

Name	Classification	Formula	Exact MW	M+H	M-H	SMILES	Parent compounds if metabolites
chlordecone	Pesticides	C10Cl10O	485.68338	486.69066	484.6761	ClC12C(=O)C3(Cl)C4(Cl)C1(Cl)C1(Cl)C2(Cl)C3(Cl)C4(Cl)C1(Cl)Cl	
chlorfenprop-methyl	Pesticides	C10H10Cl2O2	232.00579	233.01307	230.99851	COC(=O)C(Cl)Cc1ccc(Cl)cc1	
2,4-DB	Pesticides	C10H10Cl2O3	248.0007	249.00798	246.99342	OC(=O)CCCOc1ccc(Cl)cc1Cl	
camphechlor	Pesticides	C10H10Cl8	409.82908	410.83636	408.8218	ClCC1(C(Cl)Cl)C2CC(Cl)(Cl)C1(CCl)C(Cl)C2Cl	
metamiton	Pesticides	C10H10N4O	202.08546	203.09274	201.07818	CC1=NN=C(C(=O)N1N)c1ccccc1	
sulfadiazine	Pharmaceuticals	C10H10N4O2S	250.05245	251.05973	249.04517	Nc1ccc(cc1)S(=O)(=O)Nc1ncccn1	
acetamiprid	Pesticides	C10H11ClN4	222.06723	223.07451	221.05995	CN(Cc1ccc(Cl)nc1)C(C)=N\C#N	
thiacloprid-amide	Pesticides	C10H11ClN4OS	270.03421	271.04149	269.02693	NC(=O)\N=C1/SCCN1Cc1ccc(Cl)nc1	
mecoprop	Pesticides	C10H11ClO3	214.03968	215.04696	213.0324	CC(Oc1ccc(Cl)cc1C)C(O)=O	
clofibric acid	Pesticides	C10H11ClO3	214.03968	215.04696	213.0324	CC(C)(OC1=CC=C(Cl)C=C1)C(O)=O	
fluometuron	Pesticides	C10H11F3N2O	232.08235	233.08963	231.07507	CN(C)C(=O)Nc1cccc(c1)C(F)(F)F	
sulfamethoxazole	Pharmaceuticals	C10H11N3O3S	253.05212	254.0594	252.04484	Cc1cc(NS(=O)(=O)c2ccc(N)cc2)no1	
sulfamethoxazole N4-h	Metabolites	C10H11N3O4S	269.04703	270.05431	268.03975	Cc1cc(NS(=O)(=O)c2ccc(NO)cc2)no1	sulfamethoxazole
pymetrozine	Pesticides	C10H11N5O	217.09636	218.10364	216.08908	CC1=NNC(=O)N(C1)\N=C\c1ccnc1	
glyceryl p-aminobenzo	PCPs	C10H11NO5	225.06373	226.07101	224.05645	Nc1ccc(cc1)C(=O)OC(=O)C(O)CO	
bromophos-ethyl	Pesticides	C10H12BrCl2O3PS	391.88052	392.8878	390.87324	CCOP(=S)(OCC)OC1=CC(Cl)=C(Br)C=C1Cl	
carbanolate	Pesticides	C10H12ClNO2	213.05566	214.06294	212.04838	CNC(=O)Oc1ccc(C)C(C)c1Cl	
chlorpropham	Pesticides	C10H12ClNO2	213.05566	214.06294	212.04838	CC(C)OC(=O)Nc1cccc(Cl)c1	
benzofluor	Pesticides	C10H12F3NO2S2	299.02616	300.03344	298.01888	CCSc1ccc(NS(C)(=O)=O)c(c1)C(F)(F)F	
cotinine	Metabolites	C10H12N2O	176.09497	177.10225	175.08769	CN1[C@@H](CCC1=O)c1ccnc1	nicotine
bentazone	Pesticides	C10H12N2O3S	240.05687	241.06415	239.04959	CC(C)N1C(=O)c2ccccc2NS1(=O)=O	
stavudine	Pharmaceuticals	C10H12N2O4	224.07971	225.08699	223.07243	Cc1cn([C@@H]2O[C@H](CO)C=C2)c(=O)nc1O	
dinoseb	Pesticides	C10H12N2O5	240.07462	241.0819	239.06734	CCC(C)C1=CC(=CC(=C1O)[N+][O-])N+([O-])N+([O-])=O	
carbasulam	Pesticides	C10H12N2O6S	288.04161	289.04889	287.03433	COC(=O)Nc1ccc(cc1)S(=O)(=O)NC(=O)OC	
azinphos-methyl	Pesticides	C10H12N3O3PS2	317.00577	318.01305	315.99849	COP(=S)(OC)SCN1N=Nc2ccccc2C1=O	
didanosine	Pharmaceuticals	C10H12N4O3	236.09094	237.09822	235.08366	OC[C@H]1CC[C@H](O1)n1cnc2c(O)ncnc12	
tazobactam	Pharmaceuticals	C10H12N4O5S	300.05284	301.06012	299.04556	C[C@]1(Cn2ccnn2)[C@@H](N2[C@@H](CC2=O)S1(=O)=O)C(O)=O	
propylparaben	PCPs	C10H12O3	180.07865	181.08593	179.07137	CCCOC(=O)c1ccc(O)cc1	
propyl gallate	PCPs	C10H12O5	212.06848	213.07576	211.0612	CCCOC(=O)c1cc(O)c(O)c(O)c1	
meta-chlorophenylpiper	Pharmaceuticals	C10H13ClN2	196.07673	197.08401	195.06945	Clc1cccc(c1)N1CCNCC1	
chlordimeform	Pesticides	C10H13ClN2	196.07673	197.08401	195.06945	CN(C)\C=N\c1ccc(Cl)cc1C	
chlortoluron	Pesticides	C10H13ClN2O	212.07164	213.07892	211.06436	CN(C)C(=O)Nc1ccc(C)c(Cl)c1	
metoxuran	Pesticides	C10H13ClN2O2	228.06656	229.07384	227.05928	COc1ccc(NC(=O)N(C)C)cc1Cl	
zidovudine	Pharmaceuticals	C10H13N5O4	267.09676	268.10404	266.08948	Cc1cn([C@H]2C[C@H](N=[N+]=[N-])[C@@H](CO)O2)c(=O)[nH]c1=O	
N-ethyl-3-methylbenza	Metabolites	C10H13NO	163.09972	164.107	162.09244	CCNC(=O)c1cccc(C)c1	DEET
triforine	Pesticides	C10H14Cl6N4O2	431.9248	432.93208	430.91752	ClC(Cl)(Cl)C(NC=O)N1CCN(CC1)C(NC=O)C(Cl)(Cl)Cl	
nicotine	PCPs	C10H14N2	162.1157	163.12298	161.10842	CN1CCC[C@H]1c1ccnc1	
isoproturon-didemethyl	Pesticides	C10H14N2O	178.11062	179.1179	177.10334	CC(C)c1ccc(NC(N)=O)cc1	
telbivudine	Pharmaceuticals	C10H14N2O5	242.09027	243.09755	241.08299	Cc1cn([C@@H]2C[C@H](O)[C@H](CO)O2)c(=O)[nH]c1=O	
thymol	PCPs	C10H14O	150.10447	151.11175	149.09719	CC(C)c1ccc(C)cc1O	
amidothioate	Pesticides	C10H15ClNO2PS2	310.99704	312.00432	309.98976	CCNP(=S)(OC)Oc1ccc(SC)cc1Cl	
methamphetamine	Pharmaceuticals	C10H15N	149.12045	150.12773	148.11317	CN[C@@H](C)Cc1ccccc1	
ephedrine	Pharmaceuticals	C10H15NO	165.11537	166.12265	164.10809	CN[C@@H](C)[C@H](O)c1ccccc1	
fonofos	Pesticides	C10H15OPS2	246.0302	247.03748	245.02292	CCOP(=S)(CC)Sc1ccccc1	
buthidazole	Pesticides	C10H16N4O2S	256.0994	257.10668	255.09212	CN1C[C@H](O)N(C1=O)c1nnc(s1)C(C)(C)C	
cimetidine	Pharmaceuticals	C10H16N6S	252.11572	253.123	251.10844	C\N=C\NCCSCc1[nH]cnc1C)NC#N	
chrysanthemic acid	Metabolites	C10H16O2	168.11503	169.12231	167.10775	CC(C)=C[C@@H]1[C@@H](C(O)=O)C1(C)C	pyrethroids
amantadine	Pharmaceuticals	C10H17N	151.1361	152.14338	150.12882	NC12CC3CC(CC(C3)C1)C2	

amibuzin	Pesticides	C10H18N4O	210.14806	211.15534	209.14078	CN(C)c1nnc(c(=O)n1C(C)(C)C(C)C	
ametridione	Pesticides	C10H18N4O2S	258.11505	259.12233	257.10777	CCSC1=NC(=O)N(CC(C)(C)C)C(=O)N1N	
eucalyptol	PCPs	C10H18O	154.13577	155.14305	153.12849	CC12CCC(CC1)C(C)(C)O2	
prometon	Pesticides	C10H19N5O	225.15896	226.16624	224.15168	COc1nc(NC(C)C)nc(NC(C)C)n1	
terbumeton	Pesticides	C10H19N5O	225.15896	226.16624	224.15168	CCNc1nc(NC(C)(C)C)nc(OC)n1	
amicarbazone	Pesticides	C10H19N5O2	241.15388	242.16116	240.1466	CC(C)C1=NN(C(=O)NC(C)(C)C)C(=O)N1N	
prometryn	Pesticides	C10H19N5S	241.13612	242.1434	240.12884	CSc1nc(NC(C)C)nc(NC(C)C)n1	
terbutryn	Pesticides	C10H19N5S	241.13612	242.1434	240.12884	CCNc1nc(NC(C)(C)C)nc(SC)n1	
malanthion	Pesticides	C10H19O6PS2	330.03607	331.04335	329.02879	CCOC(=O)CC(SP(=S)(OC)OC)C(=O)OCC	
malaoxon	Pesticides	C10H19O7PS	314.05891	315.06619	313.05163	CCOC(=O)CC(SP(=O)(OC)OC)C(=O)OCC	
menthol	PCPs	C10H20O	156.15142	157.1587	155.14414	CC(C)[C@@H]1CC[C@@H](C)C[C@H]1O	
1-decanol	Pesticides	C10H22O	158.16707	159.17435	157.15979	CCCCCCCCCO	
tetraglyme	Industrial Chemicals	C10H22O5	222.14673	223.15401	221.13945	COCCOCCOCCOCCOCC	
2-(octylthio)ethanol	Pesticides	C10H22OS	190.13914	191.14642	189.13186	CCCCCCCCSCO	
cadusafos	Pesticides	C10H23O2PS2	270.08771	271.09499	269.08043	CCOP(=O)(SC(C)C)SC(C)CC	
ethambutol	Pharmaceuticals	C10H24N2O2	204.18378	205.19106	203.1765	CC[C@@H](CO)NCCN[C@@H](CC)CO	
amiton	Pesticides	C10H24NO3PS	269.12145	270.12873	268.11417	CCOP(=O)(OCC)SCCN(CC)CC	
perfluorooctane sulfon	Industrial Chemicals	C10H4F17NO4S	556.95896	557.96624	555.95168	OC(=O)CNS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	
quinoclorac	Pesticides	C10H5Cl2NO2	240.96974	241.97702	239.96246	OC(=O)c1c(Cl)ccc2cc(Cl)cnc12	
chlordane	Pesticides	C10H6Cl8	405.79778	406.80506	404.7905	ClC1CC2C(Cl)C1(C)C(Cl)=C(Cl)C2(Cl)C1(Cl)Cl	
sulfluramid	Pesticides	C10H6F17NO2S	526.98478	527.99206	525.9775	CCNS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	
chinomethionat	Pesticides	C10H6N2OS2	233.99216	234.99944	232.98488	Cc1ccc2nc3SC(=O)Sc3nc2c1	
3-hydroxy anagrelide	Metabolites	C10H7Cl2N3O2	270.99154	271.99882	269.98426	OC1N2Cc3c(NC2=NC1=O)ccc(Cl)c3Cl	anagrelide
thiabendazole	Pharmaceuticals	C10H7N3S	201.03607	202.04335	200.02879	c1nc(cs1)-c1nc2ccccc2[nH]1	
naphthalene	Pesticides	C10H8	128.0626	129.06988	127.05532	c1ccc2ccccc2c1	
brompyrazon	Pesticides	C10H8BrN3O	264.98508	265.99236	263.9778	Nc1cnn(-c2ccccc2)c(=O)c1Br	
chloridazon	Pesticides	C10H8ClN3O	221.03559	222.04287	220.02831	NC1=C(Cl)C(=O)N(N=C1)c1ccccc1	
rufinamide	Pharmaceuticals	C10H8F2N4O	238.06662	239.0739	237.05934	NC(=O)c1cn(Cc2c(F)cccc2F)nn1	
2-naphthalenesulfonic	Industrial Chemicals	C10H8O3S	208.01942	209.0267	207.01214	OS(=O)(=O)C1=CC2=C(C=CC=C2)C=C1	
dimethylphthalate	Pesticides	C10H8O4	192.04226	193.04954	191.03498	Cc1ccc(C([O-])=O)c(C([O-])=O)c1C	
chloranocryl	Pesticides	C10H9Cl2NO	229.00612	230.0134	227.99884	CC(=C)C(=O)Nc1ccc(Cl)c(Cl)c1	
captafol	Pesticides	C10H9Cl4NO2S	346.91081	347.91809	345.90353	ClC(Cl)(Cl)SN1C(=O)C2CC=CCC2C1=O	
tetrachlorvinphos	Pesticides	C10H9Cl4O4P	363.89926	364.90654	362.89198	COP(=O)(OC)OC(=C(Cl)c1cc(Cl)c(Cl)cc1Cl	
thiacloprid	Pesticides	C10H9ClN4S	252.02365	253.03093	251.01637	Clc1ccc(CN2CCS\C2=N/C#N)cn1	
metamitron-desamino	Pesticides	C10H9N3O	187.07457	188.08185	186.06729	CC1=NN=C(C(=O)N1)c1ccccc1	
4-nitroso sulfamethoxaz	Metabolites	C10H9N3O4S	267.03138	268.03866	266.0241	Cc1cc(NS(=O)(=O)c2ccc(cc2)N=O)no1	sulfamethoxazole
4-nitro sulfamethoxaz	Metabolites	C10H9N3O5S	283.02629	284.03357	282.01901	Cc1cc(NS(=O)(=O)c2ccc(cc2)[N+](=[O-])=O)no1	sulfamethoxazole
methoxycinnamate	PCPs	C10H9O3	177.05517	178.06245	176.04789	COc1cccc1\C=C\C([O-])=O	
perfluorocaproic acid	Industrial Chemicals	C10HF19O2	513.96732	514.9746	512.96004	OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	
sulfentrazone	Pesticides	C11H10Cl2F2N4O3S	385.98188	386.98916	384.9746	CC1=NN(C(=O)N1C(F)F)c1cc(NS(C)(=O)=O)c(Cl)cc1Cl	
chlorbufam	Pesticides	C11H10ClNO2	223.04001	224.04729	222.03273	CC(OC(=O)NC1=CC(Cl)=CC=C1)C#C	
benazolin ethyl	Pesticides	C11H10ClNO3S	271.00699	272.01427	269.99971	CCOC(=O)CN1C(=O)Sc2cccc(Cl)c12	
alpha-naphthylthioure	Pesticides	C11H10N2S	202.05647	203.06375	201.04919	NC(=S)Nc1cccc2ccccc12	
sulfapyridine	Pharmaceuticals	C11H11N3O2S	249.0572	250.06448	248.04992	Nc1ccc(cc1)S(=O)(=O)Nc1cccn1	
N4-acetyl sulfathiazole	Metabolites	C11H11N3O3S2	297.02419	298.03147	296.01691	CC(=O)Nc1ccc(cc1)S(=O)(=O)Nc1nccs1	sulfathiazole
thifensulfuron	Pesticides	C11H11N5O6S2	373.01508	374.02236	372.0078	COc1nc(C)nc(NC(=O)NS(=O)(=O)c2ccsc2C(O)=O)n1	
chloramphenicol	Pharmaceuticals	C11H12Cl2N2O5	322.01233	323.01961	321.00505	C1=CC(=CC=C1C(C(CO)NC(=O)C(Cl)Cl)O)[N+](=O)[O-]	
flufenacet OXA	Metabolites	C11H12FNO3	225.08012	226.0874	224.07284	CC(C)N(C(=O)C(O)=O)c1ccc(F)cc1	flufenacet
phenazone	Pharmaceuticals	C11H12N2O	188.09497	189.10225	187.08769	CN1N(C(=O)C=C1C)C1=CC=CC=C1	

ciobutide	Pesticides	C11H12N2O	188.09497	189.10225	187.08769	CC[C@@](C#N)(C(N)=O)c1ccccc1	
levamisol	Pharmaceuticals	C11H12N2S	204.07212	205.0794	203.06484	C1CN2C[C@@H](N=C2S1)c1ccccc1	
sulfamerazine	Pharmaceuticals	C11H12N4O2S	264.0681	265.07538	263.06082	Cc1ccnc(NS(=O)(=O)c2ccc(N)cc2)n1	
sulfamethoxyipyridazin	PCPs	C11H12N4O3S	280.06301	281.07029	279.05573	COc1ccc(NS(=O)(=O)c2ccc(N)cc2)nn1	
ethofumesate-2-keto	Metabolites	C11H12O5S	256.04055	257.04783	255.03327	CC1(C)C(=O)Oc2ccc(OS(C)(=O)=O)cc12	ethofumeaste
MCPB	Pesticides	C11H13ClO3	228.05533	229.06261	227.04805	Cc1cc(Cl)ccc1OCCCC(O)=O	
1-(3-trifluoromethylph	Pharmaceuticals	C11H13F3N2	230.10309	231.11037	229.09581	FC(F)(F)c1cccc(c1)N1CCNCCC1	
ampyrone	Pharmaceuticals	C11H13N3O	203.10587	204.11315	202.09859	CN1N(C(=O)C(N)=C1C)c1ccccc1	
sulfamoxol	PCPs	C11H13N3O3S	267.06777	268.07505	266.06049	Cc1nc(NS(=O)(=O)c2ccc(N)cc2)oc1C	
sulfisoxazole	Pharmaceuticals	C11H13N3O3S	267.06777	268.07505	266.06049	Cc1noc(NS(=O)(=O)c2ccc(N)cc2)c1C	
bentaluron	Pesticides	C11H13N3OS	235.07794	236.08522	234.07066	CC(C)NC(=O)Nc1nc2ccccc2s1	
propachlor OXA	Metabolites	C11H13NO3	207.08955	208.09683	206.08227	CC(C)N(C(=O)C(O)=O)c1ccccc1	propachlor
bendiocarb	Pesticides	C11H13NO4	223.08446	224.09174	222.07718	CNC(=O)Oc1cccc2OC(C)(C)Oc12	
propachlor	Pesticides	C11H14ClNO	211.0764	212.08368	210.06912	CC(C)N(C(=O)CCl)c1ccccc1	
cloethocarb	Pesticides	C11H14ClNO4	259.06114	260.06842	258.05386	CNC(=O)Oc1cccc1O[C@@H](CCl)OC	
flufenacet ESA	Metabolites	C11H14FNO4S	275.06276	276.07004	274.05548	CC(C)N(C(=O)CS(O)(=O)=O)c1ccc(F)cc1	flufenacet
pyrantel	Pharmaceuticals	C11H14N2S	206.08777	207.09505	205.08049	CN1CCCN=C1\C=C\c1cccs1	
butylparaben	PCPs	C11H14O3	194.0943	195.10158	193.08702	CCCCOC(=O)c1ccc(O)cc1	
chlorthiophos	Pesticides	C11H15Cl2O3PS2	359.95773	360.96501	358.95045	CCOP(=S)(OCC)Oc1cc(Cl)c(SC)cc1Cl	
chloreturon	Pesticides	C11H15ClN2O2	242.08221	243.08949	241.07493	CCOc1ccc(NC(=O)N(C)C)cc1Cl	
chlorprazophos	Pesticides	C11H15ClN3O3PS	335.02603	336.03331	334.01875	CCOP(=S)(OCC)Oc1nn2c(C)ccnc2c1Cl	
mephedrone	Pharmaceuticals	C11H15NO	177.11537	178.12265	176.10809	CNC(C)C(=O)c1ccc(C)cc1	
methiocarb	Pesticides	C11H15NO2S	225.08235	226.08963	224.07507	CNC(=O)Oc1cc(C)c(SC)c(C)c1	
propoxur	Pesticides	C11H15NO3	209.1052	210.11248	208.09792	CNC(=O)Oc1cccc1OC(C)C	
methiocarb sulfoxide	Pesticides	C11H15NO3S	241.07727	242.08455	240.06999	CNC(=O)Oc1cc(C)c(C)c1S(C)=O	
propachlor ESA	Metabolites	C11H15NO4S	257.07218	258.07946	256.0649	CC(C)N(C(=O)CS(O)(=O)=O)c1ccccc1	propachlor
proguanil	Pharmaceuticals	C11H16ClN5	253.10943	254.11671	252.10215	CC(C)NC(=N)N(C=N)Nc1ccc(Cl)cc1	
carbophenothion	Pesticides	C11H16ClO2PS3	341.97386	342.98114	340.96658	COP(=S)(OC)SCSC1=CC=C(Cl)C=C1	
2-methyl nicotine	Metabolites	C11H16N2	176.13135	177.13863	175.12407	CN1CCC[C@H]1c1cccn1C	nicotine
benzylpiperazine	Pharmaceuticals	C11H16N2	176.13135	177.13863	175.12407	C(N1CCNCC1)c1ccccc1	
isoproturon-monomer	Pesticides	C11H16N2O	192.12627	193.13355	191.11899	CNC(=O)Nc1ccc(cc1)C(C)C	
aminocarb	Pesticides	C11H16N2O2	208.12118	209.12846	207.1139	CNC(=O)Oc1ccc(N(C)C)c(C)c1	
butylated hydroxyanis	PCPs	C11H16O2	180.11503	181.12231	179.10775	COc1ccc(O)c(c1)C(C)(C)C	
dcoit	Pesticides	C11H17Cl2NOS	281.04079	282.04807	280.03351	CCCCCCCCn1sc(Cl)c(Cl)c1=O	
amiprofos-methyl	Pesticides	C11H17N2O4PS	304.06467	305.07195	303.05739	CO[P@@](S)(NC(C)C)Oc1ccc(C)cc1[N+](O-)=O	
thiopental	Pharmaceuticals	C11H18N2O2S	242.1089	243.11618	241.10162	CCC[C@@H](C)[C@@]1(C)C(C(=O)NC(S)=NC1=O	
pirimicarb	Pesticides	C11H18N4O2	238.14298	239.15026	237.1357	CN(C)C(=O)Oc1nc(nc(C)c1C)N(C)C	
irgarol	Pesticides	C11H19N5S	253.13612	254.1434	252.12884	CSc1nc(NC2CC2)nc(NC(C)(C)C)n1	
ochthilnone	Pesticides	C11H19NOS	213.11874	214.12602	212.11146	CCCCCCCCN1SC=CC1=O	
chlorazine	Pesticides	C11H20ClN5	257.14073	258.14801	256.13345	CCN(CC)c1nc(Cl)nc(n1)N(CC)CC	
2-cyclopentylhexanoic	PCPs	C11H20O2	184.14633	185.15361	183.13905	CCCCC(C1CCCC1)C(O)=O	
cycloate	Pesticides	C11H21NOS	215.13439	216.14167	214.12711	CCSC(=O)N(CC)C1CCCCC1	
methyl nonyl ketone	Pesticides	C11H22O	170.16707	171.17435	169.15979	CCCCCCCCC(C)=O	
butylate	Pesticides	C11H23NOS	217.15004	218.15732	216.14276	CCSC(=O)N(CC(C)C)CC(C)C	
barban	Pesticides	C11H9Cl2NO2	257.00104	258.00832	255.99376	ClCC#CCOC(=O)Nc1cccc(Cl)c1	
cyclanilide	Pesticides	C11H9Cl2NO3	272.99595	274.00323	271.98867	OC(=O)C1(CC1)C(=O)Nc1ccc(Cl)cc1Cl	
diatrizoic acid	Pharmaceuticals	C11H9I3N2O4	613.76964	614.77692	612.76236	CC(=O)NC1=C(I)C(C(O)=O)=C(I)C(NC(C)=O)=C1I	
bethoxazin	Pesticides	C11H9NO2S2	251.00747	252.01475	250.00019	O=S1CCON=C1C1=CC2=CC=CC=C2S1	
biphenyl	Pesticides	C12H10	154.07825	155.08553	153.07097	c1ccc(cc1)-c1ccccc1	

