabendazole	C14H9Cl3N2O5	68786-66-3	+
Triclabendazole sulfoxide	C14H9Cl3N2O2S	100648-13-3	+
Triclocarban	C13H9Cl3N2O	101-20-2	+
Triclopyr	C7H4Cl3NO3	55335-06-3	-
Tricresylphosphate	C21H21O4P	1330-78-5	+
Tricyclazole	C9H7N3S	41814-78-2	+
Tridemorph	C19H39NO	24602-86-6	+
Tridihexethyl	C21H36NO	4310-35-4	+
Trietazine	C9H16ClN5	1912-26-1	+
Trifloxystrobin	C20H19F3N2O4	141517-21-7	+
Trifloxysulfuron	C14H14F3N5O6S	145099-21-4	+
Triflumizol	C15H15ClF3N3O	68694-11-1	+
Triflumuron	C15H10ClF3N2O3	64628-44-0	+
Trifluoperazine	C21H24F3N3S	117-89-5	+
Trifluperidol	C22H23F4NO2	749-13-3	+
Triflupromazine	C18H19F3N2S	146-54-3	+
Trifluridine	C10H11F3N2O5	70-00-8	-
Triflusulfuron-methyl	C17H19F3N6O6S	126535-15-7	+
Triforine	C10H14Cl6N4O2	26644-46-2	+
Trihexyphenidyl	C20H31NO	144-11-6	+
Tri-iso-butyl phosphate	C12H27O4P	126-71-6	+
Trimazosin	C20H29N5O6	35795-16-5	+
Trimebutine	C22H29NO5	39133-31-8	+
Trimethobenzamide	C21H28N2O5	138-56-7	+
Trimethoprim	C14H18N4O3	738-70-5	+
Trimetozine	C14H19NO5	635-41-6	+
Trimipramine	C20H26N2	739-71-9	+
Tri-n-butyl phosphate	C12H27O4P	126-73-8	+
Trinexapac-ethyl	C13H16O5	95266-40-3	+

Compound Name	Formula	CAS	Polarity
Trioxysalen	C14H12O3	3902-71-4	+
Triparanol	C27H32ClNO2	78-41-1	+
Tripelenamine	C16H21N3	91-81-6	+
Tripentyl phosphate	C15H33O4P		+
Triperiden	C21H29NO	14617-17-5	+
Triprolidine	C19H22N2	486-12-4	+
Tris(2,3-dibromopropyl) phosphate	C9H15Br6O4P	126-72-7	+
Tris(2-butoxyethyl) phosphate	C18H39O7P	78-51-3	+
Tris(2-chloroethyl) phosphate	C6H12Cl3O4P	115-96-8	+
Tris(2-chloroisopropyl) phosphate	C9 H18 Cl3 O4 P	13674-84-5	+
Tris(2-ethylhexyl) phosphate	C24H51O4P	78-42-2	+
Triticonazole(I)	C17H20ClN3O	131983-72-7	+
Triticonazole(II)	C17H20ClN3O	131983-72-7	+
Tritoqualine	C26H32N2O8	14504-73-5	+
Tritosulfuron	C13H9F6N5O4S	142469-14-5	+
Trofosfamide	C9H18Cl3N2O2P	22089-22-1	+
Troleandomycin	C41H67NO15	2751-09-9	+
Tromantadine	C16H28N2O2	53783-83-8	+
Trometamol (Tris)	C4H11NO3	77-86-1	+
Tropacocaine	C15H19NO2	537-26-8	+
Tropenziline	C24H30NO4	143-92-0	+
Tropicamide	C17H20N2O2	1508-75-4	+
Tropine benzilate	C22H25NO3	3736-36-5	+
Tropisetrone	C17H20N2O2	89565-68-4	+
Trospium	C25H30NO3	10405-02-4	+
Trovafloxacin	C20H15F3N4O3	147059-72-1	+
Troxerutin	C33H42O19	7085-55-4	+ -
Tuaminoheptane	C7H17N	123-82-0	+
Tubocurarine	C37H41N2O6	57-95-4	+
Tulathromycin	C41H79N3O12	217500-96-4	+
Tulobuterol	C12H18ClNO	41570-61-0	+
Tylosin	C46H77NO17	1401-69-0	+
Tylosin A	C46H77NO17	8026-48-0	+
Tylosin B	C39H65NO14	11032-98-7	+
Tylvalosin (Aivlosin)	C53H87NO19	63409-12-1	+
Ugurol (Tranexamic acid)	C8H15NO2	1197-18-8	+
Ultralanum (Fluocortolone 21-Caproate)	C28H39FO5	303-40-2	+
Umbelliferone	C9H6O3	93-35-6	-
Uniconazole-P(I)	C15H18ClN3O	83657-22-1	+
Uniconazole-P(II)	C15H18ClN3O	83657-22-1	+
UR-144 (KM-X1)	C21H29NO	1199943-44-6	+
Uramustine (Uracil mustard)	C8H11Cl2N3O2	66-75-1	+ -
Urapidil	C20H29N5O3	34661-75-1	+ -
URB-447	C25H21ClN2O	1132922-57-6	+
URB-597 (KDS-4103)	C20H22N2O3	546141-08-6	+

