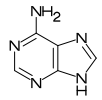
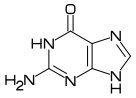
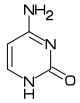
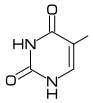
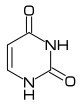
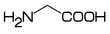
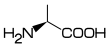
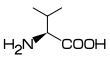
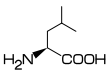
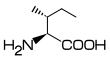
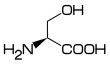
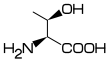
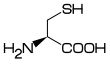
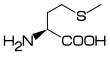
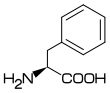
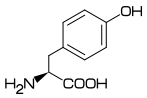
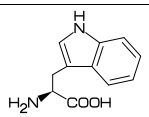
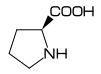
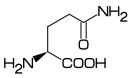
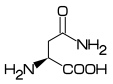
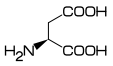
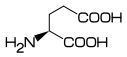
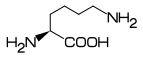
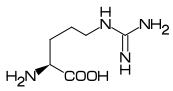
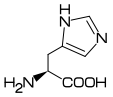
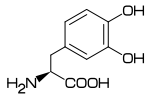
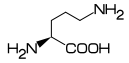
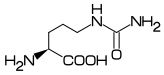
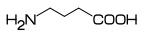
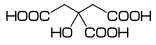
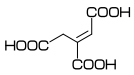
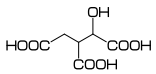
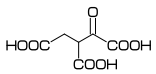
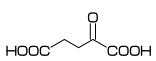
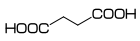
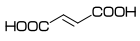
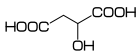
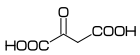
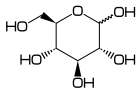
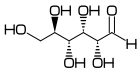
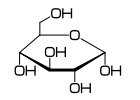
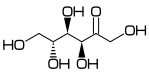
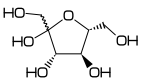
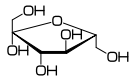
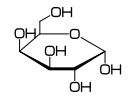
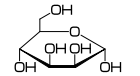
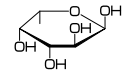
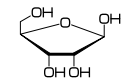
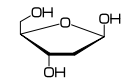
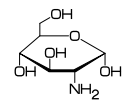
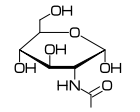
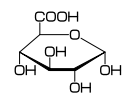
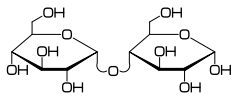
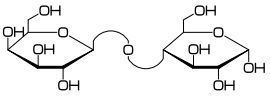
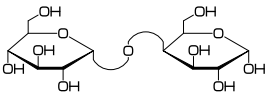
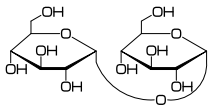
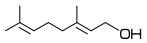
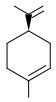
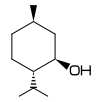
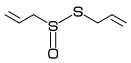
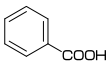
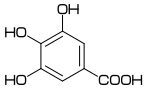