forchlorfenuron	Pesticides	C12H10CIN3O	247.05124	248.05852	246.04396	Clc1cc(NC(=O)Nc2cccc2)ccn1	
azobenzene	Pesticides	C12H10N2	182.0844	183.09168	181.07712	c1ccc(cc1)\N=N\c1ccccc1	
azoxybenzene	Pesticides	C12H10N2O	198.07932	199.0866	197.07204	[O-]\[N+](=N/c1ccccc1)c1ccccc1	
cinoxacin	Pharmaceuticals	C12H10N2O5	262.05897	263.06625	261.05169	CCn1nc(C(O)=O)c(=O)c2cc3OCOc3cc12	
biphenylol	Industrial Chemicals	C12H10O	170.07317	171.08045	169.06589	Oc1ccccc1-c1ccccc1	
2-phenylphenol	Pesticides	C12H10O	170.07317	171.08045	169.06589	Oc1ccccc1-c1ccccc1	
1-naphthylacetic acid	Pesticides	C12H10O2	186.06808	187.07536	185.0608	OC(=O)Cc1cccc2ccccc12	
2-naphthylxyacetic ac	Pesticides	C12H10O3	202.063	203.07028	201.05572	OC(=O)COc1ccc2ccccc2c1	
azaconazole	Pesticides	C12H11Cl2N3O2	299.02284	300.03012	298.01556	Clc1ccc(c(Cl)c1)C1(Cn2cncn2)OCCO1	
propyzamide	Pesticides	C12H11Cl2NO	255.02177	256.02905	254.01449	CC(C)(NC(=O)c1cc(Cl)cc(Cl)c1)C#C	
flupyradifurone	Pesticides	C12H11ClF2N2O2	288.04772	289.055	287.04044	FC(F)CN(Cc1ccc(Cl)nc1)C1=CC(=O)OC1	
furosemide	Pharmaceuticals	C12H11ClN2O5S	330.00772	331.015	329.00044	NS(=O)(=O)C1=CC(C(O)=O)=C(NCC2=CC=CO2)C=C1Cl	
ioxitalamic acid	Pharmaceuticals	C12H11I3N2O5	643.7802	644.78748	642.77292	CC(=O)NC1=C(I)C(C(O)=O)=C(I)C(C(=O)NCCO)=C1I	
1-naphthylacetamide	Pesticides	C12H11NO	185.08407	186.09135	184.07679	NC(=O)Cc1cccc2ccccc12	
carbaryl	Pesticides	C12H11NO2	201.07898	202.08626	200.0717	CNC(=O)Oc1cccc2ccccc12	
1,4-dimethylnaphthale	Pesticides	C12H12	156.0939	157.10118	155.08662	Cc1ccc(C)c2ccccc12	
chlorsulfuron	Pesticides	C12H12ClN5O4S	357.02986	358.03714	356.02258	COc1nc(C)nc(NC(=O)NS(=O)(=O)c2ccccc2Cl)n1	
diquat dibromide	Pesticides	C12H12N2Br2	341.93673	342.94401	340.92945	[Br-].[Br-].C1C[n+](c1)2ccccc2-c2cccc[n+](c1)2	
benzamacril	Pesticides	C12H12N2O2	216.08988	217.09716	215.0826	CN(Cc1ccccc1)\C=C(\C#N)C(O)=O	
dapsone	Pharmaceuticals	C12H12N2O2S	248.06195	249.06923	247.05467	Nc1ccc(cc1)S(=O)(=O)c1ccc(N)cc1	
nalidixic acid	Pharmaceuticals	C12H12N2O3	232.0848	233.09208	231.07752	CCn1cc(C(O)=O)c(=O)c2ccc(C)nc12	
N-acetyl sulfadiazine	Metabolites	C12H12N4O3S	292.06301	293.07029	291.05573	CC(=O)Nc1ccc(cc1)S(=O)(=O)Nc1ncccn1	sulfadiazine
buturon	Pesticides	C12H13ClN2O	236.07164	237.07892	235.06436	CC(C#C)N(C)C(=O)Nc1ccc(Cl)cc1	
pyrimethamine	Pharmaceuticals	C12H13ClN4	248.08288	249.09016	247.0756	CCc1nc(=N)[nH]c(N)c1-c1ccc(Cl)cc1	
pyrimethanil	Pesticides	C12H13N3	199.11095	200.11823	198.10367	Cc1cc(C)nc(Nc2ccccc2)n1	
4-formylaminoantipyri	Metabolites	C12H13N3O2	231.10078	232.10806	230.0935	Cc1c(NC=O)c(=O)n(-c2ccccc2)n1C	dipyrrone
N4-acetyl sulfamethox	Metabolites	C12H13N3O4S	295.06268	296.06996	294.0554	CC(=O)Nc1ccc(cc1)S(=O)(=O)Nc1cc(C)on1	sulfamethoxazole
prontosil	Pharmaceuticals	C12H13N5O2S	291.079	292.08628	290.07172	Nc1ccc(\N=N\c2ccc(cc2)S(N)(=O)=O)c(N)c1	
thifensulfuron-methyl	Pesticides	C12H13N5O6S2	387.03073	388.03801	386.02345	COC(=O)c1sccc1S(=O)(=O)NC(=O)Nc1nc(C)nc(OC)n1	
carboxin	Pesticides	C12H13NO2S	235.0667	236.07398	234.05942	CC1=C(SCCO1)C(=O)Nc1ccccc1	
bromfeninfos	Pesticides	C12H14BrCl2O4P	401.91902	402.9263	400.91174	CCOP(=O)(OCC)OC(=CBr)c1ccc(Cl)cc1Cl	
chlorfeninfos	Pesticides	C12H14Cl3O4P	357.96953	358.97681	356.96225	CCOP(=O)(OCC)OC(=CCl)C1=C(Cl)C=C(Cl)C=C1	
chlorphoxim	Pesticides	C12H14ClN2O3PS	332.01513	333.02241	331.00785	CCOP(=S)(OCC)O\N=C(\C#N)c1ccccc1Cl	
clomazone	Pesticides	C12H14ClNO2	239.07131	240.07859	238.06403	CC1(C)CON(Cc2ccccc2Cl)C1=O	
paraquat	Pesticides	C12H14N2	186.1157	187.12298	185.10842	C[n+](c1)ccc(cc1)-c1cc[n+](c1)cc1	
primidone	Pharmaceuticals	C12H14N2O2	218.10553	219.11281	217.09825	CCC1(C(=O)NCNC1=O)c1ccccc1	
azoluron	Pesticides	C12H14N4O	230.11676	231.12404	229.10948	CCn1nccc1NC(=O)Nc1ccccc1	
sulfadimidine	Pharmaceuticals	C12H14N4O2S	278.08375	279.09103	277.07647	Cc1cc(C)nc(NS(=O)(=O)c2ccc(N)cc2)n1	
sulfamethoxine	Pharmaceuticals	C12H14N4O4S	310.07358	311.08086	309.0663	COc1cc(NS(=O)(=O)c2ccc(N)cc2)nc(OC)n1	
thiophanate-methyl	Pesticides	C12H14N4O4S2	342.04565	343.05293	341.03837	COC(=O)NC(=S)Nc1ccccc1NC(=S)NC(=O)OC	
thien carbazole-methy	Pesticides	C12H14N4O7S2	390.03039	391.03767	389.02311	COC(=O)c1csc(C)c1S(=O)(=O)NC(=O)n1nc(OC)n(C)c1=O	
diethyl phthalate	PCPs	C12H14O4	222.08921	223.09649	221.08193	CCOC(=O)c1ccccc1C(=O)OCC	
thiamphenicol	Pharmaceuticals	C12H15Cl2NO5S	355.0048	356.01208	353.99752	CS(=O)(=O)c1ccc(cc1)[C@@H](O)[C@@H](CO)NC(=O)C(Cl)Cl	
clacyfos	Pesticides	C12H15Cl2O6P	355.99833	357.00561	354.99105	COP(=O)(OC)C(C)OC(=O)COc1ccc(Cl)cc1Cl	
albendazole	Pharmaceuticals	C12H15N3O2S	265.0885	266.09578	264.08122	CCCSc1ccc2[nH]c(NC(=O)OC)nc2c1	
musk xilene	PCPs	C12H15N3O6	297.09609	298.10337	296.08881	CC1=C(C(=C(C(C(=O)N+)([O-])=O)[N+](O)=O)C(C)(C)[N+](O)=O)C(C)(C)C1	
entecavir	Pharmaceuticals	C12H15N5O3	277.11749	278.12477	276.11021	Nc1nc2n(cnc2c(=O)[nH]1)[C@H]1C[C@H](O)[C@@H](CO)C1=C	
carbofuran	Pesticides	C12H15NO3	221.1052	222.11248	220.09792	CNC(=O)OC1=CC=CC2=C1OC(C)(C)C2	
metaxalone	Pharmaceuticals	C12H15NO3	221.1052	222.11248	220.09792	CC1=CC(OCC2CNC(=O)O2)=CC(C)=C1	

orbencarb	Pesticides	C12H16ClNO5	257.06412	258.0714	256.05684	CCN(CC)C(=O)SCc1ccccc1Cl	
carbetamide	Pesticides	C12H16N2O3	236.1161	237.12338	235.10882	CCN(C(=O)[C@H](C)OC(=O)Nc1ccccc1	
azinthos-ethyl	Pesticides	C12H16N3O3PS2	345.03707	346.04435	344.02979	CCOP(=S)(OCC)SCN1N=Nc2ccccc2C1=O	
benfuresate	Pesticides	C12H16O4S	256.07693	257.08421	255.06965	CCS(=O)(=O)Oc1ccc2OCC(C)(C)c2c1	
2,3-dihydro-2-hydroxy-	Metabolites	C12H16O5S	272.07185	273.07913	271.06457	CCS(=O)(=O)Oc1ccc2OC(C)(C)(C)c2c1	ethofumeaste
imipenem	Pharmaceuticals	C12H17N3O4S	299.09398	300.10126	298.0867	C[C@H](O)[C@H]1[C@H]2CC(SCCNC=N)=C(N2C1=O)C(O)=O	
DEET	Pesticides	C12H17NO	191.13102	192.1383	190.12374	CCN(CC)C(=O)c1cccc(C)c1	
N,N-diethyl-3-(hydroxy	Metabolites	C12H17NO2	207.12593	208.13321	206.11865	CCN(CC)C(=O)c1cccc(CO)c1	DEET
dimethenamid-OXA	Metabolites	C12H17NO4S	271.08783	272.09511	270.08055	COCC(C)N(C(=O)C(O)=O)c1c(C)csc1C	dimethenamid
dimethenamid-P	Pesticides	C12H18ClNO2S	275.07468	276.08196	274.0674	COC[C@H](C)N(C(=O)CCl)c1c(C)csc1C	
isoproturon	Pesticides	C12H18N2O	206.14192	207.1492	205.13464	CC(C)c1ccc(NC(=O)N(C)C)cc1	
oryzalin	Pesticides	C12H18N4O6S	346.09471	347.10199	345.08743	CCCN(CCC)c1c(cc(c1[N+])([O-])=O)S(N)(=O)=O[N+])([O-])=O	
butopyronoxyl	Pesticides	C12H18O4	226.12051	227.12779	225.11323	CCCCOC(=O)C1=CC(=O)CC(C)(C)O1	
1,6-dichloro-1,6-dideo-	Industrial Chemicals	C12H19Cl3O8	396.01455	397.02183	395.00727	OCC1OC(OC2(CCl)OC(CCl)C(O)C2O)C(O)C(O)C1Cl	
dimethenamid-ESA	Metabolites	C12H19NO5S2	321.07047	322.07775	320.06319	COCC(C)N(C(=O)CS(O)(=O)=O)c1c(C)csc1C	dimethenamid
sotalol	Pharmaceuticals	C12H20N2O3S	272.11947	273.12675	271.11219	CC(C)NC[C@H](O)c1ccc(NS(C)(=O)=O)cc1	
hexazinone	Pesticides	C12H20N4O2	252.15863	253.16591	251.15135	CN(C)c1nc(=O)n(C2CCCC2)c(=O)n1C	
zanamivir	Pharmaceuticals	C12H20N4O7	332.1332	333.14048	331.12592	CC(=O)N[C@H]1[C@H]2C@H(NC(N)=N)C=C(O[C@H]1[C@H](O)[C@H](O)CO)C(O)=O	
rimantadine	Pharmaceuticals	C12H21N	179.1674	180.17468	178.16012	CC(N)C12CC3CC(C(C3)C1)C2	
diazinon	Pesticides	C12H21N2O3PS	304.10105	305.10833	303.09377	CCOP(=S)(OCC)Oc1cc(C)nc(n1)C(C)C	
butathiofos	Pesticides	C12H21N2O3PS	304.10105	305.10833	303.09377	CCOP(=S)(OCC)Oc1cnc(nc1)C(C)(C)C	
picaridin	Pesticides	C12H23NO3	229.1678	230.17508	228.16052	CCC(C)OC(=O)N1CCCCC1CCO	
decyl dimethyl amine c	PCPs	C12H27NO	201.20927	202.21655	200.20199	CCCCCCCCCN(C)(C)=O	
aspon	Pesticides	C12H28O5P2S2	378.08534	379.09262	377.07806	CCCCOP(=S)(OCCC)OP(=S)(OCCC)OCCC	
fipronil-sulfone	Metabolites	C12H4Cl2F6N4O2S	451.93362	452.9409	450.92634	Nc1c(c(nn1-c1c(Cl)cc(cc1Cl)C(F)(F)F)C#N)S(=O)(=O)C(F)(F)F	fipronil
fipronil	Pesticides	C12H4Cl2F6N4OS	435.93871	436.94599	434.93143	Nc1c(c(nn1-c1c(Cl)cc(cc1Cl)C(F)(F)F)C#N)S(=O)C(F)(F)F	
fipronil-sulfide	Metabolites	C12H4Cl2F6N4S	419.94379	420.95107	418.93651	Nc1c(SC(F)(F)F)c(nn1-c1c(Cl)cc(cc1Cl)C(F)(F)F)C#N	fipronil
2,3,7,8-tetrachlorodib	Industrial Chemicals	C12H4Cl4O2	319.89654	320.90382	318.88926	Clc1cc2Oc3cc(Cl)c(Cl)cc3Oc2cc1Cl	
chlornitrofen	Pesticides	C12H6Cl3NO3	316.94133	317.94861	315.93405	[O-][N+](=O)c1ccc(Oc2c(Cl)cc(Cl)cc2Cl)cc1	
chlorfensulphide	Pesticides	C12H6Cl4N2S	349.90058	350.90786	348.8933	Clc1ccc(S\N=N\c2cc(Cl)c(Cl)cc2Cl)cc1	
bithionol	Pesticides	C12H6Cl4O2S	353.88426	354.89154	352.87698	Oc1c(Cl)cc(Cl)cc1Sc1cc(Cl)cc(Cl)c1O	
fludioxonil	Pesticides	C12H6F2N2O2	248.03974	249.04702	247.03246	FC1(F)Oc2cccc(c2O1)-c1cncc1C#N	
triclosan	PCPs	C12H7Cl3O2	287.95117	288.95845	286.94389	Oc1cc(Cl)ccc1Oc1ccc(Cl)cc1Cl	
chlorfenon	Pesticides	C12H8Cl2O3S	301.95712	302.9644	300.94984	ClC1=CC=C(OS(=O)(=O)C2=CC=C(Cl)C=C2)C=C1	
aldrin	Pesticides	C12H8Cl6	361.87572	362.883	360.86844	ClC1=C(Cl)C2(Cl)C3C4CC(C=C4)C3C1(Cl)C2(Cl)Cl	
aclonifen	Pesticides	C12H9ClN2O3	264.03017	265.03745	263.02289	Nc1c(Cl)c(Oc2ccccc2)ccc1[N+])([O-])=O	
nitazoxanide	Pharmaceuticals	C12H9N3O5S	307.02629	308.03357	306.01901	CC(=O)Oc1ccccc1C(=O)Nc1ncc(s1)[N+])([O-])=O	
acetoprole	Pesticides	C13H10Cl2F3N3O2S	398.98229	399.98957	397.97501	CC(=O)C1=NN(C(N)=C1S(C)=O)C1=C(Cl)C=C(C=C1Cl)C(F)(F)F	
carfentrazone	Pesticides	C13H10Cl2F3N3O3	383.00513	384.01241	381.99785	Cc1nn(-c2cc(CC(Cl)C(O)=O)c(Cl)cc2F)c(=O)n1C(F)F	
diclosulam	Pesticides	C13H10Cl2FN5O3S	404.98655	405.99383	403.97927	CCOc1nc(F)cc2nc(nn12)S(=O)(=O)Nc1c(Cl)cccc1Cl	
chlorbenside	Pesticides	C13H10Cl2S	267.98803	268.99531	266.98075	Clc1ccc(CSc2ccc(Cl)cc2)cc1	
benodanil	Pesticides	C13H10INO	322.98071	323.98799	321.97343	lc1cccc1C(=O)Nc1cccc1	
1-phenyl-1H-benzimid;	PCPs	C13H10N2	194.0844	195.09168	193.07712	c1nc2cccc2n1-c1cccc1	
2-phenylbenzimidazole	PCPs	C13H10N2	194.0844	195.09168	193.07712	c1ccc(cc1)-c1nc2cccc2[nH]1	
thalidomide	Pharmaceuticals	C13H10N2O4	258.06406	259.07134	257.05678	O=C1N(C2CCC(=O)NC2=O)C(=O)c2ccccc12	
benzophenone	PCPs	C13H10O	182.07317	183.08045	181.06589	O=C(c1cccc1)c1cccc1	
2,4-dihydroxybenzoph	Metabolites	C13H10O3	214.063	215.07028	213.05572	Oc1ccc(C(=O)c2ccccc2)c(O)c1	benzophenone
3-phenoxybenzoic acid	Metabolites	C13H10O3	214.063	215.07028	213.05572	OC(=O)C1=CC(OC2=CC=CC=C2)=CC=C1	pyrethroids
R41207	Pesticides	C13H10O3	214.063	215.07028	213.05572	OC(=O)c1cccc(Oc2ccccc2)c1	

2,3,4-trihydroxybenzoic acid	Metabolites	C13H10O4	230.05791	231.06519	229.05063	Oc1ccc(C(=O)c2ccccc2)c(O)c1O	benzophenone
3-(4'-hydroxy)phenoxy	Metabolites	C13H10O4	230.05791	231.06519	229.05063	OC(=O)c1cccc(Oc2ccc(O)cc2)c1	pyrethroids
bromobonil	Pesticides	C13H11Br2NO4	402.90549	403.91277	401.89821	BrC1cc(cc(Br)c1OC(=O)OC[C@H]1CCCCO1)C#N	
tetraconazole	Pesticides	C13H11Cl2F4N3O	371.02153	372.02881	370.01425	FC(F)C(F)(F)OCC(Cn1cncn1)c1ccc(Cl)cc1Cl	
chlozolinat	Pesticides	C13H11Cl2NO5	331.00143	332.00871	329.99415	CCOC(=O)C1(C)OC(=O)N(C1=O)c1cc(Cl)cc(Cl)c1	
clofencet	Pesticides	C13H11ClN2O3	278.04582	279.0531	277.03854	CCC1=C(C(O)=O)C(=O)C=NN1c1ccc(Cl)cc1	
chlorimuron	Pesticides	C13H11ClN4O6S	386.00879	387.01607	385.00151	COc1cc(Cl)nc(NC(=O)NS(=O)(=O)c2ccccc2C(O)=O)n1	
clorophene	PCPs	C13H11ClO	218.04985	219.05713	217.04257	Oc1ccc(Cl)cc1C1ccccc1	
benquinox	Pesticides	C13H11N3O2	241.08513	242.09241	240.07785	O=Nc1ccc(NNC(=O)c2ccccc2)cc1	
oxolinic acid	Pharmaceuticals	C13H11NO5	261.06373	262.07101	260.05645	CCn1cc(C(O)=O)c(=O)c2cc3OCOc3cc12	
bromuconazole	Pesticides	C13H12BrCl2N3O	374.95408	375.96136	373.9468	Clc1ccc(c(Cl)c1)C1(Cn2cncn2)CC(Br)CO1	
fluconazole	Pharmaceuticals	C13H12F2N6O	306.10407	307.11135	305.09679	OC(Cn1cncn1)(Cn1cncn1)c1ccc(F)cc1F	
flazasulfuron	Pesticides	C13H12F3N5O5S	407.05113	408.05841	406.04385	COc1cc(OC)nc(NC(=O)NS(=O)(=O)c2ncccc2C(F)(F)F)n1	
O-desmethyl naproxen	Metabolites	C13H12O3	216.07865	217.08593	215.07137	C[C@H](C(O)=O)c1ccc2cc(O)ccc2c1	naproxen
amisulbrom	Pesticides	C13H13BrFN5O4S2	464.95764	465.96492	463.95036	CN(C)S(=O)(=O)n1cnc(n1)S(=O)(=O)n1c(C)c(Br)c2ccc(F)cc12	
iprodiol	Pesticides	C13H13Cl2N3O3	329.0334	330.04068	328.02612	CC(C)NC(=O)N1CC(=O)N(C1=O)c1cc(Cl)cc(Cl)c1	
cyazofamid	Pesticides	C13H13ClN4O2S	324.04478	325.05206	323.0375	CN(C)S(=O)(=O)n1c(nc(Cl)c1-c1ccc(C)cc1)C#N	
bencarbazone	Pesticides	C13H13F4N5O3S2	427.0396	428.04688	426.03232	CCS(=O)(=O)Nc1cc(c(F)cc1C(N)=S)-n1nc(n(C)c1=O)C(F)(F)F	
ceftizoxime	Pharmaceuticals	C13H13N5O5S2	383.03581	384.04309	382.02853	CO\N=C(/C(=O)N[C@H]1[C@H]2SCC=C(N2C1=O)C(O)=O)c1csc(N)n1	
1-salicylate glucuronide	Metabolites	C13H14O9	314.06379	315.07107	313.05651	O[C@@H]1[C@@H](O)[C@H](O)[C@H](Oc2ccccc2C(O)=O)O[C@@H]1	salicylic acid
penconazole	Pesticides	C13H15Cl2N3	283.06431	284.07159	282.05703	CCCC(Cn1cncn1)c1ccc(Cl)cc1Cl	
4-acetamidoantipyrin	Metabolites	C13H15N3O2	245.11643	246.12371	244.10915	CC(=O)Nc1c(C)n(C)n(-c2ccccc2)c1=O	metamizole
imazapyr	Pesticides	C13H15N3O3	261.11134	262.11862	260.10406	COCc1cnc(C2=NC(C)(C(C)C(=O)N2)c(c1)C(O)=O	
esketamine	Pharmaceuticals	C13H16ClNO	237.09205	238.09933	236.08477	CN[C@@]1(CCCCC1=O)c1ccccc1Cl	
benfluralin	Pesticides	C13H16F3N3O4	335.10929	336.11657	334.10201	CCCCN(CC)c1c(cc(cc1[N+])([O-])=O)C(F)(F)F)[N+])([O-])=O	
2',3'-di-o-acetyl-5'-deoxy	Metabolites	C13H16FN3O6	329.10232	330.1096	328.09504	C[C@H]1O[C@H]([C@H]([C@H](OC(C)=O)[C@@H]1OC(C)=O)n1cc(F)capecitabine	
azimsulfuron	Pesticides	C13H16N10O5S	424.10259	425.10987	423.09531	COC1cc(OC)nc(NC(=O)NS(=O)(=O)c2c(cnn2C)-c2nnn(C)n2)n1	
ibuprofen carboxylic acid	Metabolites	C13H16O4	236.10486	237.11214	235.09758	CC(Cc1ccc(cc1)C(C)C(O)=O)C(O)=O	ibuprofen
trinexapac-ethyl	Pesticides	C13H16O5	252.09978	253.10706	251.0925	CCOC(=O)C1CC(=O)C(=C(C2CC2)O)C(=O)C1	
moclobemide	Pharmaceuticals	C13H17ClN2O2	268.09786	269.10514	267.09058	Clc1ccc(cc1)C(=O)NCCN1CCOCC1	
chlorprocarb	Pesticides	C13H17ClN2O4	300.08769	301.09497	299.08041	CC[C@@H](CC)NC(=O)Oc1cccc(NC(=O)OC)c1	
aminophenazone	Pharmaceuticals	C13H17N3O	231.13717	232.14445	230.12989	CN(C)C1=C(C)N(C)N(C1=O)c1ccccc1	
dioxoaminopyrine	Pharmaceuticals	C13H17N3O3	263.12699	264.13427	262.11971	CN(C)C(=O)C(=O)N(N(C)C(C)=O)c1ccccc1	
aztreonam	Pharmaceuticals	C13H17N5O8S2	435.05186	436.05914	434.04458	C[C@H]1[C@H](NC(=O)C(=N/OC(C)(C)C(O)=O)\c2csc([NH3+])n2)C(=O)N1S([O-])(=O)=O	
crotamiton	Pharmaceuticals	C13H17NO	203.13102	204.1383	202.12374	CCN(C(=O)C=CC)c1ccccc1C	
ritalinic acid	Pharmaceuticals	C13H17NO2	219.12593	220.13321	218.11865	OC(=O)C(C1CCCCN1)c1ccccc1	
dimethachlor OXA	Metabolites	C13H17NO4	251.11576	252.12304	250.10848	COCCN(C(=O)C(O)=O)c1c(C)cccc1C	dimethachlor
2-[glycoloyl(2-methoxy	Metabolites	C13H17NO5	267.11068	268.11796	266.1034	COCCN(C(=O)CO)c1c(C)cccc1C(O)=O	dimethachlor
bupropion	Pharmaceuticals	C13H18ClNO	239.1077	240.11498	238.10042	CC(NC(C)(C)C)C(=O)c1ccccc1Cl	
dimethachlor	Pesticides	C13H18ClNO2	255.10261	256.10989	254.09533	COCCN(C(=O)CC)c1c(C)cccc1C	
cisanilide	Pesticides	C13H18N2O	218.14192	219.1492	217.13464	CC1CCC(C)N1C(=O)Nc1ccccc1	
lenacil	Pesticides	C13H18N2O2	234.13683	235.14411	233.12955	O=C1NC2=C(CCC2)C(=O)N1C1CCCCC1	
pentoxifylline	Pharmaceuticals	C13H18N4O3	278.13789	279.14517	277.13061	CC(=O)CCCCn1c(=O)n(C)c2nnc(C)c2c1=O	
ibuprofen	Pharmaceuticals	C13H18O2	206.13068	207.13796	205.1234	CC(C)Cc1ccc(cc1)C(C)C(O)=O	
2-hydroxy ibuprofen	Metabolites	C13H18O3	222.1256	223.13288	221.11832	CC(C(O)=O)c1ccc(CC(C)(C)O)cc1	ibuprofen
ethofumesate	Pesticides	C13H18O5S	286.0875	287.09478	285.08022	CCOC1Oc2ccc(OS(C)=O)(=O)cc2C1(C)C	
anilofos	Pesticides	C13H19ClNO3PS2	367.02325	368.03053	366.01597	COP(=S)(OC)SCC(=O)N(C(C)C)c1ccc(Cl)cc1	
pendimethalin	Pesticides	C13H19N3O4	281.13756	282.14484	280.13028	CCC(CC)Nc1c(cc(C)C(C)c1[N+])([O-])=O)[N+])([O-])=O	
dimethachlor ESA	Metabolites	C13H19NO5S	301.0984	302.10568	300.09112	COCCN(C(=O)CS(O)(=O)=O)c1c(C)cccc1C	dimethachlor

prilocaine	Pharmaceuticals	C13H20N2O	220.15757	221.16485	219.15029	CCCN(C)C(=O)Nc1cccc1C	
butamifos	Pesticides	C13H21N2O4PS	332.09597	333.10325	331.08869	CCO[P@](=S)(N[C@H](C)CC)Oc1cc(C)ccc1[N+](O)=O	
salbutamol	Pharmaceuticals	C13H21NO3	239.15215	240.15943	238.14487	CC(C)(C)NCC(O)c1ccc(O)c(CO)c1	
trolamine salicylate	PCPs	C13H21NO6	287.13689	288.14417	286.12961	OCCN(CCO)CCO.OC(=O)c1cccc1O	
N-benzyl-N,N-dimethyl	PCPs	C13H22CIN	227.14408	228.15136	226.1368	[Cl-].CCCC[N+](C)(C)Cc1cccc1	
ranitidine	Pharmaceuticals	C13H22N4O3S	314.14126	315.14854	313.13398	CN\C(NCCSCC1=CC=C(CN(C)C)O1)=C/[N+](O)=O	
ranitidine-N-oxide	Pharmaceuticals	C13H22N4O4S	330.13618	331.14346	329.1289	CN\C(NCCSCc1ccc(CN(C)C)=O)O1)=C/[N+](O)=O	
fenamiphos	Pesticides	C13H22NO3PS	303.1058	304.11308	302.09852	CCOP(=O)(NC(C)C)Oc1ccc(SC)c(C)C1	
timolol	Pharmaceuticals	C13H24N4O3S	316.15691	317.16419	315.14963	CC(C)(C)NCC(O)COC1=NSN=C1N1CCOCC1	
bupirimate	Pesticides	C13H24N4O3S	316.15691	317.16419	315.14963	CCCCC1=C(C)N=C(NCC)N=C1OS(=O)(=O)N(C)C	
hexachlorophene	PCPs	C13H6Cl6O2	403.8499	404.85718	402.84262	Oc1c(Cl)cc(Cl)c(Cl)c1Cc1c(O)c(Cl)cc(Cl)c1Cl	
bromofenoxim	Pesticides	C13H7Br2N3O6	458.87016	459.87744	457.86288	[O-][N+](=O)C1=CC(=C(ONC=C2C=C(Br)C(=O)C(Br)=C2)C=C1)[N+](O)=O	
bifenox acid	Pesticides	C13H7Cl2NO5	326.97013	327.97741	325.96285	OC(=O)C1=CC(OC2=CC=C(C)C=C2Cl)=CC=C1[N+](O)=O	
pyraflufen-ethyl	Pesticides	C13H9Cl2F3N2O4	383.98915	384.99643	382.98187	CCOC(=O)COC1cc(-c2nn(C)c(OC(F)F)c2Cl)c(F)cc1Cl	
chlomethoxyfen	Pesticides	C13H9Cl2NO4	312.99087	313.99815	311.98359	COC1=C(C=CC(OC2=C(C)C=C(C)C=C2)=C1)[N+](O)=O	
triclocarban	PCPs	C13H9Cl3N2O	313.97805	314.98533	312.97077	O\C(Nc1ccc(Cl)cc1)=N/c1ccc(Cl)c(Cl)c1	
chlorfenazole	Pesticides	C13H9ClN2	228.04543	229.05271	227.03815	Clc1cccc1-c1nc2cccc2[nH]1	
tritosulfuron	Pesticides	C13H9F6N5O4S	445.02795	446.03523	444.02067	COc1nc(NC(=O)NS(=O)(=O)c2cccc2C(F)(F)F)nc(n1C(F)(F)F	
4-fluoro-3-phenoxyber	Metabolites	C13H9FO3	232.05358	233.06086	231.0463	OC(=O)c1ccc(F)c(Oc2cccc2)c1	cyfluthrin
anthracene oil	Pesticides	C14H10	178.07825	179.08553	177.07097	c1ccc2cc3cccc3cc2c1	
bromazepam	Pharmaceuticals	C14H10BrN3O	315.00073	316.00801	313.99345	BrC1ccc2NC(=O)CN=C(c3ccccc3)c2c1	
flufenamic acid	Pharmaceuticals	C14H10F3NO2	281.06637	282.07365	280.05909	OC(=O)c1cccc1Nc1cccc(c1)C(F)(F)F	
4,4'-dinitro-2,2'-stilben	Industrial Chemicals	C14H10N2O10S2	429.97769	430.98497	428.97041	OS(=O)(=O)c1cc(ccc1C=Cc1ccc(cc1S(O)(=O)=O)N(=O)=O)N(=O)=O	
halauxifen-methyl	Pesticides	C14H11Cl2FN2O3	344.01308	345.02036	343.0058	COC(=O)c1nc(cc(N)c1Cl)-c1ccc(Cl)c(OC)c1F	
diclofenac	Pharmaceuticals	C14H11Cl2NO2	295.01669	296.02397	294.00941	OC(=O)Cc1cccc1Nc1c(Cl)cccc1Cl	
4-hydroxy diclofenac	Metabolites	C14H11Cl2NO3	311.0116	312.01888	310.00432	OC(=O)Cc1cccc1Nc1c(Cl)cc(O)cc1Cl	aceclofenac
chlorazifop	Pesticides	C14H11Cl2NO4	327.00652	328.0138	325.99924	C[C@@H](Oc1ccc(Oc2ncc(Cl)cc2Cl)cc1)C(O)=O	
clodinafop	Pesticides	C14H11ClFNO4	311.03607	312.04335	310.02879	C[C@@H](Oc1ccc(Oc2ncc(Cl)cc2F)cc1)C(O)=O	
chlortalidone	Pharmaceuticals	C14H11ClN2O4S	338.01281	339.02009	337.00553	NS(=O)(=O)c1cc(ccc1Cl)C1(O)NC(=O)c2cccc12	
iminostilbene	Pharmaceuticals	C14H11N	193.08915	194.09643	192.08187	N1c2cccc2C=Cc2cccc12	
chlorfenethol	Pesticides	C14H12Cl2O	266.02652	267.0338	265.01924	CC(O)(c1ccc(Cl)cc1)c1ccc(Cl)cc1	
tolfenamic acid	Pharmaceuticals	C14H12ClNO2	261.05566	262.06294	260.04838	CC1=C(C=CC=C1Cl)NC2=CC=CC=C2C(=O)O	
sulfaquinoxaline	PCPs	C14H12N4O2S	300.0681	301.07538	299.06082	Nc1ccc(cc1)S(=O)(=O)N=c1/cnc2cccc2[nH]1	
benzyl benzoate	Pesticides	C14H12O2	212.08373	213.09101	211.07645	O=C(OCc1cccc1)c1cccc1	
oxybenzone	PCPs	C14H12O3	228.07865	229.08593	227.07137	COc1ccc(C(=O)c2cccc2)c(O)c1	
trans-resveratrol	Pharmaceuticals	C14H12O3	228.07865	229.08593	227.07137	Oc1ccc(\C=C\Cc2cc(O)cc(O)c2)cc1	
dioxybenzone	PCPs	C14H12O4	244.07356	245.08084	243.06628	COc1ccc(C(=O)c2cccc2O)c(O)c1	
sulisobenzene	PCPs	C14H12O6S	308.03546	309.04274	307.02818	COc1cc(O)c(cc1S(O)(=O)=O)C(=O)c1cccc1	
metosulam	Pesticides	C14H13Cl2N5O4S	417.00653	418.01381	415.99925	OCc1cc(OC)n2nc(nc2n1)S(=O)(=O)Nc1c(Cl)ccc(C)c1Cl	
sulcotrione	Pesticides	C14H13ClO5S	328.01723	329.02451	327.00995	CS(=O)(=O)c1ccc(C(=O)C2C(=O)CCCC2=O)c(Cl)c1	
pyroxulam	Pesticides	C14H13F3N6O5S	434.06203	435.06931	433.05475	COc1cc(OC)n2nc(NS(=O)(=O)c3c(OC)nccc3C(F)(F)F)nc2n1	
flufenacet	Pesticides	C14H13F4N3O2S	363.06646	364.07374	362.05918	CC(C)N(C(=O)COC1nnc(s1)C(F)(F)F)c1ccc(F)cc1	
mepanipyrim	Pesticides	C14H13N3	223.11095	224.11823	222.10367	CC#Cc1cc(C)nc(Nc2cccc2)n1	
cefdinir	Pharmaceuticals	C14H13N5O5S2	395.03581	396.04309	394.02853	NC1=NC(=CS1)C(=N\O)\C(=O)N[C@H]1[C@H]2SCC(C=C)=C(N2C1=O)C(O)=O	
mesotrione	Pesticides	C14H13NO7S	339.04128	340.04856	338.034	CS(=O)(=O)c1ccc(C(=O)C2C(=O)CCCC2=O)c(c1)[N+](O)=O	
imazalil	Pesticides	C14H14Cl2N2O	296.04832	297.0556	295.04104	Clc1ccc(C(Cn2ccnc2)OCC=C(C)Cl)c1	
azothoate	Pesticides	C14H14ClN2O3PS	356.01513	357.02241	355.00785	COP(=S)(OC)Oc1ccc(cc1)\N=N\c1ccc(Cl)cc1	
ticlopidine	Pharmaceuticals	C14H14ClNS	263.05355	264.06083	262.04627	Clc1cccc1CN1CCc2sccc2C1	
cefazolin	Pharmaceuticals	C14H14N8O4S3	454.03002	455.0373	453.02274	Cc1nnc(SCC2=C(N3[C@H](SC2)[C@H](NC(=O)Cn2cnnn2)C3=O)C(O)=O)s1	