Compound Name	Formula	CAS	Polarity
URB-602	C19H21NO2	565460-15-3	+ -
URB-754	C16H14N2O2	86672-58-4	+ -
URB-937	C20H22N2O4	1357160-72-5	+ -
Urethane	C3H7NO2	51-79-6	+
Ursodeoxycholic acid	C24H40O4	128-13-2	-
Usnic acid	C18H16O7	125-46-2	+ -
Valaciclovir	C13H20N6O4	124832-26-4	+
Valdecoxib	C16H14N2O3S	181695-72-7	+ -
Valdetamide	C9H17NO	512-48-1	+
Valethamate	C19H32NO2	90-22-2	+
Valganciclovir	C14H22N6O5	175865-59-5	+
Valproic acid	C8H16O2	99-66-1	-
Valpromide	C8H17NO	2430-27-5	+
Valsartan	C24H29N5O3	137862-53-4	+ -
Vamidothion	C8H18NO4PS2	2275-23-2	+
Vamidothion sulfone	C8H18NO6PS2	70898-34-9	+
Vanillin	C8H8O3	121-33-5	+
Vardenafil	C23H32N6O4S	224789-15-5	+
Vecuronium	C34H57N2O4	86029-43-8	+
Velnacrine (1-Hydroxytacrine)	C13H14N2O	104675-29-8	+
Venlafaxine	C17H27NO2	93413-69-5	+
Verapamil	C27H38N2O4	52-53-9	+ -
Vesamicol	C17H25NO	22232-64-0	+
Vetrabutine	C20H27NO2	3735-45-3	+
Vidarabin	C10H13N5O4	5536-17-4	+
Vigabatrin	C6H11NO2	60643-86-9	+
Viloxazine	C13H19NO3	46817-91-8	+
Viminol	C21H31ClN2O	21363-18-8	+
Vinbarbital	C11H16N2O3	2430-49-1	-
Vinblastin	C46H58N4O9	865-21-4	+
Vinburnine	C19H22N2O	4880-88-0	+
Vincamine	C21H26N2O3	1617-90-9	+
Vincristine	C46H56N4O10	57-22-7	+
Vinorelbin	C45H54N4O8	71486-22-1	+
Vinpocetine	C22H26N2O2	42971-09-5	+
Viomycin	C25H43N13O10	32988-50-4	+ -
Viquidil	C20H24N2O2	84-55-9	+
Virginiamycin S1	C43H49N7O10	23152-29-6	+ -
Visnadin	C21H24O7	477-32-7	+
Vitamin D3	C27H44O	67-97-0	-
Voriconazol	C16H14F3N5O	137234-62-9	+
Warfarin	C19H16O4	81-81-2	+ -
WIN-48098 (Pravadoline)	C23H26N2O3	92623-83-1	+
WIN-54461	C23H25BrN2O3	166599-63-9	+
Withaferin A	C28H38O6	5119-48-2	+ -

Compound Name	Formula	CAS	Polarity
Xantocilline	C18H12N2O2	580-74-5	+ -
Xenytropium	C30H34NO3	38971-12-9	+
Xipamide	C15H15ClN2O4S	14293-44-8	+
XLR-11 (5-fluoro UR-144)	C21H28FNO	1364933-54-9	+
XMC / 3,5-Xylyl methylcarbamate	C10H13NO2	2655-14-3	+
Xylazine	C12H16N2S	7361-61-7	+
Xylometazoline	C16H24N2	526-36-3	+
Yohimbic acid	C20H24N2O3	522-87-2	+ -
Yohimbine	C21H26N2O3	146-48-5	+ -
Z-10-Hydroxyamitriptyline	C20H23NO	1159-82-6	+
Z-10-Hydroxynortriptyline	C19H21NO	1156-99-6	+
Zalcitabine	C9H13N3O3	7481-89-2	+
Zaleplone	C17H15N5O	151319-34-5	+
Zaprinast	C13H13N5O2	37762-06-4	+ -
Zearalenone	C18H22O5	17924-92-4	+ -
Zidovudine	C10H13N5O4	30516-87-1	+
Zilpaterol	C14H19N3O2	117827-79-9	+
Zimelidine	C16H17BrN2	56775-88-3	+
Zipeprol	C23H32N2O3	34758-83-3	+
Ziprasidone	C21H21ClN4OS	146939-27-7	-
Zolazepam	C15H15FN4O	31352-82-6	+
Zoledronic acid	C5H10N2O7P2	118072-93-8	-
Zolmitriptan	C16H21N3O2	139264-17-8	+
Zolpidem	C19H21N3O	82626-48-0	+
Zomepirac	C15H14ClNO3	33369-31-2	+
Zonisamide	C8H8N2O3S	68291-97-4	+ -
Zopiclone	C17H17ClN6O3	43200-80-2	+
Zorubicin (Rubidazone)	C34H35N3O10	54083-22-6	+
Zotepine	C18H18ClNOS	26615-21-4	+
Zoxamide	C14H16Cl3NO2	156052-68-5	+
Zoxazolamine	C7H5ClN2O	61-80-3	+ -