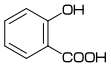
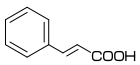
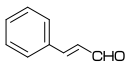
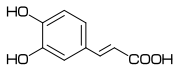
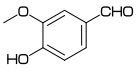
Molecular Coding Format examples

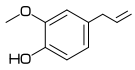
Author : Akira Yamaji Date : June 6, 2026 Located at : http://www.ctan.org/pkg/mcf2graph

[No] Molecular structure	Name	Category	Molecular Weight	MW calculated	Composition Formula calculated
	Molecular Coding Format				
[1] 	Adenine	nucleic acid	135.13	135.1267	C5H5N5
	`^30,Ph,3=?5,9=db,2'6'9:N,5:/NH2,7:NH`				
[2] 	Guanine	nucleic acid	151.13	151.1261	C5H5N5O
	`^30,?6,3=?5,1'3'9=db,2'9:N,6'7:NH,5:?O,1:/NH2`				
[3] 	Cytosine	nucleic acid	111.10	111.1019	C4H5N3O
	`^30,?6,4'6=db,4:N,3:?O,2:NH,5:/NH2`				
[4] 	Thymine	nucleic acid	126.11	126.1133	C5H6N2O2
	`^30,?6,3=db,2'6:NH,1'5:?O,4:?`				
[5] 	Uracil	nucleic acid	112.09	112.0867	C4H4N2O2
	`^30,?6,6=db,3'5:?O,2'4:NH`				
[6] 	Glycine	amino acid	75.07	75.06659	C2H5NO2
	`^30,NH2,!2,COOH`				
[7] 	L-Alanine	amino acid	89.10	89.09318	C3H7NO2
	`^30,NH2,!wb,?!,COOH`				
[8] 	L-Valine	amino acid	117.15	117.1463	C5H11NO2
	`^30,NH2,!wb,/?!,!COOH`				
[9] 	L-Leucine	amino acid	131.16	131.1729	C6H13NO2
	`^30,NH2,!wb,/!?!,!COOH`				
[10] 	L-Isoleucine	amino acid	131.16	131.1729	C6H13NO2
	`^30,NH2,!wb,/?z'!2,!COOH`				
[11] 	L-Serine	amino acid	105.09	105.0925	C3H7NO3
	`^30,NH2,!wb,/!OH,!COOH`				
[12] 	L-Threonine	amino acid	119.12	119.1191	C4H9NO3
	`^30,NH2,!wb,/?'!w'OH,!COOH`				
[13] 	L-Cysteine	amino acid	121.16	121.1581	C3H7NO2S
	`^30,NH2,!wb,/!SH,!COOH`				
[14] 	L-Methionine	amino acid	149.21	149.2113	C5H11NO2S
	`^30,NH2,!wb,/!2'S!,!COOH`				
[15] 	L-Phenylalanine	amino acid	165.19	165.1891	C9H11NO2
	`^30,NH2,!wb,/!Ph,!COOH`				
[16] 	L-Tyrosine	amino acid	181.19	181.1885	C9H11NO3
	`^30,NH2,!wb,/!Ph'5:/OH,!COOH`				

[17] 	L-Triptophan	biological	204.21	204.2251	C11H12N2O2
	^30,NH2,!wb,!COOH,2:,!2,^24,<?5,2=dr,5=dl,2=Ph,4:NH				
[18] 	L-Proline	amino acid	115.13	115.1304	C5H9NO2
	^18,?5,3:NH,4:*/COOH				
[19] 	L-Glutamine	amino acid	146.15	146.1444	C5H10N2O3
	^30,NH2,!wb,!COOH,2:,!2‘1,!?O!,NH2				
[20] 	L-Asparagine	amino acid	132.12	132.1179	C4H8N2O3
	^30,NH2,!wb,/!?O!’NH2,!COOH				
[21] 	L-Aspartic acid	amino acid	133.10	133.1026	C4H7NO4
	^30,NH2,!wb,/!COOH,!COOH				
[22] 	L-Glutamic acid	amino acid	147.13	147.1292	C5H9NO4
	^30,NH2,!wb,/!2’COOH,!COOH				
[23] 	L-Lysine	amino acid	146.19	146.1875	C6H14N2O2
	^30,NH2,!wb,/!4’NH2,!COOH				
[24] 	L-Arginine	amino acid	174.21	174.2009	C6H14N4O2