naproxen	Pharmaceuticals	C14H14O3	230.0943	231.10158	229.08702	COC1ccc2cc(ccc2c1)[C@H](C)C(O)=O	
2,2-dihydroxy-4-methc	Metabolites	C14H14O4	246.08921	247.09649	245.08193	COC1=CC(O)(O)C(C=C1)C(=O)c1ccccc1	benzophenone
bromoxynil heptanoate	Pesticides	C14H15Br2NO2	386.94696	387.95424	385.93968	CCCCCCC(=O)Oc1c(Br)cc(cc1Br)C#N	
prothioconazole-desth	Pesticides	C14H15Cl2N3O	311.05922	312.0665	310.05194	OC(Cc1ccccc1Cl)(Cn1cncn1)C1(Cl)CC1	
cyprodinil	Pesticides	C14H15N3	225.1266	226.13388	224.11932	Cc1cc(nc(Nc2ccccc2)n1)C1CC1	
metazachlor OXA	Metabolites	C14H15N3O3	273.11134	274.11862	272.10406	Cc1cccc(C)c1N(Cn1cccn1)C(=O)C(O)=O	metazachlor
metsulfuron-methyl	Pesticides	C14H15N5O6S	381.07431	382.08159	380.06703	COC(=O)c1ccccc1S(=O)(=O)NC(=O)Nc1nc(C)nc(OC)n1	
tribenuron	Pesticides	C14H15N5O6S	381.07431	382.08159	380.06703	COC1nc(C)nc(n1)N(C)C(=O)NS(=O)(=O)c1ccccc1C(O)=O	
zoxamide	Pesticides	C14H16Cl3NO2	335.02467	336.03195	334.01739	CCC(C)NC(=O)c1cc(Cl)c(C)C(Cl)c1)C(=O)CCl	
metazachlor	Pesticides	C14H16ClN3O	277.09819	278.10547	276.09091	Cc1cccc(C)c1N(Cn1cccn1)C(=O)CCl	
triadimefon	Pesticides	C14H16ClN3O2	293.09311	294.10039	292.08583	CC(C)C(C)C(=O)C(OC1=CC=C(C)C=C1)N1C=NC=N1	
triasulfuron	Pesticides	C14H16ClN5O5S	401.05607	402.06335	400.04879	COC1=NC(C)=NC(NC(=O)NS(=O)(=O)C2=CC=CC=C2OCCCl)=N1	
N4-acetylsulfamethazil	Metabolites	C14H16N4O3S	320.09431	321.10159	319.08703	C\C(O)=N/c1ccc(cc1)S(=O)(=O)Nc1nc(C)cc(C)n1	sulfamethazine
N4-acetylsulfadimetho	Metabolites	C14H16N4O5S	352.08414	353.09142	351.07686	COC1cc(OC)nc(NS(=O)(=O)c2ccc(cc2)\N=C(C)/C)O)n1	sulfadimethoxine
ethaboxam	Pesticides	C14H16N4OS2	320.07656	321.08384	319.06928	CCNc1nc(CC)c(s1)C(=O)NC(C#N)c1cccs1	
fenhexamid	Pesticides	C14H17Cl2NO2	301.06364	302.07092	300.05636	CC1(CCCCC1)C(=O)Nc1ccc(O)c(Cl)c1Cl	
imazapic	Pesticides	C14H17N3O3	275.12699	276.13427	274.11971	CC(C)C1(C)N=C(NC1=O)c1ncc(C)cc1C(O)=O	
metazachlor ESA	Metabolites	C14H17N3O4S	323.09398	324.10126	322.0867	Cc1cccc(C)c1N(Cn1cccn1)C(=O)CS(O)(=O)=O	metazachlor
rimsulfuron	Pesticides	C14H17N5O7S2	431.05694	432.06422	430.04966	CCS(=O)(=O)c1cccn1S(=O)(=O)NC(=O)Nc1nc(OC)cc(OC)n1	
acetaminophen glucur	Metabolites	C14H17NO8	327.09542	328.1027	326.08814	CC(=O)Nc1ccc(O[C@@H]2O[C@@H]([C@@H](O)[C@H](O))C(=O)Nc1ccc(O[C@@H]2O)[C@@H](O))C(=O)N	acetaminophen
triadimenol	Pesticides	C14H18ClN3O2	295.10876	296.11604	294.10148	CC(C)C(C)C(O)C(OC1ccc(Cl)cc1)n1cncn1	
methyl D-α-aspartyl-D-	Industrial Chemicals	C14H18N2O5	294.12157	295.12885	293.11429	COC(=O)[C@@H](Cc1ccccc1)NC(=O)[C@H](N)CC(O)=O	
trimethoprim	Pharmaceuticals	C14H18N4O3	290.13789	291.14517	289.13061	COC1cc(Cc2c[nH]c(N)=N)[nH]c2=N)cc(OC)c1OC	
benomyl	Pesticides	C14H18N4O3	290.13789	291.14517	289.13061	CCCCNC(=O)n1c(NC(=O)OC)nc2ccccc12	
thiophanate	Pesticides	C14H18N4O4S2	370.07695	371.08423	369.06967	CCOC(=O)NC(=S)Nc1ccccc1NC(=S)NC(=O)OCC	
abacavir	Pharmaceuticals	C14H18N6O	286.15421	287.16149	285.14693	Nc1nc(NC2CC2)c2ncn([C@@H]3C[C@H](CO)C=C3)c2n1	
cinoxate	PCPs	C14H18O4	250.12051	251.12779	249.11323	CCOCCOC(=O)C=C\c1ccc(OC)cc1	
debacarb	Pesticides	C14H19N3O4	293.13756	294.14484	292.13028	CCOCCOCCOC(=O)Nc1nc2ccccc2[nH]1	
metolachlor morpholin	Metabolites	C14H19NO2	233.14158	234.14886	232.1343	CCc1cccc(C)c1N1C(C)COCC1=O	metolachlor
alachlor OXA	Metabolites	C14H19NO4	265.13141	266.13869	264.12413	CCc1cccc(CC)c1N(COC)C(=O)C(O)=O	alachlor
alachlor	Pesticides	C14H20ClNO2	269.11826	270.12554	268.11098	CCC1=CC=CC(CC)=C1N(COC)C(=O)CCl	
acetochlor	Pesticides	C14H20ClNO2	269.11826	270.12554	268.11098	CCOCN(C(=O)CCl)c1c(C)cccc1CC	
heptylparaben	PCPs	C14H20O3	236.14125	237.14853	235.13397	CCCCCOC(=O)c1ccc(O)cc1	
butralin	Pesticides	C14H21N3O4	295.15321	296.16049	294.14593	CCC(C)NC1=C(C=C(C=C1[N+])([O-])=O)C(C)(C)[N+])([O-])=O	
N-desmethyl meptazin	Metabolites	C14H21NO	219.16232	220.1696	218.15504	CCC1(CCCNC1)c1cccc(O)c1	meptazinol
padimate A	PCPs	C14H21NO2	235.15723	236.16451	234.14995	CC(C)CCOC(=O)c1ccc(cc1)N(C)C	
atenolol acid	Pharmaceuticals	C14H21NO4	267.14706	268.15434	266.13978	CC(C)NCC(O)COC1ccc(CC(O)=O)cc1	
acetochlor ESA	Metabolites	C14H21NO5S	315.11405	316.12133	314.10677	CCOCN(C(=O)CS(O)(=O)=O)c1c(C)cccc1CC	acetochlor
alachlor ESA	Metabolites	C14H21NO5S	315.11405	316.12133	314.10677	CCc1cccc(CC)c1N(COC)C(=O)CS(O)(=O)=O	alachlor
prosulfocarb	Pesticides	C14H21NOS	251.13439	252.14167	250.12711	CCCN(CCC)C(=O)SCc1ccccc1	
metoclopramide	Pharmaceuticals	C14H22ClN3O2	299.14006	300.14734	298.13278	CCN(CC)CCNC(=O)c1cc(Cl)c(N)cc1OC	
lignocaine	Pharmaceuticals	C14H22N2O	234.17322	235.1805	233.16594	CCN(CC)CC(=O)NC1=C(C)C=CC=C1C	
rac-rivastigmine	Pharmaceuticals	C14H22N2O2	250.16813	251.17541	249.16085	CCN(C)C(=O)Oc1cccc(c1)C(C)N(C)C	
atenolol	Pharmaceuticals	C14H22N2O3	266.16305	267.17033	265.15577	CC(C)NCC(O)COC1ccc(CC(N)=O)cc1	
valganciclovir	Pharmaceuticals	C14H22N6O5	354.16517	355.17245	353.15789	CC(C)[C@H](N)C(=O)OCC(CO)OCn1cnc2c1NC(N)=NC2=O	
oseltamivir acid	Metabolites	C14H24N2O4	284.17361	285.18089	283.16633	CCC(CC)O[C@H](N)C(=O)C(C[C@H](N)[C@H]1NC(C)=O)C(O)=O	oseltamivir
spectinomycin	Pharmaceuticals	C14H24N2O7	332.15835	333.16563	331.15107	CN[C@@H]1[C@H](O)[C@H](NC)[C@H]2O[C@]3(O)[C@@H](O[C@H](C)CC3=O)O[C@@H]2[C@H]	
bensulide	Pesticides	C14H24NO4PS3	397.06051	398.06779	396.05323	CC(C)OP(=S)(OC(C)C)SCCN(S(=O)(=O)c1ccccc1	
(4R,7S)-2,4,7,9-tetram	Industrial Chemicals	C14H26O2	226.19328	227.20056	225.186	CC(C)C[C@@](C)(O)C#C[C@@](C)(O)CC(C)C	

teflubenzuron	Pesticides	C14H6Cl2F4N2O2	379.97425	380.98153	378.96697	Fc1cccc(F)c1C(=O)NC(=O)Nc1cc(Cl)c(F)c(Cl)c1F	
bromethalin	Pesticides	C14H7Br3F3N3O4	574.79388	575.80116	573.7866	CN(C1=C(Br)C=C(Br)C=C1Br)C1=C(C=C(C=C1C(F)(F)F)[N+])([O-])O[N+](O-)=O	
acifluorfen	Pesticides	C14H7ClF3NO5	360.99649	362.00377	359.98921	OC(=O)c1cc(Oc2ccc(cc2Cl)C(F)(F)F)ccc1[N+](O-)=O	
clofentezine	Pesticides	C14H8Cl2N4	302.01261	303.01989	301.00533	Clc1cccc1-c1nnc(nn1)-c1cccc1Cl	
anthraquinone	Pesticides	C14H8O2	208.05243	209.05971	207.04515	O=C1c2cccc2C(=O)c2cccc12	
bifenox	Pesticides	C14H9Cl2NO5	340.98578	341.99306	339.9785	COC(=O)c1cc(Oc2ccc(Cl)cc2Cl)ccc1[N+](O-)=O	
1-(4-chlorophenyl)-3-(4-chlorophenyl)-1H-1,2,4-triazole	Pesticides	C14H9Cl3N2O2	341.97296	342.98024	340.96568	Clc1ccc(NC(=O)NC(=O)c2c(Cl)cccc2Cl)cc1	
triclabendazole	Pesticides	C14H9Cl3N2O5	357.95012	358.9574	356.94284	CSc1nc2cc(Cl)c(Oc3cccc(Cl)c3Cl)cc2n1	
dicofol	Pesticides	C14H9Cl5O	367.90961	368.91689	366.90233	OC(c1ccc(Cl)cc1)(c1ccc(Cl)cc1)C(Cl)(Cl)Cl	
diflubenzuron	Pesticides	C14H9ClF2N2O2	310.03206	311.03934	309.02478	Fc1cccc(F)c1C(=O)NC(=O)Nc1ccc(Cl)cc1	
efavirenz	Pharmaceuticals	C14H9ClF3NO2	315.02739	316.03467	314.02011	OC1=Nc2ccc(Cl)cc2[C@@H](O1)(C#CC1CC1)C(F)(F)F	
chlorfluren	Pesticides	C14H9ClO2	244.02911	245.03639	243.02183	OC(=O)[C@H]1c2cccc2-c2ccc(Cl)cc12	
chlorflurenol	Pesticides	C14H9ClO3	260.02403	261.03131	259.01675	OC(=O)[C@H]1(O)c2cccc2-c2ccc(Cl)cc12	
2,6-dichloro-N-((4-(trifluoromethyl)phenyl)amino)-2-methylpropanamide	Pesticides	C15H10Cl2F3NO	347.00916	348.01644	346.00188	FC(F)(F)c1ccc(CNC(=O)c2c(Cl)cccc2Cl)cc1	
lorazepam	Pharmaceuticals	C15H10Cl2N2O2	320.01194	321.01922	319.00466	OC1N=C(c2cccc2Cl)c2cc(Cl)ccc2NC1=O	
genistein	Pharmaceuticals	C15H10O5	270.05283	271.06011	269.04555	Oc1ccc(cc1)-c1coc2cc(O)cc(O)c2c1=O	
chlorfenapyr	Pesticides	C15H11BrClF3N2O	405.96954	406.97682	404.96226	CCOCn1c(c(C#N)c(Br)c1C(F)(F)F)-c1ccc(Cl)cc1	
oxyfluorfen	Pesticides	C15H11ClF3NO4	361.03287	362.04015	360.02559	CCOC1cc(Oc2ccc(cc2Cl)C(F)(F)F)ccc1[N+](O-)=O	
oxazepam	Pharmaceuticals	C15H11ClN2O2	286.05091	287.05819	285.04363	O[C@H]1N=C(c2cccc2)c2cc(Cl)ccc2NC1=O	
chlorfluren methyl	Pesticides	C15H11ClO2	258.04476	259.05204	257.03748	COC(=O)[C@H]1c2cccc2-c2ccc(Cl)cc12	
chlorflurenol methyl	Pesticides	C15H11ClO3	274.03968	275.04696	273.0324	COC(=O)[C@H]1(O)c2cccc2-c2ccc(Cl)cc12	
diclofop	Pesticides	C15H12Cl2O4	326.01127	327.01855	325.00399	CC(Oc1ccc(Oc2ccc(Cl)cc2Cl)cc1)C(O)=O	
diflufenzopyr	Pesticides	C15H12F2N4O3	334.08775	335.09503	333.08047	C\C(=N/NC(=O)Nc1cc(F)cc(F)c1)c1Ncccc1C(O)=O	
fluzazifop	Pesticides	C15H12F3NO4	327.07185	328.07913	326.06457	[C@H](O)(Cc1ccc(Oc2ccc(nc2)C(F)(F)F)cc1)C(O)=O	
isoxaflutole	Pesticides	C15H12F3NO4S	359.04392	360.0512	358.03664	CS(=O)(=O)c1cc(ccc1C(=O)c1cnoc1C1CC1)C(F)(F)F	
carbamazepine	Pharmaceuticals	C15H12N2O	236.09497	237.10225	235.08769	NC(=O)N1c2cccc2C=Cc2cccc12	
2-hydroxy carbamazep	Metabolites	C15H12N2O2	252.08988	253.09716	251.0826	OC(=N)N1c2cccc2C=Cc2cc(O)ccc12	carbamazepine
oxcarbazepine	Pharmaceuticals	C15H12N2O2	252.08988	253.09716	251.0826	NC(=O)N1c2cccc2CC(=O)c2cccc12	
phenytoin	Pharmaceuticals	C15H12N2O2	252.08988	253.09716	251.0826	OC1=NC(C(O)=N1)(c1cccc1)c1cccc1	
3-hydroxy carbamazep	Metabolites	C15H12N2O2	252.08988	253.09716	251.0826	NC(=O)N1c2cccc2C=Cc2ccc(O)cc12	carbamazepine
carbamazepine-10, 11-	Metabolites	C15H12N2O2	252.08988	253.09716	251.0826	NC(=O)N1c2cccc2C2OC2c2cccc12	carbamazepine
azafenidin	Pesticides	C15H13Cl2N3O2	337.03849	338.04577	336.03121	Clc1cc(Cl)c(cc1OCC#C)N1N=C2CCCCN2C1=O	
clofop	Pesticides	C15H13ClO4	292.05024	293.05752	291.04296	CC(Oc1ccc(Oc2ccc(Cl)cc2)cc1)C(O)=O	
carfentrazone-ethyl	Pesticides	C15H14Cl2F3N3O3	411.03643	412.04371	410.02915	CCOC(=O)[C@H](Cl)Cc1cc(c(F)cc1Cl)-n1nc(C)n(C(F)F)c1=O	
ceftaclor	Pharmaceuticals	C15H14ClN3O4S	367.03936	368.04664	366.03208	N[C@H](C(=O)N[C@H]1[C@H]2SCC(Cl)=C(N2C1=O)C(O)=O)c1cccc1	
clopidogrel carboxylic acid	Metabolites	C15H14ClNO2S	307.04338	308.05066	306.0361	CN1[C@H](C@H]1[C@H]2CC[C@H]1[C@H](C@H](C2)OC(=O)c1cccc1	clopidogrel
chlorazate	Pesticides	C15H14ClNO3	291.06622	292.0735	290.05894	CCn1c(C)cc(=O)c(C(O)=O)c1-c1ccc(Cl)cc1	
10,11-trans-dihydroxy-carbamazepine	Metabolites	C15H14N2O3	270.10045	271.10773	269.09317	O[C@H]1[C@H](O)c2cccc2N(C(O)=N)c2cccc12	carbamazepine
carbamazepine-10,11-dihydroxy	Metabolites	C15H14N2O3	270.10045	271.10773	269.09317	NC(=O)N1c2cccc2[C@@H](O)[C@H](O)c2cccc12	carbamazepine
nevirapine	Pharmaceuticals	C15H14N4O	266.11676	267.12404	265.10948	Cc1cnc2N(C3CC3)c3ncccc3C(=O)Nc12	
sulfaphenazole	PCPs	C15H14N4O2S	314.08375	315.09103	313.07647	Nc1ccc(cc1)S(=O)(=O)Nc1ccnn1-c1cccc1	
ceftibuten	Pharmaceuticals	C15H14N4O6S2	410.03548	411.04276	409.0282	Nc1nc(cs1)C(=C\CC(O)=O)\C(O)N[C@H]1[C@H]2SCC=C(N2C1=O)C(O)=O	
chloroxuron	Pesticides	C15H15ClN2O2	290.08221	291.08949	289.07493	CNC(=O)Nc1ccc(Oc2ccc(Cl)cc2)cc1	
1-(4-chloro-1,3-dihydroxyphenyl)-3-methyl-5-phenylisoxazolin-4-one	Pesticides	C15H15ClN2O3	306.07712	307.0844	305.06984	NC(=O)C1(CCCCC1)N1C(=O)c2cccc(Cl)c2C1=O	
chlorimuron-ethyl	Pesticides	C15H15ClN4O6S	414.04009	415.04737	413.03281	CCOC(=O)c1cccc1S(=O)(=O)NC(=O)Nc1nc(Cl)cc(OC)n1	
flurprimidol	Pesticides	C15H15F3N2O2	312.10857	313.11585	311.10129	CC(C)C(O)(C1=CC=C(C(OC(F)(F)F)C=C1)C1=CN=CN=C1	
mefenamic acid	Pharmaceuticals	C15H15NO2	241.11028	242.11756	240.103	Cc1cccc(Nc2cccc2C(O)=O)c1C	
prochloraz	Pesticides	C15H16Cl3N3O2	375.03081	376.03809	374.02353	CCCN(CCOc1c(Cl)cc(Cl)cc1Cl)C(=O)N1C=CN=C1	
dithiopyr	Pesticides	C15H16F5N2O2S2	401.05426	402.06154	400.04698	CSC(=O)c1c(nc(c(Cl)C(=O)SC)c1CC(C)C)C(F)(F)F	

ancymidol	Pesticides	C15H16N2O2	256.12118	257.12846	255.1139	COc1ccc(cc1)C(O)(C1CC1)c1cncnc1	
ticarcillin	Pharmaceuticals	C15H16N2O6S2	384.04498	385.05226	383.0377	CC1(C)S[C@@H]2[C@H](NC(=O)[C@H](C(O)=O)c3ccsc3)C(=O)N2[C@H]1C(O)=O	
sulfometuron-methyl	Pesticides	C15H16N4O5S	364.08414	365.09142	363.07686	COC(=O)c1cccc1S(=O)(=O)NC(=O)Nc1nc(C)cc(C)n1	
bensulfuron	Pesticides	C15H16N4O7S	396.07397	397.08125	395.06669	COc1cc(OC)nc(NC(=O)NS(=O)(=O)Cc2ccccc2C(O)=O)n1	
bisphenol A	Industrial Chemicals	C15H16O2	228.11503	229.12231	227.10775	CC(C)(c1ccc(O)cc1)c1ccc(O)cc1	
bromoxynil octanoate	Pesticides	C15H17Br2NO2	400.96261	401.96989	399.95533	CCCCCCCC(=O)Oc1c(Br)cc(cc1Br)C#N	
propiconazole	Pesticides	C15H17Cl2N3O2	341.06979	342.07707	340.06251	CCCC1COC(Cn2cncn2)(O1)c1ccc(Cl)cc1Cl	
climbazole	Pesticides	C15H17ClN2O2	292.09786	293.10514	291.09058	CC(C)(C)C(=O)C(Oc1ccc(Cl)cc1)n1cncnc1	
myclobutanil	Pesticides	C15H17ClN4	288.11418	289.12146	287.1069	CCCCC(Cn1cncn1)(C#N)c1ccc(Cl)cc1	
enoxacin	Pharmaceuticals	C15H17FN4O3	320.12847	321.13575	319.12119	CCn1cc(C(O)=O)c(=O)c2cc(F)c(nc12)N1CCNCC1	
tribenuron-methyl	Pesticides	C15H17N5O6S	395.08996	396.09724	394.08268	COC(=O)C1=CC=CC=C1S(=O)(=O)NC(=O)N(C)C1=NC(OC)=NC(C)=N1	
cefpodoxime	Pharmaceuticals	C15H17N5O6S2	427.06203	428.06931	426.05475	COCC1=C(N2[C@H](SC1)[C@H](NC(=O)C(=N/OC)\c1csc(N)n1)C2=O)C(O)=O	
oxadiazon	Pesticides	C15H18Cl2N2O3	344.06945	345.07673	343.06217	CC(C)OC1=C(C)C=C(C)C(=C1)N1N=C(OC1=O)C(C)(C)C	
carpropamid	Pesticides	C15H18Cl3NO	333.0454	334.05268	332.03812	CCC1(C(C)C1(C)Cl)C(=O)NC(C)c1ccc(Cl)cc1	
cyproconazole	Pesticides	C15H18ClN3O	291.11384	292.12112	290.10656	CC(C1CC1)C(O)(CN1C=NC=N1)c1ccc(Cl)cc1	
uniconazole	Pesticides	C15H18ClN3O	291.11384	292.12112	290.10656	CC(C)(C)[C@H](O)C(=C/c1ccc(Cl)cc1)\n1cncn1	
benthiavalicarb	Pesticides	C15H18FN3O3S	339.10529	340.11257	338.09801	CC(C)[C@@H](NC(O)=O)C(=O)N[C@H](C)c1nc2ccc(F)cc2s1	
binapacryl	Pesticides	C15H18N2O6	322.11649	323.12377	321.10921	CCC(C)c1cc(ccc1OC(=O)C=C(C)C)[N+](O-)=O[N+](O-)=O	
nicosulfuron	Pesticides	C15H18N6O6S	410.10086	411.10814	409.09358	COc1cc(OC)nc(NC(=O)NS(=O)(=O)c2cccc2C(=O)N(C)C)n1	
dimefuron	Pesticides	C15H19ClN4O3	338.11457	339.12185	337.10729	CN(C)C(=O)Nc1ccc(N2N=C(OC2=O)C(C)(C)C)c(Cl)c1	
imazethapyr	Pesticides	C15H19N3O3	289.14264	290.14992	288.13536	CCc1cnc(C2=NC(C)(C)C)C(=O)N2)c(c1)C(O)=O	
imazamox	Pesticides	C15H19N3O4	305.13756	306.14484	304.13028	COCC1cnc(C2=NC(C)(C)C)C(=O)N2)c(c1)C(O)=O	
cinosulfuron	Pesticides	C15H19N5O7S	413.10052	414.1078	412.09324	COCCOc1ccccc1S(=O)(=O)NC(=O)Nc1nc(OC)nc(OC)n1	
strongid	Pharmaceuticals	C15H20N2O6S	356.10421	357.11149	355.09693	O[C@H]([C@@H](O)C(O)=O)C(O)=O.CN1CCCN=C1\C=C\c1cccs1	
metalaxyl	Pesticides	C15H21NO4	279.14706	280.15434	278.13978	COCC(=O)N(C(C)C(=O)OC)c1c(C)cccc1C	
metolachlor OXA	Metabolites	C15H21NO4	279.14706	280.15434	278.13978	C\C=C1\N(C)[C@H](C)CC1(c1ccccc1)c1ccccc1	metolachlor
bromobutide	Pesticides	C15H22BrNO	311.08848	312.09576	310.0812	CC(C)(C)[C@@H](Br)C(=O)NC(C)(C)c1ccccc1	
metolachlor	Pesticides	C15H22ClNO2	283.13391	284.14119	282.12663	CCc1cccc(C)c1N([C@H](C)COC)C(=O)CCl	
capecitabine	Pharmaceuticals	C15H22FN3O6	359.14927	360.15655	358.14199	CCCCCO\C(O)=N\c1nc(=O)n(cc1F)[C@@H]1O[C@H](C)[C@@H](O)[C@H]1O	
mepivacaine	Pharmaceuticals	C15H22N2O	246.17322	247.1805	245.16594	CN1CCCCC1C(=O)Nc1c(C)cccc1C	
gemfibrizil	Pharmaceuticals	C15H22O3	250.1569	251.16418	249.14962	Cc1ccc(C)c(OCCCC(C)(C)C(O)=O)c1	
octisalate	PCPs	C15H22O3	250.1569	251.16418	249.14962	CCCCCCCCOC(=O)c1ccccc1O	
aramite	Pesticides	C15H23ClO4S	334.10056	335.10784	333.09328	C[C@@H](COc1ccc(cc1)C(C)(C)C)O[S@](=O)OCCCCI	
sulpiride	Pharmaceuticals	C15H23N3O4S	341.14093	342.14821	340.13365	CCN1CCCC1CNC(=O)c1cc(ccc1OC)S(N)(=O)=O	
meptazinol	Pharmaceuticals	C15H23NO	233.17797	234.18525	232.17069	CCC1(CCCCN(C)C1)c1cccc(O)c1	
tebutam	Pesticides	C15H23NO	233.17797	234.18525	232.17069	CC(C)N(Cc1ccccc1)C(=O)C(C)(C)C	
N,N-didesmethyl	Metabolites	C15H23NO2	249.17288	250.18016	248.1656	COC1=CC=C(C=C1)C(CN)C1(O)CCCCC1	venlafaxine
N,O-didesmethyl venla	Metabolites	C15H23NO2	249.17288	250.18016	248.1656	CNCC(c1ccc(O)cc1)C1(O)CCCCC1	venlafaxine
oxprenolol	Pharmaceuticals	C15H23NO3	265.1678	266.17508	264.16052	CC(C)NCC(O)COc1ccccc1OCC=C	
metolachlor ESA	Metabolites	C15H23NO5S	329.1297	330.13698	328.12242	CCC1=C(N(C(C)COC)C(=O)CS(O)(=O)=O)C(C)=CC=C1	metolachlor
tiapride	Pharmaceuticals	C15H24N2O4S	328.14568	329.15296	327.1384	CCN(CC)CC\N=C(/O)c1cc(ccc1OC)S(C)(=O)=O	
doripenem	Pharmaceuticals	C15H24N4O6S2	420.11373	421.12101	419.10645	C[C@@H](O)[C@@H]1[C@H]2[C@@H](C)C(S[C@@H]3CN[C@H](CNS(N)(=O)=O)C3)=C(N2C1=O)C	
butylated hydroxytoluene	PCPs	C15H24O	220.18272	221.19	219.17544	Cc1cc(c(O)c(c1)C(C)(C)C(C)(C)C	
ametoctradin	Pesticides	C15H25N5	275.211	276.21828	274.20372	CCCCCCCCc1c(CC)nc2cncn2c1N	
metoprolol	Pharmaceuticals	C15H25NO3	267.18345	268.19073	266.17617	COCCCC1=CC=C(OCC(O)CNC(C)C)C=C1	
prohydrojasmon	Pesticides	C15H26O3	254.1882	255.19548	253.18092	CCCC[C@@H]1[C@@H](CC(=O)OCCC)CCC1=O	
peramivir	Pharmaceuticals	C15H28N4O4	328.21106	329.21834	327.20378	CCC(CC)[C@H](NC(C)=O)[C@@H]1[C@H](O)[C@H](C[C@H]1NC(N)=N)C(O)=O	
dodine	Pesticides	C15H33N3O2	287.25728	288.26456	286.25	CC(O)=O.CCCCCCCCCCN=C(N)N	
quinoxifen	Pesticides	C15H8Cl2FNO	306.9967	308.00398	305.98942	Fc1ccc(Oc2ccnc3cc(Cl)cc(Cl)c23)cc1	

benzoylprop	Pesticides	C16H13Cl2NO3	337.02725	338.03453	336.01997	CC(N(C(=O)c1cccc1)c1ccc(Cl)c(Cl)c1)C(O)=O	
flufenpyr-ethyl	Pesticides	C16H13ClF4N2O4	408.05	409.05728	407.04272	CCOC(=O)COCc1cc(c(F)cc1Cl)-n1ncc(c(C)c1=O)C(F)(F)F	
diazepam	Pharmaceuticals	C16H13ClN2O	284.07164	285.07892	283.06436	CN1C2=C(C=C(Cl)C=C2)C(=NCC1=O)C1=CC=CC=C1	
mebendazole	Pharmaceuticals	C16H13N3O3	295.09569	296.10297	294.08841	COC(=O)Nc1nc2cc(ccc2[nH]1)C(=O)c1cccc1	
chlorobenzilate	Pesticides	C16H14Cl2O3	324.032	325.03928	323.02472	CCOC(=O)C(O)(c1ccc(Cl)cc1)c1ccc(Cl)cc1	
voriconazole	Pharmaceuticals	C16H14F3N5O	349.11505	350.12233	348.10777	C[C@H](c1ncncc1F)[C@H](O)(C1ncn1)c1ccc(F)cc1F	
2-methyl carbamazepine	Metabolites	C16H14N2O	250.11062	251.1179	249.10334	Cc1ccc2N(C(N)=O)c3cccc3C=Cc2c1	carbamazepine
ketoprofen	Pharmaceuticals	C16H14O3	254.0943	255.10158	253.08702	CC(C(O)=O)c1cccc(c1)C(=O)c1cccc1	
N-desmethyl sertraline	Metabolites	C16H15Cl2N	291.05816	292.06544	290.05088	N[C@H]1CC[C@H](c2ccc(Cl)c(Cl)c2)c2cccc12	sertraline
clomeprop	Pesticides	C16H15Cl2NO2	323.04799	324.05527	322.04071	C[C@H](Oc1ccc(Cl)c(c1Cl)C(=O)Nc1cccc1	
methoxychlor	Pesticides	C16H15Cl3O2	344.01377	345.02105	343.00649	COc1ccc(cc1)C(c1ccc(OC)cc1)C(Cl)Cl	
medazepam	Pharmaceuticals	C16H15ClN2	270.09238	271.09966	269.0851	CN1CCN=C(c2cccc2)c2cc(Cl)cc12	
pantoprazole	Pharmaceuticals	C16H15F2N3O4S	383.07514	384.08242	382.06786	COc1ccnc(CS(=O)c2nc3cc(OC(F)F)ccc3[nH]2)c1OC	
sitagliptin	Pharmaceuticals	C16H15F6N5O	407.11808	408.12536	406.1108	N[C@H](CC(=O)N1CCn2c(C1)nn2C(F)(F)F)Cc1cc(F)c(F)cc1F	
5-methyl-5-phenyl-3-(f	Metabolites	C16H15N3O2	281.11643	282.12371	280.10915	C[C@]11(NC(=O)N(NC2=CC=CC=C2)C1=O)C1=CC=CC=C1	fenamidone
cefixime	Pharmaceuticals	C16H15N5O7S2	453.04129	454.04857	452.03401	Nc1nc(cs1)C(=N\OCC(O)=O)\C(=O)N[C@H]1[C@H]2SCC(C=C)=C(N2C1=O)C(O)=O	
etoxinol	Pesticides	C16H16Cl2O2	310.05274	311.06002	309.04546	CCOCC(O)(c1ccc(Cl)cc1)c1ccc(Cl)cc1	
loracarbef	Pharmaceuticals	C16H16ClN3O4	349.08294	350.09022	348.07566	[NH3+][C@@H](C(=O)N[C@H]1[C@H]2CCC(Cl)=C(N2C1=O)C([O-])=O)c1cccc1	
clopidogrel	Pharmaceuticals	C16H16ClNO2S	321.05903	322.06631	320.05175	COC(=O)[C@@H](N1CCc2sc2c2C1)c1cccc1Cl	
norfluoxetine	Metabolites	C16H16F3NO	295.1184	296.12568	294.11112	NCCC(Oc1ccc(cc1)C(F)(F)F)c1cccc1	fluoxetine
desmedipham	Pesticides	C16H16N2O4	300.11101	301.11829	299.10373	CCOC(=O)Nc1cccc(OC(=O)Nc2cccc2)c1	
phenmedipham	Pesticides	C16H16N2O4	300.11101	301.11829	299.10373	COC(=O)Nc1cccc(OC(=O)Nc2cccc(C)c2)c1	
cefalotin	Pharmaceuticals	C16H16N2O6S2	396.04498	397.05226	395.0377	CC(=O)OCC1=C(N2[C@H](SC1)[C@H](NC(=O)Cc1cccs1)C2=O)C(O)=O	
cefuroxime	Pharmaceuticals	C16H16N4O8S	424.06889	425.07617	423.06161	CO\N=C/(C(=O)N[C@H]1[C@H]2SCC(OC(N)=O)C(N2C1=O)C(O)=O)c1ccco1	
triflurosulfuron	Pesticides	C16H17F3N6O6S	478.08824	479.09552	477.08096	CN(C)c1nc(NC(=O)NS(=O)(=O)c2c(C)cccc2C(O)=O)nc(OCC(F)(F)F)n1	
cefalexin	Pharmaceuticals	C16H17N3O4S	347.09398	348.10126	346.0867	CC1=C(N2[C@H](SC1)[C@H](NC(=O)[C@H](N)c1ccccc1)C2=O)C(O)=O	
cefadroxil	Pharmaceuticals	C16H17N3O5S	363.08889	364.09617	362.08161	CC1=C(N2[C@H](SC1)[C@H](NC(=O)[C@H](N)c1ccc(O)cc1)C2=O)C(O)=O	
cefoxitin	Pharmaceuticals	C16H17N3O7S2	427.05079	428.05807	426.04351	CO[C@]11(NC(=O)CC2cccs2)[C@H]2SCC(COC(N)=O)C(N2C1=O)C(O)=O	
cefotaxime	Pharmaceuticals	C16H17N5O7S2	455.05694	456.06422	454.04966	CC(=O)OCC1=C(N2C(C(C2=O)NC(=O)C(=NOC)C3=CSC(=N3)N)SC1)C(=O)O	
mefenpyr-diethyl	Pesticides	C16H18Cl2N2O4	372.06437	373.07165	371.05709	CCOC(=O)C1=NN(c2ccc(Cl)cc2Cl)C(Cl)(C1)C(=O)OCC	
norfloxacin	Pharmaceuticals	C16H18FN3O3	319.13322	320.1405	318.12594	CCn1cc(C(O)=O)c(=O)c2cc(F)c(cc12)N1CCNCC1	
benzylpenicillin	Pharmaceuticals	C16H18N2O4S	334.09873	335.10601	333.09145	CC1(C(N2C(S1)C(C2=O)NC(=O)CC3=CC=CC(=C3)C(=O)O)C	
phenoxymethylpenicillin	Pharmaceuticals	C16H18N2O5S	350.09365	351.10093	349.08637	CC1(C)S[C@@H]2[C@H](NC(=O)COC3cccc3)C(=O)N2[C@H]1C(O)=O	
temopen	Pharmaceuticals	C16H18N2O7S2	414.05555	415.06283	413.04827	CO[C@]11(NC(=O)C(C(O)=O)c2ccsc2)[C@H]2SCC(C)(C)[C@@H](N2C1=O)C(O)=O	
bensulfuron-methyl	Pesticides	C16H18N4O7S	410.08962	411.0969	409.08234	COC(=O)c1cccc1CS(=O)(=O)NC(=O)Nc1nc(OC)cc(OC)n1	
chlorpheniramine	Pharmaceuticals	C16H19ClN2	274.12368	275.13096	273.1164	CN(C)CCC(c1ccc(Cl)cc1)c1cccn1	
clofibric acid glucuronide	Metabolites	C16H19ClO9	390.07176	391.07904	389.06448	CC(C)(Oc1ccc(Cl)cc1)C(=O)O[C@@H]1O[C@@H]([C@@H](O)clofibric acid	
ampicillin	Pharmaceuticals	C16H19N3O4S	349.10963	350.11691	348.10235	CC1(C(N2C(S1)C(C2=O)NC(=O)C(C3=CC=CC(=C3)N)C(=O)O)C	
cephradine	Pharmaceuticals	C16H19N3O4S	349.10963	350.11691	348.10235	CC1=C(N2[C@H](SC1)[C@H](NC(=O)[C@H](N)C1=CCC=CC1)C2=O)C(O)=O	
amoxicillin	Pharmaceuticals	C16H19N3O5S	365.10454	366.11182	364.09726	CC1(C(N2C(S1)C(C2=O)NC(=O)C(C3=CC=CC(=C3)O)N)C(=O)O)C	
sanguinine	Metabolites	C16H19NO3	273.1365	274.14378	272.12922	CN1CC[C@@]23C=C[C@H](O)C[C@@H]2Oc2c3c(C1)ccc2O	galanthamine
benzoyl ecgonine	Metabolites	C16H19NO4	289.13141	290.13869	288.12413	CN1C2CCCC1(C(C2)OC(=O)c1ccccc1)C(O)=O	cocaine
penthipyrad	Pesticides	C16H20F3N3OS	359.12792	360.1352	358.12064	CC(C)C(C)[C@H](C)c1sc2c1NC(=O)c1cn(C)nc1(F)(F)F	
linezolid	Pharmaceuticals	C16H20FN3O4	337.14379	338.15107	336.13651	CC(=O)NC[C@H]1CN(C(=O)O1)c1ccc(N2CCOCC2)c(F)c1	
benzamacril isobutyl	Pesticides	C16H20N2O2	272.15248	273.15976	271.1452	CC(C)COC(=O)C(=CN(C)CC1=CC=CC=C1)C#N	
imazamethabenz-methyl	Pesticides	C16H20N2O3	288.1474	289.15468	287.14012	COC(=O)c1ccc(Cl)cc1C1=NC(C)(C(C)C)C(=O)N1.COC(=O)c1cc(Cl)ccc1C1=NC(C)(C(C)C)C(=O)N1	
torasemide	Pharmaceuticals	C16H20N4O3S	348.12561	349.13289	347.11833	CC(C)NC(=O)NS(=O)(=O)c1cnccc1Nc1cccc(C)c1	
orthosulfamuron	Pesticides	C16H20N6O6S	424.11651	425.12379	423.10923	COC1cc(OC)nc(NC(=O)NS(=O)(=O)Nc2cccc2C(=O)N(C)C)n1	
propranolol	Pharmaceuticals	C16H21NO2	259.15723	260.16451	258.14995	CC(C)NC[C@H](O)COC1cccc2cccc12	

tebuconazole	Pesticides	C16H22ClN3O	307.14514	308.15242	306.13786	CC(C)(C)[C@@](O)(CCc1ccc(Cl)cc1)Cn1cncn1	
pethoxamid	Pesticides	C16H22ClNO2	295.13391	296.14119	294.12663	CCOCCN(C(=O)CC)C(=C(C)C)c1ccccc1	
allyxycarb	Pesticides	C16H22N2O2	274.16813	275.17541	273.16085	CNC(=O)Oc1cc(C)c(N(CC=C)CC=C(C)C)c1	
cafenstrole	Pesticides	C16H22N4O3S	350.14126	351.14854	349.13398	CCN(CC)C(=O)n1cnc(n1)S(=O)(=O)c1c(C)cc(C)cc1C	
homomenthyl salicylat	PCPs	C16H22O3	262.1569	263.16418	261.14962	CC1CC(CC(C)C)C1)OC(=O)c1ccccc1O	
dibutyl phthalate	PCPs	C16H22O4	278.15181	279.15909	277.14453	CCCCOC(=O)c1ccccc1C(=O)OCCCC	
buprofezin	Pesticides	C16H23N3OS	305.15619	306.16347	304.14891	CC(C)N1\C(SCN(C1=O)c1ccccc1)=N\C(C)(C)C	
xylometazoline	Pharmaceuticals	C16H24N2	244.19395	245.20123	243.18667	Cc1cc(cc(C)c1CC1=NCCN1)(C)(C)C	
O-desmethylvenlafaxin	Pharmaceuticals	C16H25NO2	263.18853	264.19581	262.18125	CN(C)CC(c1ccc(O)cc1)C1(O)CCCCC1	venlafaxine
tramadol	Pharmaceuticals	C16H25NO2	263.18853	264.19581	262.18125	COC1=CC=CC(=C1)[C@@]1(O)CCCC[C@@H]1CN(C)C	
cilastatin	Pharmaceuticals	C16H26N2O5S	358.15625	359.16353	357.14897	CC1(CC1C(=O)NC(=CCCCSCC(C(=O)O)N)C(=O)O)C	
iso-E-super	PCPs	C16H26O	234.19837	235.20565	233.19109	C[C@@H]1CC2=C(C[C@@]1(C)C(C)=O)C(C)(C)CCC2	
artemether	Pharmaceuticals	C16H26O5	298.17803	299.18531	297.17075	CO[C@H]1O[C@H]2O[C@H]3(C)CC[C@H]4[C@H](C)CC[C@@H]1[C@H]1C[C@@]24OO3	
oseltamivir	Pharmaceuticals	C16H28N2O4	312.20491	313.21219	311.19763	CCC(CC)OC1C=C(CCC(C1NC(=O)C)N)C(=O)OCC	
bistrifluron	Pesticides	C16H7ClF8N2O2	446.00683	447.01411	444.99955	Fc1cccc(F)c1C(=O)NC(=O)Nc1cc(cc(c1Cl)C(F)(F)F)C(F)(F)F	
hexaflumuron	Pesticides	C16H8Cl2F6N2O3	459.98162	460.9889	458.97434	FC(F)C(F)(F)Oc1c(Cl)cc(NC(=O)NC(=O)c2c(F)cccc2F)cc1Cl	
fenarimol	Pesticides	C17H12Cl2N2O	330.03267	331.03995	329.02539	OC(c1ccc(Cl)cc1)(c1cncnc1)c1ccccc1Cl	
chlorazifop propargyl	Pesticides	C17H13Cl2NO4	365.02217	366.02945	364.01489	C[C@@H](Oc1ccc(Oc2ncc(Cl)cc2Cl)cc1)C(=O)OCC#C	
epoxiconazole	Pesticides	C17H13ClFN3O	329.07312	330.0804	328.06584	Fc1ccc(cc1)C1(Cn2cncn2)OC1c1cccc1Cl	
clodinafop-propargyl	Pesticides	C17H13ClFNO4	349.05172	350.059	348.04444	C[C@@H](Oc1ccc(Oc2ncc(Cl)cc2F)cc1)C(=O)OCC#C	
alprazolam	Pharmaceuticals	C17H13ClN4	308.08288	309.09016	307.0756	Cc1nnc2CN=C(c3ccccc3)c3cc(Cl)ccc3-n12	
tefluthrin	Pesticides	C17H14ClF7O2	418.05706	419.06434	417.04978	Cc1c(F)c(F)c(COC(=O)C2C(\C=C(/Cl)C(F)(F)F)C2(C)C)c(F)c1F	
fibracor	Pharmaceuticals	C17H15ClO4	318.06589	319.07317	317.05861	CC(C)(Oc1ccc(cc1)C(=O)c1ccc(Cl)cc1)C(O)=O	
tedizolid	Pharmaceuticals	C17H15FN6O3	370.11897	371.12625	369.11169	CN1N=NC(=N1)C1=NC=C(C=C1)C1=C(F)C=C(C=C1)N1C[C@H]1(CO)OC1=O	
bromopropylate	Pesticides	C17H16Br2O3	425.94662	426.9539	424.93934	CC(C)OC(=O)C(O)(C1=CC=C(Br)C=C1)C1=CC=C(Br)C=C1	
anisuron	Pesticides	C17H16Cl2N2O3	366.0538	367.06108	365.04652	COc1ccc(cc1)C(=O)N(C(=O)N(C)C)c1ccc(Cl)c(Cl)c1	
chloropropylate	Pesticides	C17H16Cl2O3	338.04765	339.05493	337.04037	CC(C)OC(=O)C(O)(c1ccc(Cl)cc1)c1ccc(Cl)cc1	
tembotrione	Pesticides	C17H16ClF3O6S	440.03082	441.0381	439.02354	CS(=O)(=O)c1ccc(C(=O)C2C(=O)CCCC2=O)c(Cl)c1COCC(F)(F)F	
flutolanil	Pesticides	C17H16F3NO2	323.11332	324.1206	322.10604	CC(C)OC1=CC=CC(NC(=O)C2=CC=CC=C2C(F)(F)F)=C1	
mefloquine	Pharmaceuticals	C17H16F6N2O	378.11669	379.12397	377.10941	O[C@H]1([C@H]1CCCCN1)c1cc(nc2c(cccc12)C(F)(F)F)C(F)(F)F	
sertraline	Pharmaceuticals	C17H17Cl2N	305.07381	306.08109	304.06653	CN[C@H]1CC[C@@H](c2ccc(Cl)c(Cl)c2)c2ccccc12	
saflufenacil	Pesticides	C17H17ClF4N4O5S	500.05443	501.06171	499.04715	CC(C)N(C)S(=O)(=O)NC(=O)c1cc(c(F)cc1Cl)-n1c(=O)cc(n(C)c1=O)C(F)(F)F	
griseofulvin	Pharmaceuticals	C17H17ClO6	352.07137	353.07865	351.06409	COC1=CC(=O)C[C@@H](C)[C@]11Oc2c(C1=O)c(OC)cc(OC)c2Cl	
difenzoquat	Pesticides	C17H17N2	249.13918	250.14646	248.1319	Cn1c(cc(-c2ccccc2)[n+]1C)-c1ccccc1	
fenamidone	Pesticides	C17H17N3OS	311.10924	312.11652	310.10196	CSC1=N[C@](C)(C)(=O)N1NC1=CC=CC=C1)C1=CC=CC=C1	
cefotetan	Pharmaceuticals	C17H17N7O8S4	575.00215	576.00943	573.99487	CN1C(=NN=N1)SCC2=C(N3C(C(C3=O)(NC(=O)C4SC(=C(C(=O)N)C(=O)O)S4)OC)SC2)C(=O)O	
fluoxetine	Pharmaceuticals	C17H18F3NO	309.13405	310.14133	308.12677	CNCCC(Oc1ccc(cc1)C(F)(F)F)c1ccccc1	
profluthrin	Pesticides	C17H18F4O2	330.1243	331.13158	329.11702	CNCCC(C1=CC=CC=C1)OC2=CC=C(C=C2)C(F)(F)F	
ciprofloxacin	Pharmaceuticals	C17H18FN3O3	331.13322	332.1405	330.12594	OC(=O)c1cn(C2CC2)c2cc(N3CCNCC3)c(F)cc2c1=O	
nifedipine	Pharmaceuticals	C17H18N2O6	346.11649	347.12377	345.10921	COC(=O)C1=C(C)NC(C)=C(C1c1ccccc1[N+](=[O-])=O)C(=O)OC	
carbenicillin	Pharmaceuticals	C17H18N2O6S	378.08856	379.09584	377.08128	CC1(C)S[C@@H]2[C@H](NC(=O)C(C(=O)=O)c3ccccc3)C(=O)N2[C@H]1C(O)=O	
lomefloxacin	Pharmaceuticals	C17H19F2N3O3	351.13945	352.14673	350.13217	Cc1c(C(C(=O)=O)c(=O)c2cc(F)c(N3CCNC(C)C3)c(F)c12	
triflusalufuron-methyl	Pesticides	C17H19F3N6O6S	492.10389	493.11117	491.09661	COC(=O)c1ccccc1C1S(=O)(=O)NC(=O)Nc1nc(OCC(F)(F)F)nc(n1)N(C)C	
omeprazole	Pharmaceuticals	C17H19N3O3S	345.11472	346.122	344.10744	COc1ccc2[nH]c(nc2c1)S(=O)Cc1ncc(C)c(OC)c1C	
morphine	Pharmaceuticals	C17H19NO3	285.1365	286.14378	284.12922	CN1CC[C@@]23[C@H]4Oc5c2c[C@H]1[C@@H]3C=C[C@@H]4O)ccc5O	
fenoxycarb	Pesticides	C17H19NO4	301.13141	302.13869	300.12413	CCOC(=O)NCCOc1ccc(Oc2ccccc2)cc1	
triticonazole	Pesticides	C17H20ClN3O	317.12949	318.13677	316.12221	CC1(C)CC\C=C/C2=CC=C(Cl)C=C2)C1(O)CN1C=NC=N1	
flecainide	Pharmaceuticals	C17H20F6N2O3	414.13781	415.14509	413.13053	FC(F)(F)COc1ccc(OCC(F)(F)F)c(c1)C(=O)NCC1CCCCN1	
bifenazate	Pesticides	C17H20N2O3	300.1474	301.15468	299.14012	COc1ccc(cc1NNC(=O)OC(C)C)-c1ccccc1	