	^30,NH2,!wb,!COOH,2:,!2‘1,!2,NH!,?NH,!NH2				
[25] 	L-Hystidine	amino acid	155.16	155.1545	C6H9N3O2
	^30,NH2,!wb,!COOH,2:,!2,<?5,1’3=dl,3:N,5:NH				
[26] 	L-DOPA	amino acid	197.19	197.1879	C9H11NO4
	^30,NH2,!wb,/!Ph’(4’5:/OH),!COOH				
[27] 	Ornithine	amino acid	132.16	132.1609	C5H12N2O2
	^30,NH2,!wb,/!3’NH2,!COOH				
[28] 	Citrulline	amino acid	175.2	175.1857	C6H13N3O3
	^30,NH2,!wb,/!3’NH!’?O!’NH2,!COOH				
[29] 	GABA	amino acid	103.12	103.1197	C4H9NO2
	^30,NH2,!4,COOH				
[30] 	Citrate	biological	192.12	192.1235	C6H8O7
	^30,COOH,!2,/COOH^30,/OH^-30,!2,COOH				
[31] 	cis-Aconitate	biological	174.11	174.1082	C6H6O6
	^30,COOH,!2,/COOH,!d,60,COOH				
[32] 	Isocitrate	biological	192.12	192.1235	C6H8O7
	^30,COOH,!4,COOH,3:/COOH,4:/OH				
[33] 	Oxalosuccinate	biological	190.11	190.1076	C6H6O7
	^30,COOH,!2,/COOH,!?O!,COOH				
[34] 	alfa-Ketoglutarate	biological	146.1	146.0981	C5H6O5
	^30,COOH,!3,?O!,COOH				

[35] 	Succinate	biological	118.09	118.0880	C4H6O4
	^30,COOH,!3,COOH				
[36] 	Fumarate	biological	116.07	116.0721	C4H4O4
	^30,COOH,!!d,!COOH				
[37] 	Malate	biological	134.09	134.0874	C4H6O5
	^30,COOH,!3,COOH,3:/OH				
[38] 	Oxaloacetate	biological	132.07	132.0715	C4H4O5
	^30,COOH,!,?O!2,COOH				
[39] 	Glucose 1	sugar	180.16	180.1558	C6H12O6
	^30,?6,5:O,2:*/OH,1’3:/*OH,4:*/*OH,6:*/!OH				
[40] 	Glucose 2	sugar	180.16	180.1558	C6H12O6
	^-30,OH,!2,*/OH,!,/*OH,!,/*OH,!,/*OH,!?O!,H				
[41] 	D-Glucose	sugar	180.16	180.1558	C6H12O6
	hexose_hp,‘.5,1^$270’2^$90’3^$270’4^$270:/OH,6^$90:/!OH				
[42] 	Fructose 1	sugar	180.16	180.1558	C6H12O6
	^30,OH,!2,/*OH,!,*/OH,!,*/OH,!,?O!2,OH				
[43] 	Fructose 2	sugar	180.16	180.1558	C6H12O6
	^-18,?5,5:O,1^-48:*/*!OH,1^48:/OH,*2’3:*/OH,4:/*!OH				
[44] 	D-Fluctose	sugar	180.16	180.1558	C6H12O6
	Pyranose_hp,‘.5,1^$270:/OH,2^$270’3^$90:/OH,1^$90’4^$270:/!OH				
[45] 	D-Galactose	sugar	180.16	180.1558	C6H12O6
	hexose_hp,‘.5,1^$90’2^$90’3^$270’4^$270:/OH,6^$90:/!OH				
[46] 	D-Mannose	sugar	180.16	180.1558	C6H12O6
	hexose_hp,‘.5,1^$270’2^$90’3^$90’4^$270:/OH,6^$90:/!OH				
[47] 	L-Fucose	sugar	164.16	164.1564	C6H12O5
	hexose_hp,‘.5,1^$270’2^$270’3^$90’4^$90:/OH,6^$270:?				
[48] 	D-Ribose	sugar	150.13	150.1299	C5H10O5
	Pyranose_hp,‘.5,2^$270’3^$270’4^$90:/OH,1^$90:/!OH				
[49] 	D-Deoxyribose	sugar	134.13	134.1305	C5H10O4
	Pyranose_hp,‘.5,2^$270’4^$90:/OH,1^$90:/!OH				
[50] 	D-Glucosamine	sugar	179.17	179.1711	C6H13NO5
	hexose_hp,‘.5,1^$270’2^$90’4^$270:/OH,3^$270:/NH2,6^$90:/!OH				
[51] 	N-acetyl-Glucosamine	sugar	221.21	221.2077	C8H15NO6