methicillin	Pharmaceuticals	C17H20N2O6S	380.10421	381.11149	379.09693	COc1cccc(OC)c1C(=O)N[C@H]1[C@H]2SC(C)(C)[C@@H](N2C1=O)C(O)=O	
foramsulfuron	Pesticides	C17H20N6O7S	452.11142	453.1187	451.10414	COc1cc(OC)nc(NC(=O)NS(=O)(=O)c2c(NC=O)cccc2C(=O)N(C)C)n1	
mycophenolic acid	Pharmaceuticals	C17H20O6	320.12599	321.13327	319.11871	COc1c(C)c2COC(=O)c2c(O)c1C\C=C(/C)CCC(O)=O	
fenpyrazamine	Pesticides	C17H21N3O2S	331.13545	332.14273	330.12817	CC(C)n1n(C(=O)SCC=C)c(N)c(-c2cccc2C)c1=O	
mesosulfuron-methyl	Pesticides	C17H21N5O9S2	503.07807	504.08535	502.07079	COC(=O)c1ccc(CNS(C)(=O)=O)cc1S(=O)(=O)NC(=O)Nc1nc(OC)cc(OC)n1	
atomoxetine	Pharmaceuticals	C17H21NO	255.16232	256.1696	254.15504	CNCC[C@H](O)c1cccc1C1cccc1	
napropamide-M	Pesticides	C17H21NO2	271.15723	272.16451	270.14995	CCN(CC)C(=O)[C@@H](C)Oc1cccc2cccc12	
etodolac	Pharmaceuticals	C17H21NO3	287.15215	288.15943	286.14487	CCc1cccc2c3CCOC(CC)(CC(O)=O)c3[nH]c12	
cocaine	Pharmaceuticals	C17H21NO4	303.14706	304.15434	302.13978	COC(=O)[C@H]1[C@H]2CC[C@H](C[C@@H]1OC(=O)c1cccc1)N2C	
bensultap	Pesticides	C17H21NO4S4	431.03534	432.04262	430.02806	CN(C)C(CSS(=O)(=O)c1cccc1)CSS(=O)(=O)c1cccc1	
metconazole	Pesticides	C17H22CIN3O	319.14514	320.15242	318.13786	CC1(C)CCC(Cc2ccc(Cl)cc2)C1(O)Cn1cncn1	
iopamidol	Pharmaceuticals	C17H22I3N3O8	776.8541	777.86138	775.84682	CC(O)C(=O)NC1=C(I)C(C(=O)NC(CO)CO)=C(I)C(C(=O)NC(CO)CO)=C1I	
doxylamine	Pharmaceuticals	C17H22N2O	270.17322	271.1805	269.16594	CN(C)CCOC(C)(c1cccc1)c1cccn1	
imiprothrin	Pesticides	C17H22N2O4	318.15796	319.16524	317.15068	CC(C)=CC1C(C(=O)OCN2C(=O)CN(CC#C)C2=O)C1(C)C	
pyrantel citrate	Pharmaceuticals	C17H22N2O7S	398.11477	399.12205	397.10749	OC(=O)CC(O)(CC(O)=O)C(O)=O.CN1CCCN=C1\C=C\C1cccs1	
butenachlor	Pesticides	C17H24ClNO2	309.14956	310.15684	308.14228	CCc1cccc(CC)c1N(COC\C=C/C)C(=O)CCl	
tepraloxym	Pesticides	C17H24ClNO4	341.13939	342.14667	340.13211	CC\C(=N/OC\C=C\Cl)C1=C(O)CC(Cc1=O)C1CCOCC1	
phantolide	PCPs	C17H24O	244.18272	245.19	243.17544	CC1C(C)(C)c2cc(C)c(cc2C1(C)C)C(C)=O	
vildagliptin	Pharmaceuticals	C17H25N3O2	303.19468	304.20196	302.1874	OC12CC3CC(C1)CC(C3)(C2)NCC(=O)N1CCC[C@H]1C#N	
alanycarb	Pesticides	C17H25N3O4S2	399.12865	400.13593	398.12137	CCOC(=O)CCN(Cc1cccc1)SN(C)C(=O)O\N=C(\C)SC	
meropenem	Pharmaceuticals	C17H25N3O5S	383.15149	384.15877	382.14421	C[C@@H](O)[C@@H]1[C@@H]2[C@@H](C)C(S[C@@H]3CN[C@@H](C3)C(=O)N(C)C)=C(N2C1=O)C	
menthyl anthranilate	PCPs	C17H25NO2	275.18853	276.19581	274.18125	CC(C)[C@@H]1CC[C@@H](C)C[C@H]1OC(=O)c1cccc1N	
aloxym	Pesticides	C17H25NO5	323.17328	324.18056	322.166	CCC\C(NOCC=C)=C1/C(=O)CC(C)(C)C(C(=O)OC)C1=O	
butachlor	Pesticides	C17H26ClNO2	311.16521	312.17249	310.15793	CCCCOCN(C(=O)CCl)C1=C(CC)C=CC=C1CC	
clethodim	Pesticides	C17H26ClNO3S	359.1322	360.13948	358.12492	CCC(=C1C(=O)CC(Cc1=O)CC(C)SCC)NOC/C=C/Cl	
D-617	Metabolites	C17H26N2O2	290.19943	291.20671	289.19215	CNCCCC(C#N)(C(C)C)c1ccc(OC)c(OC)c1	verapamil
amisulpride	Pharmaceuticals	C17H27N3O4S	369.17223	370.17951	368.16495	CCN1CCC[C@H]1CN(C(=O)c1ccc(c(N)cc1OC)S(=O)(=O)CC	
padimate O	PCPs	C17H27NO2	277.20418	278.21146	276.1969	CCCC(CC)COC(=O)c1ccc(cc1)N(C)C	
venlafaxine	Pharmaceuticals	C17H27NO2	277.20418	278.21146	276.1969	COc1ccc(cc1)[C@@H](CN(C)C)C1(O)CCCC1	
cycloxydim	Pesticides	C17H27NO3S	325.17117	326.17845	324.16389	CCCC(NOCC)=C1C(=O)CC(Cc1=O)C1CCSC1	
nadolol	Pharmaceuticals	C17H27NO4	309.19401	310.20129	308.18673	CC(C)(C)NCC(O)COc1cccc2C[C@@H](O)[C@@H](O)Cc12	
noviflumuron	Pesticides	C17H7Cl2F9N2O3	527.969	528.97628	526.96172	FC(C(F)(F)F)C(F)(F)Oc1c(Cl)cc(NC(=O)NC(=O)c2c(F)cccc2F)c(F)c1Cl	
novaluron	Pesticides	C17H9ClF8N2O4	492.01231	493.01959	491.00503	FC(OC(F)(F)F)C(F)(F)Oc1ccc(NC(=O)NC(=O)c2c(F)cccc2F)cc1Cl	
bixafen	Pesticides	C18H12Cl2F3N3O	413.03096	414.03824	412.02368	Cn1cc(C(=O)Nc2ccc(F)cc2-c2ccc(Cl)c(Cl)c2)c(n1)C(F)F	
boscalid	Pesticides	C18H12Cl2N2O	342.03267	343.03995	341.02539	Clc1ccc(cc1)-c1cccc1NC(=O)c1cccn1Cl	
fluxapyroxad	Pesticides	C18H12F5N3O	381.09006	382.09734	380.08278	Cn1cc(C(=O)Nc2cccc2-c2cc(F)c(F)c(F)c2)c(n1)C(F)F	
midazolam	Pharmaceuticals	C18H13ClFN3	325.07821	326.08549	324.07093	Cc1ncc2CN=C(c3cccc3F)c3cc(Cl)ccc3-n12	
chlorantraniliprole	Pesticides	C18H14BrCl2N5O2	480.9708	481.97808	479.96352	CNC(=O)c1cc(Cl)cc(Cl)c1NC(=O)c1cc(Br)nn1-c1ncccc1Cl	
pyridalyl	Pesticides	C18H14Cl4F3NO3	488.96799	489.97527	487.96071	FC(F)(F)c1cccc(OCCOC2c(Cl)cc(OCC=C(Cl)Cl)cc2Cl)n1	
miconazole	Pharmaceuticals	C18H14Cl4N2O	413.98603	414.99331	412.97875	Clc1ccc(COC(Cn2cnc2)c2ccc(Cl)cc2Cl)c(Cl)c1	
bicalutamide	Pharmaceuticals	C18H14F4N2O4S	430.06104	431.06832	429.05376	C[C@](O)(CS(=O)(=O)c1ccc(F)cc1)C(=O)Nc1ccc(C#N)c(c1)C(F)(F)F	
sulfasalazine	Pharmaceuticals	C18H14N4O5S	398.06849	399.07577	397.06121	OC(=O)C1=C(O)C=CC(=C1)N=NC1=CC=C(C=C1)S(=O)(=O)NC1=CC=CC=N1	
benzovindiflupyr	Pesticides	C18H15Cl2F2N3O	397.05603	398.06331	396.04875	Cn1cc(C(=O)Nc2cccc3C4CCC(C4=C(Cl)Cl)c23)c(n1)C(F)F	
fenoxaprop-ethyl	Pesticides	C18H16ClNO5	361.0717	362.07898	360.06442	CCOC(=O)C(C)Oc1ccc(Oc2nc3ccc(Cl)cc3o2)cc1	
benzoylprop-ethyl	Pesticides	C18H17Cl2NO3	365.05855	366.06583	364.05127	CCOC(=O)C(C)N(C(=O)c1cccc1)c1ccc(Cl)c(Cl)c1	
beclubutamid	Pesticides	C18H17F4NO2	355.11954	356.12682	354.11226	CCC(Oc1ccc(F)c(c1)C(F)(F)F)C(=O)NCC1CCCC1	
isoxadifen-ethyl	Pesticides	C18H17NO3	295.12085	296.12813	294.11357	CCOC(=O)C1=NOC(C1)(c1cccc1)c1cccc1	
arsphenamine trimer	Pharmaceuticals	C18H18As3N3O3	548.89961	549.90689	547.89233	Nc1cc(ccc1O)-[as]1[as](-c2ccc(O)c(N)c2)[as]1-c1ccc(O)c(N)c1	
benzoximate	Pesticides	C18H18ClNO5	363.08735	364.09463	362.08007	CCO\N=C(/OC(=O)c1cccc1)c1c(OC)ccc(Cl)c1OC	

cefamandole	Pharmaceuticals	C18H18N6O5S2	462.07801	463.08529	461.07073	Cn1nnnc1SCC1=C(N2[C@H](SC1)[C@H](NC(=O)[C@H](O)c1ccccc1)C2=O)C(O)=O
ceftriaxone	Pharmaceuticals	C18H18N8O7S3	554.04606	555.05334	553.03878	CN1C(=NC(=O)C(=O)N1)SCC2=C(N3C(C(C3=O)NC(=O)C(=NOC)C4=CSC(N4)N)SC2)C(=O)O
halofenozide	Pesticides	C18H19ClN2O2	330.11351	331.12079	329.10623	CC(C)(C)N(NC(=O)C1=CC=C(Cl)C=C1)C(=O)C1=CC=CC=C1
clozapine	Pharmaceuticals	C18H19ClN4	326.12983	327.13711	325.12255	CN1CCN(CC1)C1=Nc2cc(Cl)ccc2Nc2ccccc12
sedaxane	Pesticides	C18H19F2N3O	331.14962	332.1569	330.14234	Cn1cc(C(=O)Nc2ccccc2C2CC2C2CC2)c(n1)C(F)F.Cn1cc(C(=O)Nc2ccccc2C2CC2C2CC2)c(n1)C(F)F.Cn1
cefprozil	Pharmaceuticals	C18H19N3O5S	389.10454	390.11182	388.09726	C\N=C\C1=C(N2[C@H](SC1)[C@H](NC(=O)[C@H](N)c1ccc(O)cc1)C2=O)C(O)=O
kresoxim-methyl	Pesticides	C18H19NO4	313.13141	314.13869	312.12413	CO\N=C\C(=O)OC)c1ccccc1OC1ccccc1C
levofloxacin	Pharmaceuticals	C18H20FN3O4	361.14379	362.15107	360.13651	C[C@H]1COc2c(N3CCN(C)CC3)c(F)cc3c2n1cc(C(O)=O)c3=O
gemifloxacin	Pharmaceuticals	C18H20FN5O4	389.14994	390.15722	388.14266	CO\N=C1/CN(CC1CN)C1=C(F)C=C2C(=O)C(=CN(C3CC3)C2=N1)C(O)=O
codeine	Pharmaceuticals	C18H21NO3	299.15215	300.15943	298.14487	COc1ccc2C[C@@H]3[C@H]4C=C[C@H](O)[C@H]5Oc1c2[C@@H]45CCN3C
hydrocodone	Industrial Chemicals	C18H21NO3	299.15215	300.15943	298.14487	COc1ccc2C[C@@H]3[C@H]4CCC(=O)[C@H]5Oc1c2[C@@H]45CCN3C
enzacamene	PCPs	C18H22O	254.16707	255.17435	253.15979	Cc1ccc(\C=C2/C3CCC(C)(C2=O)C3(C)C)cc1
ipconazole	Pesticides	C18H24ClN3O	333.16079	334.16807	332.15351	CC(C)C1CCC(Cc2ccc(Cl)cc2)C1(O)Cn1cncn1
penflufen	Pesticides	C18H24FN3O	317.19034	318.19762	316.18306	CC(C)CC(C)c1ccccc1NC(=O)c1c(C)nn(C)c1F
benthiavalicarb isopro	Pesticides	C18H24FN3O3S	381.15224	382.15952	380.14496	CC(C)OC(=O)N[C@H](C(C)C)C(=O)N[C@H](C)c1nc2ccc(F)cc2s1
iopromide	Pharmaceuticals	C18H24I3N3O8	790.86975	791.87703	789.86247	COCC(=O)Nc1c(I)c(C(=O)NC[C@H](O)CO)c(I)c(C(=O)N(C)C[C@H](O)CO)c1I
galaxolidone	Metabolites	C18H24O2	272.17763	273.18491	271.17035	CC1C(C)(C)c2cc3C(C)COC(=O)c3cc2C1(C)C galaxolide
dextromethorphan	Pharmaceuticals	C18H25NO	271.19362	272.2009	270.18634	COc1ccc2C[C@H]3[C@H]4CCCC[C@@H]4(CCN3C)c2c1
chloroquine	Pharmaceuticals	C18H26ClN3	319.18153	320.18881	318.17425	CCN(CC)CCCC(C)Nc1ccnc2cc(Cl)ccc12
hydroxychloroquine	Pharmaceuticals	C18H26ClN3O	335.17644	336.18372	334.16916	CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc12
galaxolide	PCPs	C18H26O	258.19837	259.20565	257.19109	CC1C(C)(C)c2cc3COCC(C)c3cc2C1(C)C
tonalide	PCPs	C18H26O	258.19837	259.20565	257.19109	CC1CC(C)(C)c2cc(C(C)=O)c(C)cc2C1(C)C
cinmethylin	Pesticides	C18H26O2	274.19328	275.20056	273.186	CC(C)C12CCC(C)(O1)C(C2)OCc1ccccc1C
3-octanyl (2E)-3-(4-me	PCPs	C18H26O3	290.1882	291.19548	289.18092	CCCCC(CC)OC(=O)\C=C\c1ccc(OC)cc1
octinoxate	PCPs	C18H26O3	290.1882	291.19548	289.18092	CCCCC(CC)COC(=O)\C=C\c1ccc(OC)cc1
iprovalicarb	Pesticides	C18H28N2O3	320.21	321.21728	319.20272	CC(C)OC(=O)NC(C(C)C)C(=O)N[C@H](C)c1ccc(C)cc1
kinoprene	Pesticides	C18H28O2	276.20893	277.21621	275.20165	CC(C)CCCC(C)\C=C\c1c(C)=C\c1(=O)OCC#C
clindamycin	Pharmaceuticals	C18H33ClN2O5S	424.17987	425.18715	423.17259	CCC[C@@H]1C[C@H](N(C)C1)C(=O)N[C@H]([C@H](C)Cl)[C@H]1O[C@H](SC)[C@H](O)[C@@H](O
lincomycin	Pharmaceuticals	C18H34N2O6S	406.21376	407.22104	405.20648	CCCC1CC(N(C1)C)C(=O)NC(C2C(C(C(O2)SC)O)O)C(C)O
spiroxamine	Pesticides	C18H35NO2	297.26678	298.27406	296.2595	CCCN(CC)[C@H]1COc2(CCC(C)C)C(C)C1O
kanamycin	Pharmaceuticals	C18H36N4O11	484.23806	485.24534	483.23078	NC[C@H]1O[C@H](O[C@@H]2[C@H](N)C[C@@H](N)[C@H](O[C@H]3O[C@H](CO)[C@@H](O
tobramycin	Pharmaceuticals	C18H37N5O9	467.25913	468.26641	466.25185	NC[C@H]1O[C@H](O[C@@H]2[C@H](N)C[C@@H](N)[C@H](O[C@H]3O[C@H](CO)[C@@H](O
aldimorph	Pesticides	C18H37NO	283.28752	284.2948	282.28024	CCCCCCCCCCCCN1C[C@@H](C)O[C@H](C)C1
buminafos	Pesticides	C18H38NO3P	347.25893	348.26621	346.25165	CCCCN1(CCCCC1)P(=O)(OCCCC)OCCCC
diflufenican	Pesticides	C19H11F5N2O2	394.07407	395.08135	393.06679	Fc1ccc(NC(=O)c2ccnc2Oc2cccc(c2)C(F)(F)F)c(F)c1
fluridone	Pesticides	C19H14F3NO	329.10275	330.11003	328.09547	CN1C=C(C(=O)C(=C1)c1cccc(c1)C(F)(F)F)c1ccccc1
pyrifluquinazon	Pesticides	C19H15F7N4O2	464.10833	465.11561	463.10105	CC(=O)N1C(=O)N(Cc2cc(c1c2)C(F)(C(F)F)C(F)(F)F)NCC1ccncn1
indometacin	Pharmaceuticals	C19H16ClNO4	357.07679	358.08407	356.06951	COC1=CC2=C(C=C1)N(C(=O)C1=CC=C(Cl)C=C1)C(C)=C2CC(O)=O
warfarin	Pharmaceuticals	C19H16O4	308.10486	309.11214	307.09758	CC(=O)CC(c1ccccc1)c1c(O)c2ccccc2oc1=O
difenoconazole	Pesticides	C19H17Cl2N3O3	405.0647	406.07198	404.05742	C[C@H]1CO[C@@H](Cn2cncn2)(O1)c1ccc(Oc2ccc(Cl)cc2)cc1Cl
dicloxacillin	Pharmaceuticals	C19H17Cl2N3O5S	469.0266	470.03388	468.01932	Cc1onc(c1C(=O)N[C@H]1[C@H]2SC(C)(C)[C@@H](N2C1=O)C(O)=O)-c1c(Cl)cccc1Cl
cinidon-ethyl	Pesticides	C19H17Cl2NO4	393.05347	394.06075	392.04619	CCOC(=O)C\Cl)=C/c1cc(c1c1Cl)N1C(=O)C2=C(CCCC2)C1=O
flucloxacillin	Pharmaceuticals	C19H17ClFN3O5S	453.05615	454.06343	452.04887	Cc1onc(c1C(=O)N[C@H]1[C@H]2SC(C)(C)[C@@H](N2C1=O)C(O)=O)-c1c(F)cccc1Cl
fenbuconazole	Pesticides	C19H17ClN4	336.11418	337.12146	335.1069	Clc1ccc(CCC(Cn2cncn2)(C#N)c2ccccc2)cc1
tolnaftate	Pharmaceuticals	C19H17NO5	307.10309	308.11037	306.09581	CN(C(=S)Oc1ccc2ccccc2c1)c1cccc(C)c1
pyraclostrobin	Pesticides	C19H18ClN3O4	387.09859	388.10587	386.09131	CON(C(=O)OC)c1ccccc1COc1ccn(n1)-c1ccc(Cl)cc1
cloxacillin	Pharmaceuticals	C19H18ClN3O5S	435.06557	436.07285	434.05829	Cc1onc(c1C(=O)N[C@H]1[C@H]2SC(C)(C)[C@@H](N2C1=O)C(O)=O)-c1ccccc1Cl
cefditoren	Pharmaceuticals	C19H18N6O5S3	506.05008	507.05736	505.0428	CO\N=C/C(=O)N[C@H]1[C@H]2SCC\C=C/C3=C(C)N=CS3=C(N2C1=O)C(O)=O)C1=CSC(N)=N1
momfluorothrin	Pesticides	C19H19F4NO3	385.13011	386.13739	384.12283	COCC1c(F)c(F)c(COC(=O)C2C(C=C(C#N)C2(C)C)c(F)c1F

N-desmethyl escitalopram	Metabolites	C19H19FN2O	310.14814	311.15542	309.14086	CNCCCC1(OCc2cc(ccc12)C#N)c1ccc(F)cc1	citalopram, escitalopram
oxacillin	Pharmaceuticals	C19H19N3O5S	401.10454	402.11182	400.09726	Cc1onc(c1C(=O)N[C@H]1[C@H]2SC(C)(C)[C@@H](N2C1=O)C(O)=O)-c1ccccc1	
bezafibrate	Pharmaceuticals	C19H20ClNO4	361.10809	362.11537	360.10081	CC(C)(Oc1ccc(CCN(C(=O)c2ccc(Cl)cc2)cc1)C(O)=O	
fluazifop-P-butyl	Pesticides	C19H20F3NO4	383.13445	384.14173	382.12717	CCCCOC(=O)[C@@H](C)Oc1ccc(Oc2ccc(cn2)C(F)(F)F)cc1	
bicyclopyrone	Pesticides	C19H20F3NO5	399.12936	400.13664	398.12208	COCCOCc1nc(ccc1C(=O)C1=C(O)C2CCC(C2)C1=O)C(F)(F)F	
paroxetine	Pharmaceuticals	C19H20FNO3	329.14272	330.15	328.13544	Fc1ccc(cc1)[C@@H]1CCNC[C@H]1COc1ccc2OCOc2c1	
metrafenone	Pesticides	C19H21BrO5	408.05724	409.06452	407.04996	COc1ccc(Br)c(C)c1C(=O)c1c(C)cc(OC)c(OC)c1OC	
Pencycuron	Pesticides	C19H21ClN2O	328.13424	329.14152	327.12696	Clc1ccc(CN(C2CCCC2)C(=O)Nc2ccccc2)cc1	
clofop-isobutyl	Pesticides	C19H21ClO4	348.11284	349.12012	347.10556	CC(C)COC(=O)C(C)Oc1ccc(Oc2ccc(Cl)cc2)cc1	
sparfloxacin	Pharmaceuticals	C19H22F2N4O3	392.166	393.17328	391.15872	C[C@H]1CN[C[C@@H](C)N1]c1c(F)c(N)c2c(c1F)n(cc(C(O)=O)c2=O)C1CC1	
enrofloxacin	Pharmaceuticals	C19H22FN3O3	359.16452	360.1718	358.15724	CCN1CCN(CC1)c1cc2n(cc(C(O)=O)c(=O)c2cc1F)C1CC1	
grepafloxacin	Pharmaceuticals	C19H22FN3O3	359.16452	360.1718	358.15724	CC1CN(CCN1)c1cc2n(cc(C(O)=O)c(=O)c2c(C)c1F)C1CC1	
gatifloxacin	Pharmaceuticals	C19H22FN3O4	375.15944	376.16672	374.15216	COc1c(N2CCNC(C)C2)c(F)cc2c1n(cc(C(O)=O)c2=O)C1CC1	
amitraz	Pesticides	C19H23N3	293.1892	294.19648	292.18192	CN(\C=N\c1ccc(C)cc1C)\C=N\c1ccc(C)cc1C	
benzipram	Pesticides	C19H23NO	281.17797	282.18525	280.17069	CC(C)N(Cc1ccccc1)C(=O)c1cc(C)cc(C)c1	
praziquantel	Pharmaceuticals	C19H24N2O2	312.18378	313.19106	311.1765	O=C(C1CCCCC1)N1CC2N(CCc3ccccc23)C(=O)C1	
pentamidine	Pharmaceuticals	C19H24N4O2	340.18993	341.19721	339.18265	NC(=N)c1ccc(OCCCCOCc2ccc(cc2)C(N)=N)cc1	
cefepime	Pharmaceuticals	C19H24N6O5S2	480.12496	481.13224	479.11768	CO\N=C(/C(=O)N[C@H]1[C@H]2SCC(C[N+](=O)C)CCCC3)=C(N2C1=O)C([O-])=O)c1csc(N)n1	
prallethrin	Pesticides	C19H24O3	300.17255	301.17983	299.16527	CC(C)=C[C@H]1[C@H](C(=O)O[C@H]2CC(=O)C(CC#C)=C2C)C1(C)C	
pyridaben	Pesticides	C19H25ClN2O5	364.13762	365.1449	363.13034	CC(C)(C)N1N=CC(SCc2ccc(cc2)C(C)C)C(=O)C1=O	
tetramethrin	Pesticides	C19H25NO4	331.17836	332.18564	330.17108	CC(C)=CC1C(C(=O)OCN2C(=O)C3=C(CCCC3)C2=O)C1(C)C	
iohexol	Pharmaceuticals	C19H26I3N3O9	820.88031	821.88759	819.87303	CC(=O)N(CC(O)CO)c1c(I)c(C(=O)NCC(O)CO)c(I)c(C(=O)NCC(O)CO)c1I	
allethrin	Pesticides	C19H26O3	302.1882	303.19548	301.18092	CC(C)=CC1C(C(=O)OC2CC(=O)C(CC=C)C2C)C1(C)C	
propargite	Pesticides	C19H26O4S	350.15518	351.16246	349.1479	CC(C)(C)c1ccc(OC2CCCCC2OS(=O)OCC#C)cc1	
valifenalate	Pesticides	C19H27ClN2O5	398.16085	399.16813	397.15357	COC(=O)CC(NC(=O)[C@@H](NC(=O)OC(C)C)C(C)C)c1ccc(Cl)cc1	
fenpropidin	Pesticides	C19H31N	273.24565	274.25293	272.23837	CC(CN1CCCCC1)Cc1ccc(cc1)C(C)(C)C	
chlorphonium	Pesticides	C19H32Cl2P	361.16187	362.16915	360.15459	CCCC[P+](CCCC)(CCCC)Cc1ccc(Cl)cc1Cl	
perindopril	Pharmaceuticals	C19H32N2O5	368.23113	369.23841	367.22385	CCC[C@H](N[C@@H](C)C(=O)N1[C@H]2CCCC[C@H]2C[C@H]1C(O)=O)C(=O)OCC	
etravirine	Pharmaceuticals	C20H15BrN6O	434.04908	435.05636	433.0418	Cc1cc(cc(C)c1Oc1nc(Nc2ccc(cc2)C#N)nc(N)c1Br)C#N	
trovafloxacin	Pharmaceuticals	C20H15F3N4O3	416.10963	417.11691	415.10235	N[C@H]1[C@@H]2CN(C[C@H]12)c1nc2n(cc(C(O)=O)c(=O)c2cc1F)-c1ccc(F)cc1F	
cyflufenamid	Pesticides	C20H17F5N2O2	412.12102	413.1283	411.11374	Fc1ccc(c(\C(NC(=O)Cc2ccccc2)=N\OCC2CC2)c1F)C(F)(F)F	
butafenacil	Pesticides	C20H18ClF3N2O6	474.08055	475.08783	473.07327	CN1C(=O)N(C(=O)C=C1C(F)(F)F)c1ccc(Cl)c(c1)C(=O)OC(C)(C)C(=O)OCC=C	
dolutegravir	Pharmaceuticals	C20H19F2N3O5	419.12928	420.13656	418.122	C[C@@H]1CCO[C@H]2Cn3cc(C(=O)NCc4ccc(F)cc4F)c(=O)c(O)c3C(=O)N12	
trifloxystrobin	Pesticides	C20H19F3N2O4	408.12969	409.13697	407.12241	CO\N=C(/C(=O)OC)c1ccccc1CO\N=C(/C)C1cccc(c1)C(F)(F)F	
fenofibrate	Pharmaceuticals	C20H21ClO4	360.11284	361.12012	359.10556	CC(C)OC(=O)C(C)(C)Oc1ccc(cc1)C(=O)c1ccc(Cl)cc1	
citalopram	Pharmaceuticals	C20H21FN2O	324.16379	325.17107	323.15651	CN(C)CCCC1(OCc2cc(ccc12)C#N)c1ccc(F)cc1	
raltegravir	Pharmaceuticals	C20H21FN6O5	444.15575	445.16303	443.14847	Cc1nnc(o1)C(=O)NC(C)(C)c1nc(C(=O)NCc2ccc(F)cc2)c(O)c(=O)n1C	
ceftobiprole	Pharmaceuticals	C20H22N8O6S2	534.11038	535.11766	533.1031	Nc1nc(ns1)C(=N\O)\C(=O)N[C@H]1[C@H]2SCC(\C=C3/CCN([C@@H]4CCNC4)C3=O)=C(N2C1=O)C(	
avobenzone	PCPs	C20H22O3	310.1569	311.16418	309.14962	OCc1ccc(cc1)C(=O)CC(=O)c1ccc(cc1)C(C)(C)C	
naproxen glucuronide	Metabolites	C20H22O9	406.12639	407.13367	405.11911	COc1ccc2cc(ccc2c1)[C@H](C)C(=O)O[C@@H]1O[C@@H]([C@H](C)naproxen	
amitriptyline	Pharmaceuticals	C20H23N	277.18305	278.19033	276.17577	CN(C)CCC=C1c2ccccc2CCc2ccccc12	
EDDP	Metabolites	C20H23N	277.18305	278.19033	276.17577	\C=C1\N(C)C(C)CC1(c1ccccc1)c1ccccc1	methadone
bitertanol	Pesticides	C20H23N3O2	337.17903	338.18631	336.17175	CC(C)(C)C(O)C(Oc1ccc(cc1)-c1ccccc1)n1cncn1	
azlocillin	Pharmaceuticals	C20H23N5O6S	461.13691	462.14419	460.12963	CC1(C)S[C@@H]2[C@H](NC(=O)[C@H](NC(=O)N3CCNC3=O)c3ccccc3)C(=O)N2[C@H]1C(O)=O	
benalaxyl	Pesticides	C20H23NO3	325.1678	326.17508	324.16052	COC(=O)C(C)N(C(=O)Cc1ccccc1)c1c(C)ccccc1C	
naltrexone	Pharmaceuticals	C20H23NO4	341.16271	342.16999	340.15543	Oc1ccc2C[C@H]3N(CC4CC4)CC[C@@H]45[C@@H](O)c1c24)C(=O)CC[C@@H]35O	
quinine	Pharmaceuticals	C20H24N2O2	324.18378	325.19106	323.1765	COc1ccc2ncccc([C@@H](O)[C@H]3C[C@@H]4CCN3C[C@@H]4C=C)c2c1	
aromasin	Pharmaceuticals	C20H24O2	296.17763	297.18491	295.17035	CC12CCC3C(CC(=C)C4=CC(=O)C=CC34C)C1CCC2=O	
trimipramine	Pharmaceuticals	C20H26N2	294.2096	295.21688	293.20232	C[C@H](CN(C)C)CN1c2ccccc2CCc2ccccc12	

enalapril	Pharmaceuticals	C20H28N2O5	376.19983	377.20711	375.19255	CCOC(=O)[C@H](CCc1ccccc1)N[C@@H](C)C(=O)N1CCC[C@H]1C(=O)=O
neotame	Industrial Chemicals	C20H30N2O5	378.21548	379.22276	377.2082	COC(=O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)=O)NCCC(C)(C)C
benfuracarb	Pesticides	C20H30N2O5S	410.18755	411.19483	409.18027	CCOC(=O)CCN(SN(C)C(=O)Oc1cccc2CC(C)(C)Oc12)C(C)C
carbosulfan	Pesticides	C20H32N2O3S	380.21337	381.22065	379.20609	CCCCN(CCCC)SN(C)C(=O)Oc1cccc2CC(C)(C)Oc12
celiprolol	Pharmaceuticals	C20H33N3O4	379.24711	380.25439	378.23983	CCN(CC)C(=O)Nc1ccc(OC(C)CNC(C)(C)C)c1C1(C)C(=O)
fenpropimorph	Pesticides	C20H33NO	303.25622	304.2635	302.24894	CC(CN1C[C@H](C)O[C@H](C)C1)Cc1ccc(cc1)C(C)(C)C
micronomicin	Pharmaceuticals	C20H41N5O7	463.3006	464.30788	462.29332	CNC[C@@H]1CC[C@@H](N)[C@@H](O[C@@H]2[C@@H](N)C[C@@H](N)[C@H](O[C@@H]3OC[C@H]3)C[C@@H]1)C1C(=O)NC(=O)NC1=CC(CI)=C(OC2=C(CI)C=C(C=N2)C(F)(F)F)C(CI)=C1
chlorfluazuron	Pesticides	C20H9Cl3F5N3O3	538.96297	539.97025	537.95569	FC1=CC=CC(F)=C1C(=O)NC(=O)NC1=CC(CI)=C(OC2=C(CI)C=C(C=N2)C(F)(F)F)C(CI)=C1
deferasirox	Pharmaceuticals	C21H15N3O4	373.10626	374.11354	372.09898	OC(=O)c1ccc(cc1)-n1nc(nc1-c1ccccc1O)-c1ccccc1O
fluoxastrobin	Pesticides	C21H16ClFN4O5	458.07933	459.08661	457.07205	CO\N=C\C1=NOCCO1)C1=CC=CC=C1OC1=C(F)C(OC2=CC=CC=C2Cl)=NC=N1
acemetacin	Pharmaceuticals	C21H18ClNO6	415.08227	416.08955	414.07499	COc1ccc2n(C(=O)c3ccc(Cl)cc3)c(C)c(CC(=O)OCC(O)=O)c2c1
temafloxacin	Pharmaceuticals	C21H18F3N3O3	417.13003	418.13731	416.12275	CC1CN(CCN1)c1cc2n(cc(C(O)=O)c(=O)c2cc1F)-c1ccc(F)cc1F
difloxacin	Pharmaceuticals	C21H19F2N3O3	399.13945	400.14673	398.13217	CN1CCN(CC1)c1cc2n(cc(C(O)=O)c(=O)c2cc1F)-c1ccc(F)cc1
cispermethrin	Pesticides	C21H20Cl2O3	390.07895	391.08623	389.07167	CC1(C)C(C=C(C(Cl)Cl)C1C(=O)OCc1ccccc1Oc2ccccc2)c1
permethrin	Pesticides	C21H20Cl2O3	390.07895	391.08623	389.07167	CC1(C)C(C=C(C(Cl)Cl)C1C(=O)OCc1ccccc1Oc2ccccc2)c1
demeclocycline	Pharmaceuticals	C21H21ClN2O8	464.09865	465.10593	463.09137	CN(C)[C@H]1[C@@H]2C[C@@H]3[C@H](O)C4=C(Cl)C=CC(O)=C4C(=O)C3=C(O)[C@]2(O)C(=O)C(C
posizolid	Pharmaceuticals	C21H21F2N3O7	465.13476	466.14204	464.12748	OC[C@H](O)C(=O)N1CCC(=CC1)c1c(F)cc(cc1F)N1C[C@H](OCc2cccon2)OC1=O
dimethomorph	Pesticides	C21H22ClNO4	387.12374	388.13102	386.11646	COc1ccc(cc1OC)C(=C/C(=O)N1CCOCC1)\c1ccc(Cl)cc1
nafcillin	Pharmaceuticals	C21H22N2O5S	414.12495	415.13223	413.11767	CCOc1ccc2ccccc2c1C(=O)N[C@H]1[C@H]2SC(C)(C)[C@@H](N2C1=O)C(O)=O
flumiclorac-pentyl	Pesticides	C21H23ClFNO5	423.12488	424.13216	422.1176	CCCCCOC(=O)COc1cc(N2C(=O)C3=C(CCCC3)C2=O)c(F)cc1Cl
etoxazole	Pesticides	C21H23F2NO2	359.16969	360.17697	358.16241	CCOC1cc(ccc1C1COC(=N1)c1c(F)cccc1F)C(C)(C)C
moxifloxacin	Pharmaceuticals	C21H24FN3O4	401.17509	402.18237	400.16781	COc1c(N2C[C@@H]3CCCN[C@H]3C2)c(F)cc2c1n(cc(C(O)=O)c2=O)C1CC1
levocetirizine	Pharmaceuticals	C21H25ClN2O3	388.15537	389.16265	387.14809	OC(=O)COCCN1CCN(CC1)[C@H](c1ccccc1)c1ccc(Cl)cc1
terbinafine	Pharmaceuticals	C21H25N	291.1987	292.20598	290.19142	CN(C)C=C\C#CC(C)(C)C)Cc1ccccc1c1ccccc12
mezlocillin	Pharmaceuticals	C21H25N5O8S2	539.11446	540.12174	538.10718	CC1(C)S[C@@H]2[C@H](NC(=O)[C@H](NC(=O)N3CCN(C3=O)S(C)(=O)=O)c3ccccc3)C(=O)N2[C@H]
prednisone	Pharmaceuticals	C21H26O5	358.17803	359.18531	357.17075	C[C@]12CC(=O)[C@H]3[C@@H](CCC4=CC(=O)C=C[C@]34C)[C@@H]1CC[C@]2(O)C(=O)CO
methadone	Pharmaceuticals	C21H27NO	309.20927	310.21655	308.20199	CCC(=O)C(CCC(C)N(C)C)c1ccccc1c1ccccc1
spirotetramat	Pesticides	C21H27NO5	373.18893	374.19621	372.18165	CCOC(=O)OC1=C(C(=O)N[C@@H]11CC[C@@H](CC1)OC)c1cc(C)ccc1C
buthiobate	Pesticides	C21H28N2S2	372.16939	373.17667	371.16211	CCCCS\CScc1ccc(cc1)C(C)(C)C)=N\c1ccccc1
cortisone	Pharmaceuticals	C21H28O5	360.19368	361.20096	359.1864	C[C@]12CC(=O)[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@]2(O)C(=O)CO
prednisolone	Pharmaceuticals	C21H28O5	360.19368	361.20096	359.1864	C[C@]12CC[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)C=C[C@]34C)[C@@H]1CC[C@]2(O)C(=O)CO
progesterone	Pharmaceuticals	C21H30O2	314.22458	315.23186	313.2173	CC(=O)[C@H]1CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C
corticosterone	Pharmaceuticals	C21H30O4	346.21441	347.22169	345.20713	C[C@]12C[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@]2(O)CO
cortisol	Pharmaceuticals	C21H30O5	362.20933	363.21661	361.20205	C[C@]12C[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@]2(O)C(=O)CO
streptomycin	Pharmaceuticals	C21H39N7O12	581.26567	582.27295	580.25839	CN[C@H]1[C@H](O)[C@@H](O)[C@H](CO)O[C@H]1O[C@H]1[C@H](O)[C@H]2[C@H](O)[C@@H]
netilmicin	Pharmaceuticals	C21H41N5O7	475.3006	476.30788	474.29332	CCN[C@@H]1C[C@H](N)[C@@H](O[C@H]2OC(CN)=CC[C@H]2N)[C@H](O)[C@H]1O[C@H]1OC[C
miltefosine	Pharmaceuticals	C21H46NO4P	407.31645	408.32373	406.30917	CCCCCCCCCCCCCCCCOP([O-])(=O)OCC[N+](C)(C)C
indoxacarb	Pesticides	C22H17ClF3N3O7	527.07072	528.078	526.06344	COC(=O)N(C(=O)N1CO[C@H]2(Cc3cc(Cl)ccc3C2=N1)C(=O)OC)c1ccc(OC(F)(F)F)cc1
clotrimazole	Pharmaceuticals	C22H17ClN2	344.10803	345.11531	343.10075	Clc1ccccc1C(c1ccccc1)(c1ccccc1)n1ccnc1
azoxystrobin	Pesticides	C22H17N3O5	403.11682	404.1241	402.10954	CO\C=C\C(=O)OC)c1ccccc1Oc1cc(OC2ccccc2C#N)ncn1
cyfluthrin	Pesticides	C22H18Cl2FNO3	433.06478	434.07206	432.0575	CC1(C)C(C=C(C(Cl)Cl)C1C(=O)OC(C#N)c1ccc(F)c(Oc2ccccc2)c1
famoxadone	Pesticides	C22H18N2O4	374.12666	375.13394	373.11938	CC1(OC(=O)N(Nc2ccccc2)C1=O)c1ccc(OC2ccccc2)cc1
rilpivirine	Pharmaceuticals	C22H18N6	366.1593	367.16658	365.15202	Cc1cc(\C=C\C#N)cc(C)c1Nc1ccnc(Nc2ccc(cc2)C#N)n1
decamethrin	Pesticides	C22H19Br2NO3	502.97317	503.98045	501.96589	CC1(C)[C@@H](C=C(Br)Br)[C@H]1C(=O)O[C@H](C#N)c1ccccc1Oc2ccccc2)c1
tralomethrin	Pesticides	C22H19Br4NO3	660.80985	661.81713	659.80257	CC1(C)C(C(Br)C(Br)(Br)Br)C1C(=O)OC(C#N)c1ccccc1Oc2ccccc2)c1
cypermethrin	Pesticides	C22H19Cl2NO3	415.0742	416.08148	414.06692	CC1(C)[C@@H](C=C(C(Cl)Cl)[C@H]1C(=O)O[C@H](C#N)c1ccccc1Oc2ccccc2)c1
atovaquone	Pharmaceuticals	C22H19ClO3	366.10228	367.10956	365.095	OC1=C([C@H]2CC[C@@H](CC2)C2=CC=C(CI)C=C2)C(=O)C2=CC=CC=C2C1=O
benzobicyclon	Pesticides	C22H19ClO4S2	446.04133	447.04861	445.03405	CS(=O)(=O)c1ccc(C(=O)C2=C(C3ccccc3)C3CCC(C3)C2=O)c(Cl)c1
benzofenap	Pesticides	C22H20Cl2N2O3	430.0851	431.09238	429.07782	Cc1nn(C)c(OC(C)=O)c2ccc(C)cc2)c1C(=O)c1ccc(Cl)c(C)c1Cl

ceftaroline	Pharmaceuticals	C22H20N8O5S4	604.04395	605.05123	603.03667	CCO\N=C/(C(=O)N[C@H]1[C@H]2SCC(SC3=NC(=CS3)C3=CC=[N+](C)C=C3)=C(N2C1=O)C([O-])=O)C:
ceftaroline fosamil	Pharmaceuticals	C22H21N8O8PS4	684.01028	685.01756	683.003	CCO\N=C/(C(=O)N[C@H]1[C@H]2SCC(SC3=NC(=CS3)C3=CC=[N+](C)C=C3)=C(N2C1=O)C([O-])=O)C:
propaquizafop	Pesticides	C22H22ClN3O5	443.1248	444.13208	442.11752	C[C@H](O)c1ccc(Oc2cnc3cc(Cl)ccc3n2)cc1C(=O)OCCON=C(C)C
ceftazidime	Pharmaceuticals	C22H22N6O7S2	546.09914	547.10642	545.09186	CC(C)(O)\N=C/(C(=O)N[C@H]1[C@H]2SCC(C[n+3cccc3]=C(N2C1=O)C([O-])=O)c1csc(N)n1C(C)=O
chlortetracycline	Pharmaceuticals	C22H23ClN2O8	478.1143	479.12158	477.10702	CN(C)[C@H]1[C@H]2C[C@H]3C(=C(O)[C@H]2(O)C(=O)C(C(O)=N)=C1O)C(=O)c1c(O)ccc(Cl)c1[C@H]3
losartan	Pharmaceuticals	C22H23ClN6O	422.16219	423.16947	421.15491	CCCCc1nc(Cl)c(CO)n1Cc1ccc(cc1)-c1cccc1-c1nnnn1
razeolid	Pharmaceuticals	C22H23FN6O3	438.18157	439.18885	437.17429	CC(=O)NC[C@H]1CN(C(=O)O)C1=CC(F)=C(C=C1)C1=CC=C(CNCC2=CN=NN2)C=C1
fenpropathrin	Pesticides	C22H23NO3	349.1678	350.17508	348.16052	CC1(C)C(C(=O)OC(C#N)c2cccc(Oc3cccc3)c2)C1(C)C
narcotine	Pharmaceuticals	C22H23NO7	413.14746	414.15474	412.14018	COc1ccc2[C@H](OC(=O)c2c1OC)[C@H]1N(C)CCc2cc3OCOC3c(OC)c12
tetracycline	Pharmaceuticals	C22H24N2O8	444.15327	445.16055	443.14599	CN(C)[C@H]1[C@H]2C[C@H]3C(=C(O)[C@H]2(O)C(=O)C(C(N)=O)=C1O)C(=O)c1c(O)cccc1[C@@H]3
oxytetracycline	Pharmaceuticals	C22H24N2O9	460.14818	461.15546	459.1409	CN(C)[C@H]1[C@H]2C[C@H](O)[C@H]3C(=C(O)[C@H]2(O)C(=O)C(C(N)=O)=C1O)C(=O)C1=C(C=C
ertapenem	Pharmaceuticals	C22H25N3O7S	475.14132	476.1486	474.13404	C[C@H](O)[C@H]1[C@H]2[C@H](C)C(S[C@@H]3CN[C@H](C3)C(=O)Nc3cccc(c3)C(O)=O):
diltiazem	Pharmaceuticals	C22H26N2O4S	414.16133	415.16861	413.15405	COc1ccc(cc1)[C@@H]1Sc2cccc2N(CCN(C)C)C(=O)[C@H]1OC(C)=O
bioresmethrin	Pesticides	C22H26O3	338.1882	339.19548	337.18092	CC(C)=CC1C(C(=O)OCc2coc(Cc3cccc3)c2)C1(C)C
rosuvastatin	Pharmaceuticals	C22H28FN3O6S	481.16829	482.17557	480.16101	CC(C)c1nc(nc(-c2ccc(F)cc2)c1\C=C\C[C@H](O)C[C@H](O)CC(O)=O)N(C)S(C(=O)=O
tebufenozide	Pesticides	C22H28N2O2	352.21508	353.22236	351.2078	CCc1ccc(cc1)C(=O)NN(C(=O)c1cc(C)cc(C)c1)C(C)(C)C
methoxyfenozide	Pesticides	C22H28N2O3	368.21	369.21728	367.20272	COc1cccc(C(=O)NN(C(=O)c2cc(C)cc(C)c2)C(C)(C)C)c1C
delavirdine	Pharmaceuticals	C22H28N6O3S	456.19436	457.20164	455.18708	CC(C)Nc1ccnc1N1CCN(CC1)C(=O)c1cc2cc(NS(C)(=O)=O)ccc2[nH]1
sofosbuvir	Pharmaceuticals	C22H29FN3O9P	529.16255	530.16983	528.15527	CC(C)OC(=O)[C@H](C)N[P@](=O)(OC[C@H]1O[C@@H](n2ccc(=O)[nH]c2=O)[C@](C)(F)[C@@H]1C
betamethasone	Pharmaceuticals	C22H29FO5	392.19991	393.20719	391.19263	C[C@H]1C[C@H]2[C@@H]3CCCC4=CC(=O)C=C[C@H]4(C)[C@@]3(F)[C@H](O)C[C@H]2(C)[C@@]1(F
chlorhexidine	PCPs	C22H30Cl2N10	504.2032	505.21048	503.19592	Clc1ccc(CN(=N)NC(=N)NCCCCCNC(=N)NC(=N)Nc2ccc(Cl)cc2)cc1
methylprednisolone	Pharmaceuticals	C22H30O5	374.20933	375.21661	373.20205	[H][C@@]12CC[C@](O)(C(=O)CO)[C@@]1(C)C[C@H](O)[C@@]1([H])[C@@]2([H])C[C@]([H])(C)C:
oxybutynin	Pharmaceuticals	C22H31NO3	357.2304	358.23768	356.22312	CCN(CC)CC#CCOC(=O)C(O)(C1CCCCC1)c1cccc1
quicifal	PCPs	C22H38O7	414.26176	415.26904	413.25448	CCCCCCCCCCCCC(=O)OC[C@H](O)[C@H]1OC(=O)C(O)=C1O
benzamorf	Pesticides	C22H39NO4S	413.25998	414.26726	412.2527	C1OCC[NH2+].CCCCCCCCCCCCc1ccc(cc1)S([O-])(=O)=O
amikacin	Pharmaceuticals	C22H43N5O13	585.28574	586.29302	584.27846	C1C(C(C(C1NC(=O)C(CCN)O)OC2C(C(C(C(O2)CO)O)N)O)OC3C(C(C(C(O3)CN)O)O)O)N
chlorophacinone	Pesticides	C23H15ClO3	374.07098	375.07826	373.0637	Clc1ccc(cc1)C(C(=O)C1C(=O)c2cccc2C1=O)c1cccc1
diphacinone	Pesticides	C23H16O3	340.10995	341.11723	339.10267	O=C(C(c1cccc1)c1cccc1)C1(C(=O)c2cccc2C1=O
gamma-cyhalothrin	Pesticides	C23H19ClF3NO3	449.10056	450.10784	448.09328	CC1(C(C1C(=O)OC(C#N)C2=CC(=CC=C2)OC3=CC=CC=C3)C=C(C(F)(F)F)Cl)C
bifenthrin	Pesticides	C23H22ClF3O2	422.12605	423.13333	421.11877	Cc1c(COC(=O)C2C(\C=C(Cl)C(F)(F)F)C2(C)C)cccc1-c1cccc1
mandipropamid	Pesticides	C23H22ClNO4	411.12374	412.13102	410.11646	COC1=C(OCC#C)C=CC(CN(C(=O)C(OCC#C)C2=CC=C(C)C=C2)=C1
elvitegravir	Pharmaceuticals	C23H23ClFNO5	447.12488	448.13216	446.1176	COc1cc2n(cc(C(O)=O)c(=O)c2cc1Cc1cccc(Cl)c1F)[C@H](CO)C(C)C
eprosartan	Pharmaceuticals	C23H24N2O4S	424.14568	425.15296	423.1384	CCCCc1ncc(\C=C(\Cc2cccs2)C(O)=O)n1Cc1ccc(cc1)C(O)=O
phenothrin	Pesticides	C23H26O3	350.1882	351.19548	349.18092	CC(C)=CC1C(C(=O)OCC2=CC(OC3=CC=CC=C3)=CC=C2)C1(C)C
minocycline	Pharmaceuticals	C23H27N3O7	457.1849	458.19218	456.17762	CN(C)[C@H]1[C@@H]2C[C@H]3Cc4c(ccc(O)c4C(=O)C3=C(O)[C@H]2(O)C(=O)C(C(O)=N)=C1O)N(C
piperacillin	Pharmaceuticals	C23H27N5O7S	517.16312	518.1704	516.15584	CCN1CCN(C(=O)C1=O)C(=O)NC(C2=CC=CC=C2)C(=O)NC3C4N(C3=O)C(C(S4)(C)C)C(=O)O
6-O-desmethyl donepezil	Metabolites	C23H27NO3	365.1991	366.20638	364.19182	COc1cc2CC(CC3CCN(Cc4cccc4)CC3)C(=O)c2cc1O donepezil
ceftolozane	Pharmaceuticals	C23H30N12O8S2	666.1751	667.18238	665.16782	Cn1c(N)c(NC(=O)NCCN)c[n+1]CC1=C(N2[C@H](SC1)[C@H](NC(=O)C(=N/OC(C)(C)C(O)=O)\c1nsc(N
spiromesifen	Pesticides	C23H30O4	370.21441	371.22169	369.20713	Cc1cc(C)C(C2=C(C(OC(=O)CC(C)(C)C(CCCC3)OC2=O)c(C)C1
fludrocortisone acetate	Pharmaceuticals	C23H31FO6	422.21047	423.21775	421.20319	CC(=O)OCC(=O)[C@@H]1(O)CC(C[C@H]2[C@@H]3CCCC4=CC(=O)CC[C@H]4(C)[C@@]3(F)[C@@H](O)C[
diafenthuiuron	Pesticides	C23H32N2O5	384.22354	385.23082	383.21626	CC(C)c1cc(Oc2cccc2)cc(C(C)C)c1NC(=S)NC(C)(C)C
pravastatin	Pharmaceuticals	C23H36O7	424.24611	425.25339	423.23883	CC[C@H](C)C(=O)O[C@H]1C[C@H](O)C=C2C=C[C@H](C)[C@H](CC[C@@H](O)C[C@H](O)CC(
paromomycin	Pharmaceuticals	C23H45N5O14	615.2963	616.30358	614.28902	NC[C@@H]1O[C@H](O)[C@@H]2[C@@H](CO)O[C@@H](O)[C@@H]3[C@H](O)[C@H](N)C[C@H]1
neomycin B	Pharmaceuticals	C23H46N6O13	614.31229	615.31957	613.30501	NC[C@@H]1O[C@H](O)[C@@H]2[C@@H](CO)O[C@@H](O)[C@@H]3[C@H](O)[C@H](N)C[C@H]1
10,10'-oxybisphenoxar	Pesticides	C24H16As2O3	501.95314	502.96042	500.94586	O([As]1c2cccc2Oc2cccc12)[As]1c2cccc2Oc2cccc12
metaflumizone	Pesticides	C24H16F6N4O2	506.11775	507.12503	505.11047	FC(F)(F)OC1ccc(NC(=O)N\N=C(\Cc2ccc(cc2)C#N)c2cccc(c2)C(F)(F)F)cc1
candesartan	Pharmaceuticals	C24H20N6O3	440.15969	441.16697	439.15241	CCOc1nc2cccc(C(O)=O)c2n1Cc1ccc(cc1)-c1cccc1-c1nnnn[nH]1
2,4-DEP	Pesticides	C24H21Cl6O6P	645.92069	646.92797	644.91341	Clc1ccc(OCCOP(OCCOc2ccc(Cl)cc2Cl)OCCOc2ccc(Cl)cc2Cl)c(Cl)c1
cyflumetofen	Pesticides	C24H24F3NO4	447.16575	448.17303	446.15847	COCCOC(=O)C(C#N)(C(=O)c1cccc1C(F)(F)F)c1ccc(cc1)C(C)(C)C

cyphenothrin	Pesticides	C24H25NO3	375.18345	376.19073	374.17617	CC(C)=CC1C(C(=O)OC(C#N)c2cccc(Oc3ccccc3)c2)C1(C)C
fluvastatin	Pharmaceutials	C24H26FNO4	411.18459	412.19187	410.17731	CC(C)n1c(\C=C\ [C@H](O)C[C@H](O)CC(O)=O)c(-c2ccc(F)cc2)c2ccccc12
octocrylene	PCPs	C24H27NO2	361.20418	362.21146	360.1969	CCCC(C)COC(=O)C(C#N)=C(c1cccc1)c1cccc1
platensimycin	Pharmaceutials	C24H27NO7	441.17876	442.18604	440.17148	[C@H]12C[C@H]34C[C@H]1C[C@H](O2)[C@H]3[C@H](C)(CCC(=O)Nc1c(O)ccc(C(=O)c1O)C(=O)C
valsartan	Pharmaceutials	C24H29N5O3	435.22704	436.23432	434.21976	CCCC(=O)N(CC1=CC=C(C=C1)C1=C(C=CC=C1)C1=NN=NN1)[C@H](C(C)C)C(O)=O
chromafenozide	Pesticides	C24H30N2O3	394.22565	395.23293	393.21837	Cc1cc(C)cc(c1)C(=O)N(NC(=O)c1ccc2OCCCC2c1C)C(C)C
dexamethasone acetat	Metabolites	C24H31FO6	434.21047	435.21775	433.20319	[C@H]1C[C@H]2[C@H]3CCC4=CC(=O)C=C[C@H]4(C)[C@H]3C[C@H]2O
acequinocyl	Pesticides	C24H32O4	384.23006	385.23734	383.22278	CCCCCCCCCCCC1=C(OC(C)=O)C(=O)c2ccccc2C1=O
butroxydim	Pesticides	C24H33NO4	399.24096	400.24824	398.23368	CCCC(=O)c1c(C)cc(C)c(C2CC(O)=C(\C(CC)=N\OCC)C(=O)C2)c1C
lovastatin	Pharmaceutials	C24H36O5	404.25628	405.26356	403.249	CC[C@H](C)C(=O)O[C@H]1C[C@H](C)C=C2C=C[C@H](C)[C@H](CC[C@H]3C[C@H](O)CC(=O
fenvalerate	Pesticides	C25H22ClNO3	419.12882	420.1361	418.12154	CC(C)C(C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1)c1ccc(Cl)cc1
hydramethylnon	Pesticides	C25H24F6N4	494.19052	495.1978	493.18324	CC1(C)CNC(NN=C(\C=C\c2ccc(cc2)C(F)F)/C=C/c2ccc(cc2)C(F)F)=NC1
benzfendione	Pesticides	C25H25F3N2O6	506.16647	507.17375	505.15919	CCc1ccc(COc2ccc(cc2)N2C(=O)C=C(N(C)C2=O)C(F)F)c(OC(C)C(=O)OC)c1
sertraline carbamoyl gl	Metabolites	C25H27Cl2NO8	539.11138	540.11866	538.1041	CN([C@H]1CC[C@H](c2ccc(Cl)c(Cl)c2)c2ccccc12)C(=O)O[C] sertraline
cefoperazone	Pharmaceutials	C25H27N9O8S2	645.1424	646.14968	644.13512	CCN1CCN(C(=O)N[C@H](C(=O)N[C@H]2[C@H]3SCC(CSc4nnnn4C)=C(N3C2=O)C(O)=O)c2ccc(O)cc2
irbesartan	Pharmaceutials	C25H28N6O	428.23246	429.23974	427.22518	CCCCC1=NC2(CCCCC2)C(=O)N1Cc1ccc(cc1)-c1cccc1-c1nn[nH]n1
etofenprox	Pesticides	C25H28O3	376.20385	377.21113	375.19657	CCOc1ccc(cc1)C(C)(C)COCc1cccc(Oc2ccccc2)c1
tropium	Pharmaceutials	C25H30ClNO3	427.19142	428.1987	426.18414	[Cl-].OC(C(=O)O[C@H]1CC2CCC(C1)[N+]21CCCC1)(c1cccc1)c1cccc1
2-hydroxy imipramine	Metabolites	C25H32N2O7	472.22095	473.22823	471.21367	CN(C)CCCN1c2ccccc2Cc2cc(O[C@H]3O[C@H]([C@H] imipramine
budesonide	Pharmaceutials	C25H34O6	430.23554	431.24282	429.22826	CCCC1O[C@H]2C[C@H]3[C@H]4CCCC5=CC(=O)C=C[C@H]5(C)[C@H]4[C@H](O)C[C@H]3(C)[C@
amprenavir	Pharmaceutials	C25H35N3O6S	505.22466	506.23194	504.21738	CC(C)CN(CC(C)CC1=CC=CC=C1)NC(=O)OC2CCOC2)O)S(=O)(=O)C3=CC=C(C=C3)N
simvastatin	Pharmaceutials	C25H38O5	418.27193	419.27921	417.26465	CCC(C)C(C(=O)O[C@H]1C[C@H](C)C=C2C=C[C@H](C)[C@H](CC[C@H]3C[C@H](O)CC(=O)O
acrinathrin	Pesticides	C26H21F6NO5	541.1324	542.13968	540.12512	CC1(C)C(\C=C\C(=O)OC(C(F)F)C(F)F)C1C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1
brofluthrinat	Pesticides	C26H22BrF2NO4	529.07003	530.07731	528.06275	CC(C)C(C(=O)OC(C#N)C1=CC(OC2=CC=C(Br)C=C2)=CC=C1)C1=CC=C(OC(F)F)C=C1
tau-fluvalinate	Pesticides	C26H22ClF3N2O3	502.12711	503.13439	501.11983	CC(C)[C@H](Nc1ccc(cc1Cl)C(F)F)C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1
cambendichlor	Pesticides	C26H23Cl4NO6	585.02795	586.03523	584.02067	COc1c(Cl)ccc(Cl)c1C(=O)OCCN(CCOc(=O)c1c(Cl)ccc(Cl)c1OC)c1cccc1
dasabuvir	Pharmaceutials	C26H27N3O5S	493.16714	494.17442	492.15986	COc1c(cc(c1C(C)C(C)C)-n1ccc(=O)[nH]c1=O)-c1ccc2cc(NS(C)(=O)=O)ccc2c1
ketoconazole	Pharmaceutials	C26H28Cl2N4O4	530.14876	531.15604	529.14148	CC(=O)N1CCN(CC1)C1=CC=C(OC[C@H]2CO[C@H](CN3C=CN=C3)(O2)C2=C(Cl)C=C(Cl)C=C2)C=C1
halofantrine	Pharmaceutials	C26H30Cl2F3NO	499.16566	500.17294	498.15838	CCCCN(CCCC)CCC(O)c1cc2c(Cl)cc(Cl)cc2c2cc(ccc12)C(F)F
bufen carb	Pesticides	C26H38N2O4	442.28316	443.29044	441.27588	CCC[C@H](C)c1cccc(OC(=O)NC)c1.CCC(CC)c1cccc(OC(=O)NC)c1
mupirocin	Pharmaceutials	C26H44O9	500.29854	501.30582	499.29126	[C@H](O)[C@H](C)[C@H]1O[C@H]1C[C@H]1CO[C@H](C)C(C)=C\C(=O)OCCCCCCCC(O)=O
clofazimine	Pharmaceutials	C27H22Cl2N4	472.12216	473.12944	471.11488	CC(C)\N=c1/cc2-c(cc1Nc1ccc(Cl)cc1)nc1cccc1n2-c1ccc(Cl)cc1
darunavir	Pharmaceutials	C27H37N3O7S	547.23522	548.2425	546.22794	CC(C)CN(C[C@H](O)[C@H](Cc1ccccc1)NC(=O)O[C@H]1CO[C@H]2OCC[C@H]12)S(=O)(=O)c1c
verapamil	Pharmaceutials	C27H38N2O4	454.28316	455.29044	453.27588	COC1=C(OC)C=C(CCN(C)CCCC(C#N)(C(C)C)C2=CC(OC)=C(OC)C=C2)C=C1
cholecalciferol	Pesticides	C27H44O	384.33922	385.3465	383.33194	CC(C)CCC[C@H](C)[C@H]1CC[C@H]2\C(CCC[C@H]12C)=C\C=C1\C[C@H](O)CCC1=C
boceprevir	Pharmaceutials	C27H45N5O5	519.34207	520.34935	518.33479	CC(C)(C)NC(=O)N[C@H](C(=O)N1C[C@H]2[C@H]([C@H]1C(=O)NC(C1CCC1)C(=O)C(N)=O)C2(C)
ecamsule	PCPs	C28H34O8S2	562.16951	563.17679	561.16223	CC1(C)C2CCC1(CS(O)(=O)=O)C(=O)\C2=C/c1ccc(\C=C2\C3CCC(CS(O)(=O)=O)(C2=O)C3(C)C)cc1
neohesperidin dihydro	Industrial Chemicals	C28H36O15	612.20542	613.2127	611.19814	COc1ccc(CCC(=O)c2c(O)cc(O[C@H]3O[C@H](CO)[C@H](O)[C@H](O)[C@H]3O[C@H]3O[C@H]3O[C@
calciferol	Pesticides	C28H44O	396.33922	397.3465	395.33194	CC(C)[C@H](C)\C=C\ [C@H](C)[C@H]1CC[C@H]2\C(CCC[C@H]12C)=C\C=C1\C[C@H](O)CCC1=
tokoferol	PCPs	C28H48O2	416.36543	417.37271	415.35815	CC(C)CCCC(C)CCCC(C)CCCC1(C)CCc2cc(O)c(C)C(C)c2O1
brassinolide	Pesticides	C28H48O6	480.34509	481.35237	479.33781	CC(C)[C@H](C)[C@H](O)[C@H](O)[C@H](C)[C@H]1CC[C@H]2[C@H]3COC(=O)[C@H]4C[C@
tigecycline	Pharmaceutials	C29H39N5O8	585.27987	586.28715	584.27259	CN(C)[C@H]1[C@H]2C[C@H]3CC4=C(C=C(NC(=O)CNC(C)(C)C)O)=C4C(=O)C3=C(O)[C@H]2(O)
geldanamycin	Pharmaceutials	C29H40N2O9	560.27338	561.28066	559.2661	CC1CC(C(C(=C(C(C(=CC(=O)NC2=CC(=O)C=C(C1)C2=O)OC)C)OC(=O)N(C)C)O)OC
maraviroc	Pharmaceutials	C29H41F2N5O	513.32792	514.3352	512.32064	CC(C)c1nn(C)n1[C@H]1C[C@H]2CC[C@H](C1)N2CC[C@H](NC(=O)C1CCC(F)(F)CC1)c1cccc1
bis-trichloromethyl sul	Pesticides	C2Cl6O2S	297.77498	298.78226	296.7677	ClC(Cl)(Cl)S(=O)(=O)C(Cl)(Cl)Cl
chloral hydrate	Pesticides	C2H3Cl3O2	163.91987	164.92715	162.91259	OC(O)C(Cl)(Cl)Cl
1,2-dibromoethane	Pesticides	C2H4Br2	185.86798	186.87526	184.8607	BrCCBr
amitrole	Pesticides	C2H4N4	84.0436	85.05088	83.03632	Nc1ncnn1
peroxyacetic acid	Pesticides	C2H4O3	76.01605	77.02333	75.00877	CC(=O)OO