	hexose_hp,‘.5,1^$270’2^$90’4^$270:/OH,3^$270^lr:/NH!’?O!,6^$90:/!OH				
[52] 	Glucuronic acid	sugar	194.14	194.1393	C6H10O7
	hexose_hp,‘.5,1^$270’2^$90’3^$270’4^$270:/OH,6^$90:/COOH				

[53] 	Maltose	sugar	342.3	342.2964	C12H22O11
	`hexose_hp,‘.5,1^$270’2^$90’3^$270:/OH,6^$90:/!OH,‘, 4:,$310~arc_lb‘1,0,$50~arc_br‘1,^$0, <hexose_hp,‘.5,2^$90’3^$270’4^$270:/OH,6^$90:/!OH`				
[54] 	Lactose	sugar	342.3	342.2964	C12H22O11
	`hexose_hp,‘.5,1^$90’2^$90’3^$270:/OH,6^$90:/!OH,‘, 4:,$0~arc_ltr,0,$0~arc_lbr, <hexose_hp,‘.5,2^$90’3^$270’4^$270:/OH,6^$90:/!OH`				
[55] 	Cellobiose	sugar	342.3	342.2964	C12H22O11
	`hexose_hp,‘.5,1^$270’2^$90’3^$270:/OH,6^$90:/!OH,‘, 4:,$0~arc_lbr,0,$0~arc_ltr, <hexose_hp,‘.5,2^$90’3^$270’4^$270:/OH,6^$90:/!OH`				
[56] 	Trehalose	sugar	342.3	342.2964	C12H22O11
	`hexose_hp,‘.5,1^$270’2^$90’3^$270:/OH,6^$90:/!OH,‘, 4:,(1’0):,<hexose_hp,‘.5,1^$270’2^$90’3^$270:/OH,6^$90:/!OH,‘, $4:,$323~arc_lb‘3.25,0,:4~arc_br`				
[57] 	Geraniol	biological	154.25	154.2493	C10H18O
	`^30,!8,OH,2’6=dr,2’6:?`				
[58] 	Limonene	biological	136.24	136.2340	C10H16
	`^30,?6,2=dl,2:?,5:*/?!d`				
[59] 	l-Menthol	biological	156.27	156.2652	C10H20O
	`^30,?6,2:/*?!,5:?w,3:*/OH`				
[60] 	Allicin	biological	162.28	162.2729	C6H10OS2
	`^-30,!d,!2,S?O,!S,!2,!d`				
[61] 	Benzoic acid	biological	122.12	122.1213	C7H6O2
	`^30,Ph,3:/COOH`				
[62] 	Gallic acid	biological	170.12	170.1195	C7H6O5
	`^30,Ph,3:/COOH,1’5’6:/OH`				
[63] 	Salicylic acid	biological	138.12	138.1207	C7H6O3
	`^30,Ph,3:/COOH,4:/OH`				
[64] 	Cinnamic acid	biological	148.16	148.1586	C9H8O2
	`^30,Ph,3:/!dr’!COOH`				
[65] 	Cinnamaldehyde	biological	132.16	132.1592	C9H8O
	`^30,Ph,3:/!dr’!CHO`				
[66] 	Caffeic acid	biological	180.16	180.1574	C9H8O4
	`^30,Ph,1’6:/OH,3:/!d’!COOH`				
[67] 	Vanillin	biological	152.15	152.1473	C8H8O3
	`^30,Ph,1:/OH,6:/O!,4:/CHO`				
[68]	alfa-Terpinene	biological	136.24	136.2340	C10H16
	`^30,?6,3:/?!,6:?,3’5=db`				
[69]	beta-Terpinene	biological	136.24	136.2340	C10H16
	`^30,?6,3:/?!,6:?d,3=db`				
[70]	gamma-Terpinene	biological	136.24	136.2340	C10H16
	`^30,?6,3:/?!,6:?,3’6=db`				

[71]	delta-Terpinene	biological	136.24	136.2340	C10H16
	^30,?6,3://?!,6:?,5=db				
[72] 	Eugenol	biological	164.20	164.2010	C10H12O2
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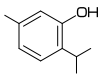
[73] 	Thymol	biological	150.22	150.2175	C10H14O
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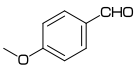
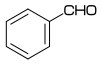
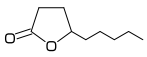
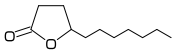