ethephon	Pesticides	C2H6ClO3P	143.97431	144.98159	142.96703 OP(O)(=O)CCCl
dimethyl disulfide	Pesticides	C2H6S2	93.99109	94.99837	92.98381 CSSC
cacodylic acid	Pesticides	C2H7AsO2	137.9662	138.97348	136.95892 C[As](C)(O)=O
2-hydrazinoethanol	Pesticides	C2H8N2O	76.06367	77.07095	75.05639 NNCCO
methamidophos	Pesticides	C2H8NO2PS	141.00134	142.00862	139.99406 COP(N)(=O)SC
bromadiolone	Pesticides	C30H23BrO4	526.07798	527.08526	525.0707 OC(CC(C1=CC=CC=C1)C1=C(O)OC2=CC=CC=C2C1=O)C1=CC=C(C=C1)C1=CC=C(Br)C=C1
lumefantrine	Pharmaceuticals	C30H32Cl3NO	527.15495	528.16223	526.14767 CCCC(N(CCCC)CC(O)c1cc(Cl)cc2\C=C/c3ccc(Cl)cc3)c3cc(Cl)ccc3-c12
herbimycin	Pharmaceuticals	C30H42N2O9	574.28903	575.29631	573.28175 CC1CC(C(C(C=C(C(C(C=CC=C(C(=O)NC2=CC(=O)C=C(C1OC)C2=O)C)OC)OC(=O)N)C)OC)OC
enoxolone	Pharmaceuticals	C30H46O4	470.33961	471.34689	469.33233 CC1(C)[C@H](O)CC[C@H]2(C)[C@H]1CC[C@H]1(C)[C@H]2C(=O)C=C2[C@H]3C[C@H](C)(CC(C
aliskiren	Pharmaceuticals	C30H53N3O6	551.39344	552.40072	550.38616 COCCCCOC1=C(OC)C=CC(C[C@H](C[C@H](N)[C@H](O)C[C@H](C(C)C)C(=O)NCC(C)(C)C(N)=O
difethialone	Pesticides	C31H23BrO2S	538.06022	539.0675	537.05294 OC1=C(C2CC(Cc3cccc23)c2ccc(cc2)-c2ccc(Br)cc2)C(=O)c2cccc2S1
brodifacoum	Pesticides	C31H23BrO3	522.08306	523.09034	521.07578 OC1=C(C2CC(Cc3=CC=CC=C23)C2=CC=C(C=C2)C2=CC=C(Br)C=C2)C(=O)C2=CC=CC=C2O1
difenacoum	Pesticides	C31H24O3	444.17255	445.17983	443.16527 OC1=C(C2CC(Cc3cccc23)c2ccc(cc2)-c2cccc2)C(=O)c2cccc2O1
tipranavir	Pharmaceuticals	C31H33F3N2O5S	602.20623	603.21351	601.19895 C[C@H]1(C)CC2=CC=CC=C2C(C)C(=O)C([C@H](CC)C2=CC(NS(=O)F)=O)C3=NC=C(C=C3)C(F)(F)F)=CC=
dronedarone	Pharmaceuticals	C31H44N2O5S	556.2971	557.30438	555.28982 CCCC(N(CCCC)CCCOc1ccc(cc1)C(=O)c1(CCCC)oc2ccc(NS(C)(=O)F)=O)cc12
fusidic acid	Pharmaceuticals	C31H48O6	516.34509	517.35237	515.33781 CC1C2CCC3(C(C2(CCC1O)C)C(CC4C3(CC(C4=C(CCC=C(C)C)C(
bedaquiline	Pharmaceuticals	C32H31BrN2O2	554.15689	555.16417	553.14961 COc1nc2ccc(Br)cc2cc1[C@H](c1cccc1)[C@H](O)(CCN(C)C)c1cccc2cccc12
fexofenadine	Pharmaceuticals	C32H39NO4	501.28791	502.29519	500.28063 CC(C)(C(O)=O)c1ccc(cc1)C(O)CCCN1CCC(CC1)C(O)(c1cccc1)c1cccc1
nelfinavir	Pharmaceuticals	C32H45N3O4S	567.31308	568.32036	566.3058 CC1=C(C=CC=C1O)C(=O)NC(CSC2=CC=CC=C2)C(CN3CC4CCCC4CC3C(=O)NC(C)(C)C)O
telmisartan	Pharmaceuticals	C33H30N4O2	514.23688	515.24416	513.2296 CCCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1cccc1C(O)=O)c1nc2cccc2n1C
atorvastatin	Pharmaceuticals	C33H35FN2O5	558.253	559.26028	557.24572 CC(C)c1c(C(=O)Nc2cccc2)c(c(-c2ccc(F)cc2)n1CC[C@H](O)C[C@H](O)CC(O)=O)-c1cccc1
afidopyropen	Pesticides	C33H39NO9	593.26248	594.26976	592.2552 [H][C@H]12C[C@H](O)[C@H]3(C)OC4=C([C@H](O)[C@H]3([H]))[C@H]1(C)CC[C@H](OC(=O)C1CC1)[I
reserpine	Pharmaceuticals	C33H40N2O9	608.27338	609.28066	607.2661 CO[C@H]1[C@H](O)[C@H]2CN3CCc4c([nH]c5cc(OC)ccc45)[C@H]3C[C@H]2[C@H]1C(=O)OC
dalfopristin	Pharmaceuticals	C34H50N4O9S	690.32985	691.33713	689.32257 CCN(CC)CCS(=O)(=O)C1CCN2C1C(=O)OC(C(C)C)C(C)C=C\C(=O)N\C=C\C(=O)O)CC(=O)Cc1nc(
isavuconazonium	Pharmaceuticals	C35H35F2N8O5S	717.24192	718.2492	716.23464 CNCC(=O)OCC1=C(N=CC=C1)N(C)C(=O)OC(C)[N+]=CN(C[C@H](O)([C@H](C)C2=NC(=CS2)C2=C(
itraconazole	Pharmaceuticals	C35H38Cl2N8O4	704.23931	705.24659	703.23201 CCC(C)n1ncn(-c2ccc(cc2)N2CCN(CC2)c2ccc(OC[C@H]3CO[C@H](Cn4cncn4)(O3)c3ccc(Cl)cc3Cl)cc2
oleandomycin	Pharmaceuticals	C35H61NO12	687.41938	688.42666	686.4121 CO[C@H]1C[C@H](O)[C@H]2(C)[C@H](O)[C@H]3(C)[C@H](O)[C@H]3O)N(C)C(
indinavir	Pharmaceuticals	C36H47N5O4	613.36281	614.37009	612.35553 CC(C)(C)NC(=O)C1CN(CCN1CC(CC(C2=CC=CC=C2)C(=O)NC3C(CC4=CC=CC=C34)O)O)CC5=CN=CC=
telaprevir	Pharmaceuticals	C36H53N7O6	679.40574	680.41302	678.39846 CCC[C@H](NC(=O)[C@H]1[C@H]2CCC[C@H]2CN1C(=O)[C@H](NC(=O)[C@H](NC(=O)c1cnc1
retinyl palmitate	PCPs	C36H60O2	524.45933	525.46661	523.45205 CCCCCCCCCCCCCC(=O)OC\C=C(/C)\C=C\C=C(/C)\C=C\C=C(C)CCCC1(C)C
posaconazole	Pharmaceuticals	C37H42F2N8O4	700.32971	701.33699	699.32243 CC[C@H]([C@H](C)O)n1ncn(-c2ccc(cc2)N2CCN(CC2)c2ccc(OC[C@H]3CO[C@H](Cn4cncn4)(C3)c
lopinavir	Pharmaceuticals	C37H48N4O5	628.36247	629.36975	627.35519 CC(C)[C@H](N1CCNC1=O)C(=O)N[C@H](C[C@H](O)[C@H](Cc1cccc1)NC(=O)COc1c(C)cccc1C)Cc:
ritonavir	Pharmaceuticals	C37H48N6O5S2	720.31276	721.32004	719.30548 CC(C)C1=NC(=CS1)CN(C)C(=O)NC(C(C)C)C(=O)NC(CC2=CC=CC=C2)CC(C(Cc3=CC=CC=C3)NC(=O)OC
erythromycin	Pharmaceuticals	C37H67NO13	733.46124	734.46852	732.45396 CC[C@H]1OC(=O)[C@H](C)[C@H]2(C)[C@H](O)[C@H]2C[C@H](C)(OC)[C@H](O)[C@H](C)O2)[C@H](C)(C
simeprevir	Pharmaceuticals	C38H47N5O7S2	749.29169	750.29897	748.28441 COc1ccc2c(O[C@H]3C[C@H]4[C@H]3(C)C(=O)N(C)CCCC\C=C/[C@H]3C[C@H]3(NC4=O)C(=
bis-ethylhexyloxypheni	PCPs	C38H49N3O5	627.36722	628.3745	626.35994 CCCCC(CC)COC1=CC(O)=C(C=C1)C1=NC(=NC(=N1)C1=CC=C(OC)C=C1)C1=C(O)C=C(OC(C)CCCC)C:
saquinavir	Pharmaceuticals	C38H50N6O5	670.38427	671.39155	669.37699 CC(C)(C)NC(=O)C1CC2CCCC2CN1CC(C(Cc3=CC=CC=C3)NC(=O)C(Cc(=O)N)NC(=O)C4=NC5=CC=CC=
grazoprevir	Pharmaceuticals	C38H50N6O9S	766.336	767.34328	765.32872 COc1ccc2nc3CCCC[C@H]4C[C@H]4OC(=O)N[C@H](C(=O)N4C[C@H](C[C@H]4C(=O)N(C)C@H
atazanavir	Pharmaceuticals	C38H52N6O7	704.38975	705.39703	703.38247 COC(=O)N(C)[C@H](C(=O)N[C@H](Cc1cccc1)[C@H](O)CN(Cc1ccc(cc1)-c1cccc1)NC(=O)[C@H
clarithromycin	Pharmaceuticals	C38H69NO13	747.47689	748.48417	746.46961 CC[C@H]1OC(=O)[C@H](C)[C@H]2(C)[C@H](O)[C@H]2C[C@H](C)(OC)[C@H](O)[C@H](C)O2)[C@H](C)(C
azithromycin	Pharmaceuticals	C38H72N2O12	748.50853	749.51581	747.50125 CC[C@H]1OC(=O)[C@H](C)[C@H]2(C)[C@H](O)[C@H]2C[C@H](C)(OC)[C@H](O)[C@H](C)O2)[C@H](C)(C
tris-biphenyl triazine	PCPs	C39H27N3	537.2205	538.22778	536.21322 c1ccc(cc1)-c1ccc(cc1)-c1nc(nc(n1)-c1ccc(cc1)-c1cccc1)-c1ccc(cc1)-c1cccc1
bisthiosemi	Pesticides	C3H10N6S2	194.04084	195.04812	193.03356 NC(=S)NNCNNC(N)=S
ampropylfos	Pesticides	C3H10NO3P	139.03983	140.04711	138.03255 CCC(N)P(O)(O)=O
DBNPA	Pesticides	C3H2Br2N2O	239.85339	240.86067	238.84611 NC(=O)C(Br)(Br)C#N
chloropon	Pesticides	C3H3Cl3O2	175.91987	176.92715	174.91259 OC(=O)C(Cl)(Cl)CCl
acrylonitrile	Pesticides	C3H3N	53.02655	54.03383	52.01927 C=CC#N
1,3-dichloropropene	Pesticides	C3H4Cl2	109.96901	110.97629	108.96173 ClCC=CCl
acrolein	Pesticides	C3H4O	56.02622	57.0335	55.01894 C=CC=O

[illegible]

heptafluorobutyric acid	Industrial Chemicals	C4HF7O2	213.98648	214.99376	212.9792	OC(=O)C(F)(F)C(F)(F)C(F)(F)F
ombitasvir	Pharmaceuticals	C50H67N7O8	893.50512	894.5124	892.49784	COC(=O)N[C@@H](C(C)C)C(=O)N1CCC[C@H]1C(=O)Nc1ccc(cc1)[C@@H]1CC[C@H](N1c1ccc(cc1)C
capreomycin	Pharmaceuticals	C50H88N28O15	1320.6984	1321.70568	1319.69112	C[C@@H]1NC(=O)[C@@H](N)CNC(=O)[C@@H](NC(=O)C(NC(=O)[C@@H](CNC(=O)C[C@@H](N)CC
fidaxomicin	Pharmaceuticals	C52H74Cl2O18	1056.42522	1057.4325	1055.41794	CC[C@H]1C=C(C)C[C@@H](O)C=C(C)C=CCO[C@@H]2O[C@H](C)[C@@H](OC(=O)C3=C(CC)C(Cl):
caspofungin	Pharmaceuticals	C52H88N10O15	1092.64307	1093.65035	1091.63579	CCCC(C)CC(C)CCCCCCCC(=O)N[C@H]1C[C@@H](O)[C@@H](NCCN)NC(=O)[C@@H]2[C@@H](O)C
colistin	Pharmaceuticals	C52H98N16O13	1154.74993	1155.75721	1153.74265	CCC(C)CCCC(=O)N[C@@H](CCN)C(=O)N[C@@H]([C@@H](C)O)C(=O)N[C@@H](CCN)C(=O)N[C@H
quinupristin	Pharmaceuticals	C53H67N9O10S	1021.47316	1022.48044	1020.46588	CC[C@H]1NC(=O)[C@@H](NC(=O)c2ncccc2O)[C@@H](C)OC(=O)[C@@H](NC(=O)[C@@H]2CC(=O
micalfungin	Pharmaceuticals	C56H71N9O23S	1269.43835	1270.44563	1268.43107	CCCCCOC1ccc(cc1)-c1cc(nO1)-c1ccc(cc1)C(=O)N[C@H]1C[C@@H](O)[C@@H](O)NC(=O)[C@@H]2
anidulafungin	Pharmaceuticals	C58H73N7O17	1139.5063	1140.51358	1138.49902	CCCCCOC1ccc(cc1)-c1ccc(cc1)-c1ccc(cc1)C(=O)N[C@H]1C[C@@H](O)[C@@H](O)NC(=O)[C@@H]2
teixobactin	Pharmaceuticals	C58H95N15O15	1241.71321	1242.72049	1240.70593	CC[C@H](C)[C@H](NC(=O)[C@@H](Cc1ccccc1)NC)C(=O)N[C@@H](CO)C(=O)N[C@H](CCC(N)=O)C
1,3-dimethyl-2-imidaz	Industrial Chemicals	C5H10N2O	114.07932	115.0866	113.07204	CN1CCN(C)C1=O
kipsin	Metabolites	C5H10N2O2S	162.0463	163.05358	161.03902	CS\C(C)=N\O\C(O)=N\C
methomyl	Pesticides	C5H10N2O2S	162.0463	163.05358	161.03902	CNC(=O)O\N=C(/C)SC
dazomet	Pesticides	C5H10N2S2	162.02854	163.03582	161.02126	CN1CSC(=S)N(C)C1
4,4-dimethyloxazolidin	Pesticides	C5H11NO	101.08407	102.09135	100.07679	CC1(C)COCN1
chlormephos	Pesticides	C5H12ClO2PS2	233.97049	234.97777	232.96321	CCOP(=S)(OCC)SCCl
dimethoate	Pesticides	C5H12NO3PS2	228.99962	230.0069	227.99234	CNC(=O)CSP(=S)(OC)OC
choline chloride	Pesticides	C5H14ClNO	139.0764	140.08368	138.06912	[Cl-].C[N+](C)(C)CCO
etridiazole	Pesticides	C5H5Cl3N2OS	245.91882	246.9261	244.91154	CCOc1nc(ns1)C(Cl)(Cl)Cl
pyrazinamide	Pharmaceuticals	C5H5N3O	123.04327	124.05055	122.03599	OC(=N)c1cncn1
chloridazone-methyl-d	Pesticides	C5H6ClN3O	159.01994	160.02722	158.01266	CN1N=CC(N)=C(Cl)C1=O
4-aminopyridine	Pesticides	C5H6N2	94.0531	95.06038	93.04582	Nc1ccncc1
deisopropylatrazine	Pesticides	C5H8ClN5	173.04683	174.05411	172.03955	CCNc1nc(N)nc(Cl)n1
4-methoxy-6-methyl-1,	Metabolites	C5H8N4O	140.06981	141.07709	139.06253	COc1nc(C)nc(N)n1
glutaral	PCPs	C5H8O2	100.05243	101.05971	99.04515	O=CCCCC=O
acetylcysteine	PCPs	C5H9NO3S	163.03032	164.0376	162.02304	CC(=O)NC(CS)C(=O)O
alorac	Pesticides	C5HCl5O3	283.83684	284.84412	282.82956	OC(=O)C(Cl)=C(Cl)C(=O)C(Cl)(Cl)Cl
perfluoropentane-1-su	Industrial Chemicals	C5HF11O3S	349.94708	350.95436	348.9398	[O-]S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
perfluoropentanoic acid	Industrial Chemicals	C5HF9O2	263.98329	264.99057	262.97601	OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
bacitracin	Pharmaceuticals	C65H101N17O16S	1407.73329	1408.74057	1406.72601	CC[C@@H](C)[C@H](NC(=O)[C@H](CCC(O)=O)NC(=O)[C@H](CC(C)C)NC(=O)C1CN=C(S1)[C@H](N)
vancomycin	Pharmaceuticals	C66H75Cl2N9O24	1447.4302	1448.43748	1446.42292	CN[C@H](CC(C)C)C(=O)N[C@@H]1[C@H](O)c2ccc(Oc3cc4cc(Oc5ccc(cc5Cl)[C@@H](O)[C@@H]5N
bacitracin F	Pharmaceuticals	C66H98N16O17S	1418.70166	1419.70894	1417.69438	CCCC(C)C(NC(=O)C(CCC(O)=O)NC(=O)C(C(C)C)NC(=O)c1csc(n1)C(=O)C(C)CC(C(=O)NC1CCCCNC(=O)
bacitracin A	Pharmaceuticals	C68H103N17O16S	1445.74894	1446.75622	1444.74166	CC[C@H](C)[C@H](N)C1=N[C@@H](CS1)C(=O)N[C@@H](CC(C)C)C(=O)N[C@H](CCC(O)=O)C(=O)N
chloranil	Pesticides	C6Cl4O2	243.865234	244.872514	242.857954	ClC1=C(Cl)C(=O)C(Cl)=C(Cl)C1=O
atrazine-desethyl	Pesticides	C6H10ClN5	187.06248	188.06976	186.0552	CC(C)Nc1nc(N)nc(Cl)n1
cyromazine	Pesticides	C6H10N6	166.0967	167.10398	165.08942	Nc1nc(N)nc(NC2CC2)n1
dimethipin	Pesticides	C6H10O4S2	210.00205	211.00933	208.99477	CC1=C(C)S(=O)(=O)CCS1(=O)=O
chlorethoxyfos	Pesticides	C6H11Cl4O3PS	333.89207	334.89935	332.88479	CCOP(=S)(OCC)OC(Cl)(Cl)Cl
methidathion	Pesticides	C6H11N2O4PS3	301.96186	302.96914	300.95458	COC1=NN(CSP(=S)(OC)OC)C(=O)S1
atrazine-desethyl-2-hy	Pesticides	C6H11N5O	169.09636	170.10364	168.08908	CC(C)Nc1nc(N)nc(O)n1
TCEP	Industrial Chemicals	C6H12Cl3O4P	283.95388	284.96116	282.9466	ClCCOP(=O)(OCCCl)OCCCl
daminozide	Pesticides	C6H12N2O3	160.0848	161.09208	159.07752	CN(C)NC(=O)CCC(O)=O
thiram	Pesticides	C6H12N2S4	239.98833	240.99561	238.98105	CN(C)C(=S)SSC(=S)N(C)C
hexamine	Pharmaceuticals	C6H12N4	140.1062	141.11348	139.09892	C1N2CN3CN1CN(C2)C3
cyclamic acid	Industrial Chemicals	C6H13NO3S	179.06162	180.0689	178.05434	OS(=O)(=O)NC1CCCCC1
azithiram	Pesticides	C6H14N4S4	270.01013	271.01741	269.00285	CN(C)NC(=S)SSC(=S)NN(C)C
triethanolamine	PCPs	C6H15NO3	149.1052	150.11248	148.09792	OCCN(CCO)CCO
triethylphosphate	Industrial Chemicals	C6H15O4P	182.0708	183.07808	181.06352	CCOP(=O)(OCC)OCC
glyphosate trimesium	Pesticides	C6H16NO5PS	245.04868	246.05596	244.0414	C[S+](C)C.OP(O)(=O)CNCC([O-])=O

clpyralid	Pesticides	C6H3Cl2NO2	190.95409	191.96137	189.94681	OC(=O)c1nc(Cl)ccc1Cl
2,4,5-trichlorophenol	Pesticides	C6H3Cl3O	195.92495	196.93223	194.91767	Oc1cc(Cl)c(Cl)cc1Cl
aminopyralid	Pesticides	C6H4Cl2N2O2	205.96499	206.97227	204.95771	Nc1cc(Cl)nc(C(O)=O)c1Cl
dicloran	Pesticides	C6H4Cl2N2O2	205.96499	206.97227	204.95771	Nc1c(Cl)cc(cc1Cl)[N+]{([O-])=O
1,2,3-benzotriazole	Industrial Chemicals	C6H5N3	119.04835	120.05563	118.04107	c1ccc2[nH]nnc2c1
hydroxybenzotriazole	Industrial Chemicals	C6H5N3O	135.04327	136.05055	134.03599	On1nnc2cccc12
lindane	Pesticides	C6H6Cl6	287.86007	288.86735	286.85279	ClC1C(Cl)C(Cl)C(Cl)C(Cl)C1Cl
niacinamide	PCPs	C6H6N2O	122.04802	123.0553	121.04074	OC(=N)c1ccncc1
isoniazid	Pharmaceuticals	C6H7N3O	137.05892	138.0662	136.05164	NNC(=O)c1ccncc1
clothianidin	Pesticides	C6H8ClN5O2S	249.00873	250.01601	248.00145	C\N=C(\NCc1cnc(Cl)s1)N[N+]{([O-])=O
sulfanilamide	Pharmaceuticals	C6H8N2O2S	172.03065	173.03793	171.02337	Nc1ccc(cc1)S(N)(=O)=O
metronidazole	Pharmaceuticals	C6H9N3O3	171.06439	172.07167	170.05711	Cc1ncc(n1CCO)[N+]{([O-])=O
perfluorohexanoic acid	Industrial Chemicals	C6HF11O2	313.98009	314.98737	312.97281	OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
ambamide	Pharmaceuticals	C7H10N2O2S	186.0463	187.05358	185.03902	Nc1ccc(cc1)S(N)(=O)=O
cymoxanil	Pesticides	C7H10N4O3	198.07529	199.08257	197.06801	CCNC(=O)NC(=O)C(=N/OC)\C#N
avibactam	Pharmaceuticals	C7H11N3O6S	265.03686	266.04414	264.02958	NC(=O)[C@@H]1CC[C@@H]2C[N@]1C(=O)N2OS(O)(=O)=O
aziprotryne	Pesticides	C7H11N7S	225.07967	226.08695	224.07239	CSc1nc(NC(C)C)nc(N=[N+]=[N-])n1
desethylterbutylazine	Pesticides	C7H12ClN5	201.07813	202.08541	200.07085	CC(C)(C)Nc1nc(N)nc(Cl)n1
simazine	Pesticides	C7H12ClN5	201.07813	202.08541	200.07085	CCNc1nc(Cl)nc(NCC)n1
simazine-2-hydroxy	Pesticides	C7H13N5O	183.11201	184.11929	182.10473	CCNc1nc(O)nc(NCC)n1
terbutylazine-desethyl-	Pesticides	C7H13N5O	183.11201	184.11929	182.10473	CC(C)(C)Nc1nc(N)nc(O)n1
aldicarb	Pesticides	C7H14N2O2S	190.0776	191.08488	189.07032	CNC(=O)O\N=C\C(C)(C)SC
butocarboxim	Pesticides	C7H14N2O2S	190.0776	191.08488	189.07032	CNC(=O)O\N=C\C(C)(C)SC
aldoxycarb	Pesticides	C7H14N2O4S	222.06743	223.07471	221.06015	CNC(=O)O\N=C\C(C)(C)S(C)(=O)=O
butoxycarboxim	Pesticides	C7H14N2O4S	222.06743	223.07471	221.06015	CNC(=O)ON=C(C)C(C)S(C)(=O)=O
cyclophosphamide	Pharmaceuticals	C7H15Cl2N2O2P	260.02482	261.0321	259.01754	CICCN(CCCl)P1(=O)NCCCO1
ifosfamide	Pharmaceuticals	C7H15Cl2N2O2P	260.02482	261.0321	259.01754	CICCNCP1(=O)OCCCN1CCCl
cartap	Pesticides	C7H15N3O2S2	237.06057	238.06785	236.05329	CN(C)C(CSC(N)=O)CSC(N)=O
amidithion	Pesticides	C7H16NO4PS2	273.02584	274.03312	272.01856	COCCNC(=O)CSP(=S)(OC)OC
brofmoxynil	Pesticides	C7H3Br2NO	274.85814	275.86542	273.85086	Oc1c(Br)cc(cc1Br)C#N
dichlobenil	Pesticides	C7H3Cl2N	170.96426	171.97154	169.95698	Clc1cccc(Cl)c1C#N
chloroxynil	Pesticides	C7H3Cl2NO	186.95917	187.96645	185.95189	Oc1c(Cl)cc(cc1Cl)C#N
2,3,6-TBA	Pesticides	C7H3Cl3O2	223.91987	224.92715	222.91259	OC(=O)c1c(Cl)ccc(Cl)c1Cl
ioxynil	Pesticides	C7H3I2NO	370.8304	371.83768	369.82312	Oc1c(I)cc(cc1I)C#N
2,3,5-tri-iodobenzoic a	Pesticides	C7H3I3O2	499.72671	500.73399	498.71943	OC(=O)c1cc(I)cc(I)c1I
triclopyr	Pesticides	C7H4Cl3NO3	254.92568	255.93296	253.9184	OC(=O)COC1=C(Cl)C=C(Cl)C(Cl)=N1
clodinate	Pesticides	C7H4ClI2NO2	422.802	423.80928	421.79472	CC(=O)Oc1c(I)cnc(Cl)c1I
benclothiaz	Pesticides	C7H4ClNS	168.9753	169.98258	167.96802	Clc1cccc2cncs12
3,5-dibromo-4-hydroxy	Metabolites	C7H5Br2NO2	292.86871	293.87599	291.86143	NC(=O)c1cc(Br)c(O)c(Br)c1
4-bromo-3-(trifluoromethyl)	Industrial Chemicals	C7H5BrF3NO2S	302.91765	303.92493	301.91037	NS(=O)(=O)c1ccc(Br)c(c1)C(F)(F)F
fluroxypyr	Pesticides	C7H5Cl2FN2O3	253.96613	254.97341	252.95885	Nc1c(Cl)c(F)nc(OCC(O)=O)c1Cl
BAM	Pesticides	C7H5Cl2NO	188.97482	189.9821	187.96754	OC(=N)c1c(Cl)cccc1Cl
chloramben	Pesticides	C7H5Cl2NO2	204.96974	205.97702	203.96246	Nc1cc(Cl)cc(C(O)=O)c1Cl
chlorthiamid	Pesticides	C7H5Cl2NS	204.95198	205.95926	203.9447	NC(=S)c1c(Cl)cccc1Cl
2-chloro-4-(trifluoromethyl)	Industrial Chemicals	C7H5ClF3NO2S	258.96816	259.97544	257.96088	NS(=O)(=O)c1ccc(cc1Cl)C(F)(F)F
fluensulfone	Pesticides	C7H5ClF3NO2S2	290.94024	291.94752	289.93296	FC(F)=C(F)CCS(=O)(=O)C1=NC=C(Cl)S1
saccharin	Industrial Chemicals	C7H5NO3S	182.99902	184.0063	181.99174	OC1=NS(=O)(=O)c2ccccc12
1,2-benzisothiazolin-3-	Pesticides	C7H5NOS	151.00919	152.01647	150.00191	O=c1[nH]sc2cccc12
benzisothiazolinone	PCPs	C7H5NOS	151.00919	152.01647	150.00191	Oc1nsc2cccc12

bromoxynil

salicylate	PCPs	C7H5O3	137.02387	138.03115	136.01659	Oc1ccccc1C([O-])=O	
diuron-desdimethyl	Pesticides	C7H6Cl2N2O	203.98572	204.993	202.97844	OC(=N)Nc1ccc(Cl)c(Cl)c1	
benzoic acid	Pesticides	C7H6O	106.04187	107.04915	105.03459	OC(=O)c1ccccc1	
salicylic acid	PCPs	C7H6O3	138.0317	139.03898	137.02442	OC(=O)c1ccccc1O	
chlorpyrifos-methyl	Pesticides	C7H7Cl3NO3PS	320.89499	321.90227	319.88771	COP(=S)(OC)Oc1nc(Cl)c(Cl)cc1Cl	
1-methylbenzotriazole	Industrial Chemicals	C7H7N3	133.064	134.07128	132.05672	Cn1nnc2ccccc12	
2-amino-1H-benzimida	Pesticides	C7H7N3	133.064	134.07128	132.05672	NC1=NC2=C(N1)C=CC=C2	
para amino benzoic aci	PCPs	C7H7NO2	137.04768	138.05496	136.0404	Nc1ccc(cc1)C(O)=O	
aminosalicylic acid	Pharmaceuticals	C7H7NO3	153.0426	154.04988	152.03532	Nc1ccc(C(O)=O)c(O)c1	
hydrochlorothiazide	Pharmaceuticals	C7H8ClN3O4S2	296.96448	297.97176	295.9572	NS(=O)(=O)C1=CC2=C(NCNS2(=O)=O)C=C1Cl	
paraxanthine	Metabolites	C7H8N4O2	180.06473	181.07201	179.05745	Cn1cnc2nc(O)n(C)c(=O)c12	caffeine
1,7-dimethyluric acid	Metabolites	C7H8N4O3	196.05964	197.06692	195.05236	Cn1c2c([nH]c1=O)[nH]c(=O)n(C)c2=O	caffeine
4-methylphenol	PCPs	C7H8O	108.05752	109.0648	107.05024	Cc1ccc(O)cc1	
perfluoroheptanoic aci	Industrial Chemicals	C7HF13O2	363.9769	364.98418	362.96962	OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	
chlorothalonil	Pesticides	C8Cl4N2	263.88158	264.88886	262.8743	Clc1c(Cl)c(C#N)c(Cl)c(C#N)c1Cl	
perfluorooctanesulfoni	Industrial Chemicals	C8F17O3S	498.93018	499.93746	497.9229	[O-]S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	
deltamethric acid	Metabolites	C8H10Br2O2	295.90476	296.91204	294.89748	CC1(C)[C@@H](C=C(Br)Br)[C@H]1C(O)=O	deltamethrin
permethric acid	Metabolites	C8H10Cl2O2	208.00579	209.01307	206.99851	CC1(C)C(C=C(Cl)Cl)C1C(O)=O	permethrin
thiamethoxam	Pesticides	C8H10ClN5O3S	291.01929	292.02657	290.01201	CN1COCN(Cc2cnc(Cl)s2)\C1=N\[N+][([O-])=O	
emtricitabine	Pharmaceuticals	C8H10FN3O3S	247.04269	248.04997	246.03541	Nc1nc(=O)n(cc1F)[C@@H]1CS[C@H](CO)O1	
sulfacetamide	Pharmaceuticals	C8H10N2O3S	214.04122	215.0485	213.03394	CC(=O)NS(=O)(=O)c1ccc(N)cc1	
asulam	Pesticides	C8H10N2O4S	230.03613	231.04341	229.02885	COC(=O)NS(=O)(=O)c1ccc(N)cc1	
ethionamide	Pharmaceuticals	C8H10N2S	166.05647	167.06375	165.04919	CCc1cc(ccn1)C(S)=N	
caffeine	Pharmaceuticals	C8H10N4O2	194.08038	195.08766	193.0731	Cn1cnc2n(C)c(=O)n(C)c(=O)c12	
parathion-methyl	Pesticides	C8H10NO5PS	263.00173	264.00901	261.99445	COP(=S)(OC)Oc1ccc(cc1)[N+][([O-])=O	
2,4-dimethylphenol	Pesticides	C8H10O	122.07317	123.08045	121.06589	Cc1ccc(O)c(C)c1	
phenoxxyethanol	PCPs	C8H10O2	138.06808	139.07536	137.0608	OCCOc1ccccc1	
endothal	Pesticides	C8H10O5	186.05283	187.06011	185.04555	OC(=O)C1C2CCC(O2)C1C(O)=O	
chloralose	Pesticides	C8H11Cl3O6	307.96212	308.9694	306.95484	C(C([C@@H]1[C@@H]([C@@H]2 C(O1)O[C@@H](O2)C(Cl)(~*+I)O)O)O	
lamivudine	Pharmaceuticals	C8H11N3O3S	229.05212	230.0594	228.04484	Nc1ccn([C@@H]2CS[C@H](CO)O2)c(=O)n1	
sulbactam	Pharmaceuticals	C8H11NO5S	233.0358	234.04308	232.02852	CC1(C)[C@@H](N2[C@@H](CC2=O)S1(=O)=O)C(O)=O	
allidochlor	Pesticides	C8H12ClNO	173.06075	174.06803	172.05347	C1CC(=O)N(CC=C)CC=C	
iodopropynyl butylcarb	Pesticides	C8H12INO2	280.99127	281.99855	279.98399	CCCCNC(=O)OCC#Cl	
adefovir	Pharmaceuticals	C8H12N5O4P	273.06269	274.06997	272.05541	Nc1ncnc2n(CCOCP(O)(O)=O)cnc12	
tinidazole	Pharmaceuticals	C8H13N3O4S	247.06268	248.06996	246.0554	CCS(=O)(=O)CCn1c(C)ncc1[N+][([O-])=O	
metribuzin-desamino	Pesticides	C8H13N3OS	199.07794	200.08522	198.07066	CSc1nc(=O)c(n[nH]1)C(C)(C)C	
butonate	Pesticides	C8H14Cl3O5P	325.96445	326.97173	324.95717	CCCC(=O)OC(C(Cl)(Cl)Cl)P(=O)(OC)OC	
atrazine	Pesticides	C8H14ClN5	215.09378	216.10106	214.0865	CCNc1nc(Cl)nc(NC(C)C)n1	
levetiracetam	Pharmaceuticals	C8H14N2O2	170.10553	171.11281	169.09825	CC[C@H](N1CCCC1=O)C(N)=O	
metribuzin	Pesticides	C8H14N4OS	214.08884	215.09612	213.08156	CSC1=NN=C(C(=O)N1N)C(C)(C)C	
2-propyl-4-pentenoic a	Metabolites	C8H14O2	142.09938	143.10666	141.0921	CCCC(CC=C)C(O)=O	valproic acid
athidathion	Pesticides	C8H15N2O4PS3	329.99316	331.00044	328.98588	CCOP(=S)(OCC)SCn1nc(OC)sc1=O	
hydroxyatrazine	Pesticides	C8H15N5O	197.12766	198.13494	196.12038	CCNc1nc(O)nc(NC(C)C)n1	
simeton	Pesticides	C8H15N5O	197.12766	198.13494	196.12038	CCNc1nc(NCC)nc(OC)n1	
ilrgarol-descyclopropyl	Pesticides	C8H15N5S	213.10482	214.1121	212.09754	CSc1nc(N)nc(NC(C)(C)C)n1	
carbamorph	Pesticides	C8H16N2OS2	220.07041	221.07769	219.06313	CN(C)C(=S)SCN1CCOCC1	
dicrotophos	Pesticides	C8H16NO5P	237.07661	238.08389	236.06933	COP(=O)(OC)O\C(C)=C\C(=O)N(C)C	
valproic acid	Pharmaceuticals	C8H16O2	144.11503	145.12231	143.10775	CCCC(CCC)C(O)=O	
metaldehyde	Pesticides	C8H16O4	176.10486	177.11214	175.09758	CC1OC(C)OC(C)OC(C)O1	

acethion	Pesticides	C8H17O4PS2	272.03059	273.03787	271.02331 CCOC(=O)CSP(=S)(OCC)OCC
disulfoton	Pesticides	C8H19O2PS3	274.02848	275.03576	273.0212 CCOP(=S)(OCC)SCCSCC
chlorquinox	Pesticides	C8H2Cl4N2	265.89721	266.90449	264.88993 Clc1c(Cl)c(Cl)c2nccnc2c1Cl
chlorfluazole	Pesticides	C8H3Cl2F3N2	253.96254	254.96982	252.95526 FC(F)(F)c1nc2c(Cl)c(Cl)ccc2[nH]1
2,4,5-trichloro-3-cyano	Pesticides	C8H3Cl3N2O2	263.92601	264.93329	262.91873 OC(=N)c1c(O)c(Cl)c(Cl)c(C#N)c1Cl
bromocyclen	Pesticides	C8H5BrCl6	389.77058	390.77786	388.7633 ClC1=C(Cl)C2(Cl)C(CBr)CC1(Cl)C2(Cl)Cl
chlorfenac	Pesticides	C8H5Cl3O2	237.93552	238.9428	236.92824 OC(=O)Cc1c(Cl)ccc(Cl)c1Cl
2,4,5-trichlorophenoxy	Pesticides	C8H5Cl3O3	253.93043	254.93771	252.92315 OC(=O)COc1cc(Cl)c(Cl)cc1Cl
dicamba	Pesticides	C8H6Cl2O3	219.9694	220.97668	218.96212 COc1c(Cl)ccc(Cl)c1C(O)=O
2,4-D	Pesticides	C8H6Cl2O3	219.9694	220.97668	218.96212 OC(=O)COc1ccc(Cl)cc1Cl
chlorthal-dimethyl	Pesticides	C8H6Cl4O4	305.90202	306.9093	304.89474 COC(=O)c1c(Cl)c(Cl)c(C(=O)OC)c(Cl)c1Cl
chlobenthiазone	Pesticides	C8H6ClNOS	198.98587	199.99315	197.97859 Cn1c2c(Cl)cccc2sc1=O
perfluorooctyl phospho	Industrial Chemicals	C8H6F13O4P	443.97962	444.9869	442.97234 OP(O)(=O)OCCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
acibenzolar-S-methyl	Pesticides	C8H6N2OS2	209.99216	210.99944	208.98488 OC(=S)c1cccc2nnsc12
nitrofurantoin	Pharmaceuticals	C8H6N4O5	238.03382	239.0411	237.02654 [O-][N+](=O)c1ccc(\C=N\N2CC(=O)NC2=O)o1
2,5-dichlorobenzoic ac	Pesticides	C8H6O2Cl2	203.97449	204.98177	202.96721 COC(=O)c1cc(Cl)ccc1Cl
4-CPA	Pesticides	C8H7ClO3	186.00838	187.01566	185.0011 OC(=O)COc1ccc(Cl)cc1
2-chloro-4-(methylsulfi	Pesticides	C8H7ClO4S	233.97536	234.98264	232.96808 CS(=O)(=O)c1ccc(C(O)=O)c(Cl)c1
furazolidone	Pharmaceuticals	C8H7N3O5	225.03857	226.04585	224.03129 [O-][N+](=O)c1ccc(\C=N\N2CCOC2=O)o1
bromophos	Pesticides	C8H8BrCl2O3PS	363.84922	364.8565	362.84194 COP(=S)(OC)Oc1cc(Cl)c(Br)cc1Cl
diuron-desmethyl	Pesticides	C8H8Cl2N2O	218.00137	219.00865	216.99409 CNC(=O)Nc1ccc(Cl)c(Cl)c1
chloroneb	Pesticides	C8H8Cl2O2	205.99014	206.99742	204.98286 COc1cc(Cl)c(OC)cc1Cl
aminocyclopyrachlor	Pesticides	C8H8ClN3O2	213.03051	214.03779	212.02323 Nc1nc(nc(C(O)=O)c1Cl)C1CC1
zonisamide	Pharmaceuticals	C8H8N2O3S	212.02557	213.03285	211.01829 NS(=O)(=O)Cc1noc2ccccc12
methyl salicylate	PCPs	C8H8O3	152.04735	153.05463	151.04007 COC(=O)c1ccccc1O
methylparaben	PCPs	C8H8O3	152.04735	153.05463	151.04007 COC(=O)c1ccc(O)cc1
chloroxylenol	PCPs	C8H9ClO	156.0342	157.04148	155.02692 Cc1cc(O)cc(C)c1Cl
chloroxylenol	Pesticides	C8H9ClO	156.0342	157.04148	155.02692 Cc1cc(O)cc(C)c1Cl
paracetamol	Pharmaceuticals	C8H9NO2	151.06333	152.07061	150.05605 CC(=O)NC1=CC=C(O)C=C1
methyl 2-sulfamoylben	Pesticides	C8H9NO4S	215.02523	216.03251	214.01795 COC(=O)C1=C(C=C=C1)S(N)(=O)=O
clavulanate	Pharmaceuticals	C8H9NO5	199.04808	200.05536	198.0408 OCC=C1O[C@H]2CC(=O)N2[C@H]1C(O)=O
chlorthion	Pesticides	C8H9O5NSCIP	296.96276	297.97004	295.95548 COP(=S)(OC)Oc1ccc(c(Cl)c1)[N+](O-)=O
perfluorooctanoic acid	Industrial Chemicals	C8HF15O2	413.97371	414.98099	412.96643 OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
chlorbromuron	Pesticides	C9H10BrClN2O2	291.96142	292.9687	290.95414 CON(C)C(=O)NC1=CC(Cl)=C(Br)C=C1
diuron	Pesticides	C9H10Cl2N2O	232.01702	233.0243	231.00974 CN(C)C(=O)Nc1ccc(Cl)c(Cl)c1
linuron	Pesticides	C9H10Cl2N2O2	248.01194	249.01922	247.00466 CON(C)C(=O)Nc1ccc(Cl)c(Cl)c1
azamethiphos	Pesticides	C9H10ClN2O5PS	323.97366	324.98094	322.96638 COP(=O)(OC)SCN1C(=O)Oc2cc(Cl)cnc12
imidacloprid-urea	Pesticides	C9H10ClN3O	211.05124	212.05852	210.04396 Clc1ccc(CN2CCNC2=O)cn1
imidacloprid	Pesticides	C9H10ClN5O2	255.05231	256.05959	254.04503 Clc1ccc(CN2CCNC2=NN(=O)=O)cn1
2',2'-difluorodeoxyurid	Metabolites	C9H10F2N2O5	264.05578	265.06306	263.0485 OC[C@H]1O[C@H](n2ccc(=O)[nH]c2=O)C(F)(F)[C@@H]1O gemcitabine
sulfamethizole	Pharmaceuticals	C9H10N4O2S2	270.02452	271.0318	269.01724 Cc1nnc(NS(=O)(=O)c2ccc(N)cc2)s1
ethylparaben	PCPs	C9H10O3	166.063	167.07028	165.05572 CCOC(=O)c1ccc(O)cc1
bromuron	Pesticides	C9H11BrN2O	242.00548	243.01276	240.9982 CN(C)C(=O)Nc1ccc(Br)cc1
chlorpyrifos	Pesticides	C9H11Cl3N3O3PS	348.92629	349.93357	347.91901 CCOP(=S)(OCC)Oc1nc(Cl)c(Cl)cc1Cl
monuron	Pesticides	C9H11ClN2O	198.05599	199.06327	197.04871 CN(C)C(=O)Nc1ccc(Cl)cc1
monolinuron	Pesticides	C9H11ClN2O2	214.05091	215.05819	213.04363 CON(C)C(=O)Nc1ccc(Cl)cc1
desnitro-imidacloprid	Metabolites	C9H11ClN4	210.06723	211.07451	209.05995 ClC1=NC=C(CN2CCNC2=N)C=C1 imidacloprid
gemcitabine	Pharmaceuticals	C9H11F2N3O4	263.07177	264.07905	262.06449 NC1=NC(=O)N(C=C1)[C@H]1O[C@H](CO)[C@H](O)C1(F)F
N-(2,4-dimethyl-	Pesticides	C9H11NO	149.08407	150.09135	148.07679 [H]C(=O)NC1=C(C)C=C(C)C=C1

nornicotine	Metabolites	C9H12N2	148.10005	149.10733	147.09277	C1CNC(C1)c1ccccc1	nicotine
p-amino-N-methylacet	Industrial Chemicals	C9H12N2O	164.09497	165.10225	163.08769	CN(C(C)=O)c1ccc(N)cc1	
bromacil	Pesticides	C9H13BrN2O2	260.01604	261.02332	259.00876	CCC(C)N1C(=O)NC(C)=C(Br)C1=O	
terbacil	Pesticides	C9H13ClN2O2	216.06656	217.07384	215.05928	CC1=C(Cl)C(=O)N(C(=O)N1)C(C)(C)C	
amphetamine	Pharmaceuticals	C9H13N	135.1048	136.11208	134.09752	CC(N)Cc1ccccc1	
zalcitabine	Pharmaceuticals	C9H13N3O3	211.09569	212.10297	210.08841	OC[C@@H]1CC[C@@H](O1)n1ccc(=N)nc1O	
N,N-dimethyl-N'-p-toly	Pesticides	C9H14N2O2S	214.0776	215.08488	213.07032	CN(C)S(=O)(=O)Nc1ccc(C)cc1	
carboxazole	Pesticides	C9H14N2O3	198.10045	199.10773	197.09317	COC(=O)Nc1cc(on1)C(C)(C)C	
tenofovir	Pharmaceuticals	C9H14N5O4P	287.07834	288.08562	286.07106	C[C@H](Cn1cnc2c(N)ncnc12)OCP(O)(O)=O	
amidosulfuron	Pesticides	C9H15N5O7S2	369.04129	370.04857	368.03401	COc1cc(OC)nc(NC(=O)NS(=O)(=O)N(C)S(C)(=O)=O)n1	
tris(2-carboxyethyl)phc	Industrial Chemicals	C9H15O6P	250.06063	251.06791	249.05335	OC(=O)CCP(CCC(O)=O)CCC(O)=O	
terbuthylazine	Pesticides	C9H16ClN5	229.10943	230.11671	228.10215	CCNc1nc(Cl)nc(NC(C)(C)C)n1	
buthiuron	Pesticides	C9H16N4O3S2	292.06639	293.07367	291.05911	CCCCS(=O)(=O)c1nnc(s1)N(C)C(=O)NC	
tebuthiuron	Pesticides	C9H16N4O5	228.10449	229.11177	227.09721	CNC(=O)N(C)c1nnc(s1)C(C)(C)C	
2-hydroxypropazine	Pesticides	C9H17N5O	211.14331	212.15059	210.13603	CC(C)Nc1nc(O)nc(NC(C)C)n1	
terbutylazine-2-hydrox	Pesticides	C9H17N5O	211.14331	212.15059	210.13603	CCNC1=NC(O)=NC(NC(C)(C)C)=N1	
atraton	Pesticides	C9H17N5O	211.14331	212.15059	210.13603	CCNc1nc(NC(C)C)nc(OC)n1	
ametryn	Pesticides	C9H17N5S	227.12047	228.12775	226.11319	CCNc1nc(NC(C)C)nc(SC)n1	
gabapentin	Pharmaceuticals	C9H17NO2	171.12593	172.13321	170.11865	NCC1(CC(O)=O)CCCCC1	
asomate	Pesticides	C9H18AsN3S6	434.9041	435.91138	433.89682	CN(C)C(=S)S[As](SC(=S)N(C)C)SC(=S)N(C)C	
meprobamate	Pharmaceuticals	C9H18N2O4	218.12666	219.13394	217.11938	CCCC(C)(COC(N)=O)COC(N)=O	
EPTC	Pesticides	C9H19NOS	189.11874	190.12602	188.11146	CCCN(CCC)C(=O)SCC	
propamocarb	Pesticides	C9H20N2O2	188.15248	189.15976	187.1452	CCCCO(=O)NCCCN(C)C	
terbufos	Pesticides	C9H21O2PS3	288.04413	289.05141	287.03685	CCOP(=S)(OCC)SCSC(C)(C)C	
folpet	Pesticides	C9H4Cl3NO2S	294.90284	295.91012	293.89556	ClC(Cl)(Cl)SN1C(=O)c2ccccc2C1=O	
anilazine	Pesticides	C9H5Cl3N4	273.95798	274.96526	272.9507	Clc1ccccc1Nc1nc(Cl)nc(Cl)n1	
iodoquinol	Pharmaceuticals	C9H5I2NO	396.84605	397.85333	395.83877	Oc1c(I)cc(I)c2ccccc12	
endosulfan	Pesticides	C9H6Cl6O3S	403.81688	404.82416	402.8096	ClC1=C(Cl)C2(Cl)C3COS(=O)OCC3C1(Cl)C2(Cl)Cl	
chlorbicyclen	Pesticides	C9H6Cl8	393.79778	394.80506	392.7905	ClCC1C(CCl)C2(Cl)C(Cl)=C(Cl)C1(Cl)C2(Cl)Cl	
benazolin	Pesticides	C9H6ClNO3S	242.97569	243.98297	241.96841	OC(=O)CN1C(=O)Sc2cccc(Cl)c12	
flonicamid	Pesticides	C9H6F3N3O	229.0463	230.05358	228.03902	FC(F)(F)c1ccncc1C(=O)NCC#N	
2-(thiocyanomethylthi	Pesticides	C9H6N2S3	237.96931	238.97659	236.96203	N#CSCSC1nc2ccccc2s1	
lamotrigine	Pharmaceuticals	C9H7Cl2N5	255.00785	256.01513	254.00057	Nc1nnc(c(N)n1)-c1cccc(Cl)c1Cl	
chloraniformethan	Pesticides	C9H7Cl5N2O	333.9001	334.90738	332.89282	Clc1ccc(N[C@@H](NC=O)C(Cl)(Cl)Cl)cc1Cl	
8-hydroxyquinoline	Pesticides	C9H7NO	145.05277	146.06005	144.04549	Oc1cccc2ccncc12	
cinnamate	PCPs	C9H7O2	147.04461	148.05189	146.03733	[O-]C(=O)\C=C\c1ccccc1	
dichlorprop	Pesticides	C9H8Cl2O3	233.98505	234.99233	232.97777	C[C@@H](O)c1ccc(Cl)cc1Cl)C(O)=O	
captan	Pesticides	C9H8Cl3NO2S	298.93414	299.94142	297.92686	ClC(Cl)(Cl)SN1C(=O)[C@H]2CC=CC[C@H]2C1=O	
thidiazuron	Pesticides	C9H8N4O5	220.04188	221.04916	219.0346	O=C(Nc1cnns1)Nc1ccccc1	
aspirin	Pharmaceuticals	C9H8O4	180.04226	181.04954	179.03498	CC(=O)Oc1ccccc1C(O)=O	
3-hydroxy guanfacine	Metabolites	C9H9Cl2N3O2	261.00719	262.01447	259.99991	NC(N)=NC(=O)Cc1c(Cl)ccc(O)c1Cl	guanfacine
propanil	Pesticides	C9H9Cl2NO	217.00612	218.0134	215.99884	CCC(=O)Nc1ccc(Cl)c(Cl)c1	
MCPA	Pesticides	C9H9ClO3	200.02403	201.03131	199.01675	Cc1cc(Cl)ccc1OCC(O)=O	
carbendazim	Pesticides	C9H9N3O2	191.06948	192.07676	190.0622	COC(=O)NC1=NC2=CC=CC=C2N1	
sulfathiazole	Pharmaceuticals	C9H9N3O2S2	255.01362	256.0209	254.00634	Nc1ccc(cc1)S(=O)(=O)Nc1nccs1	
benzthiazuron	Pesticides	C9H9N3O5	207.04664	208.05392	206.03936	CNC(=O)Nc1nc2ccccc2s1	
benzadox	Pesticides	C9H9NO4	195.05316	196.06044	194.04588	OC(=O)CONC(=O)c1ccccc1	
perfluorononanoic acic	Industrial Chemicals	C9HF17O2	463.97051	464.97779	462.96323	OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	
chloropicrin	Pesticides	CCl3NO2	162.89946	163.90674	161.89218	[O-][N+](=O)C(Cl)(Cl)Cl	

foscarnet	Pharmaceuticals	CH3O5P	125.97181	126.97909	124.96453	<chem>OC(=O)P(O)(O)=O</chem>
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