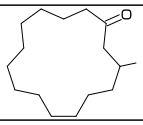
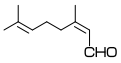
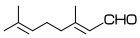
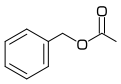
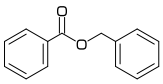
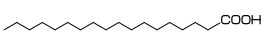
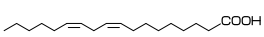
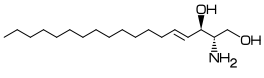
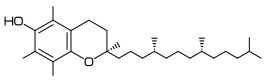
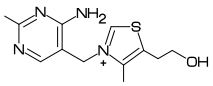
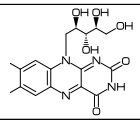
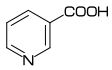
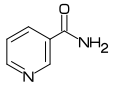
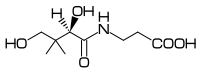
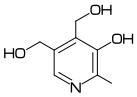
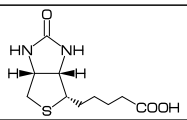
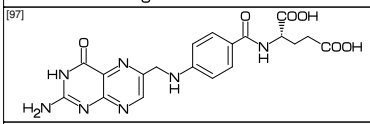
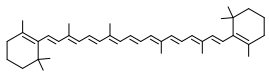
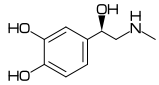
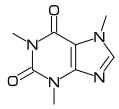
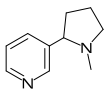
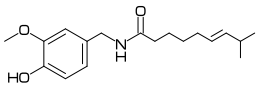
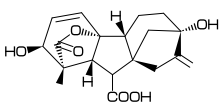
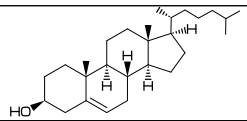
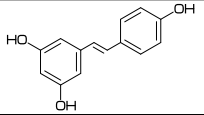
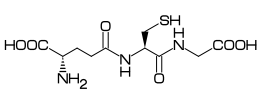
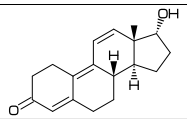
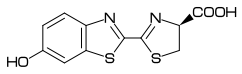
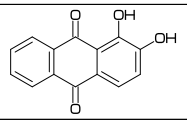
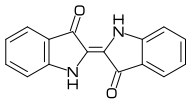
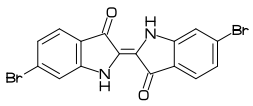
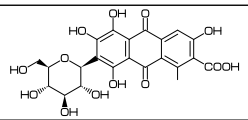
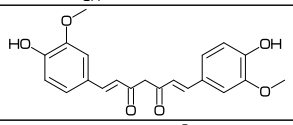
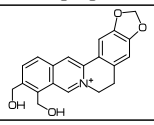
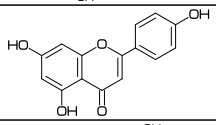
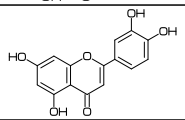
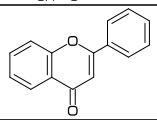
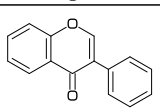
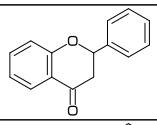
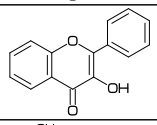
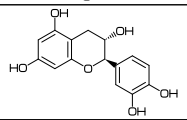
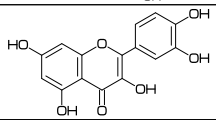
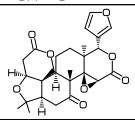
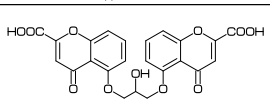
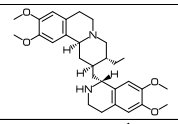
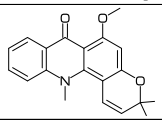
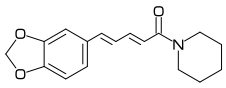
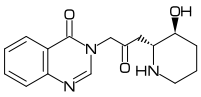
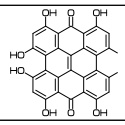
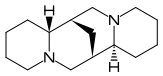
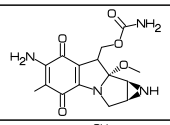
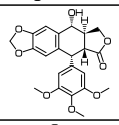
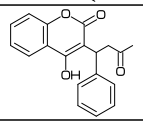
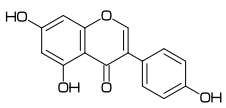
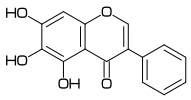
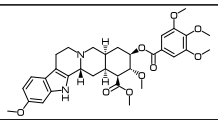
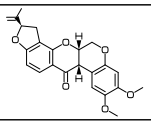
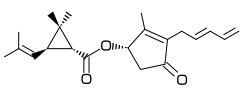
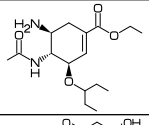
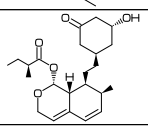
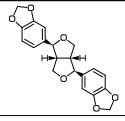
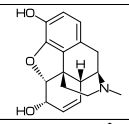
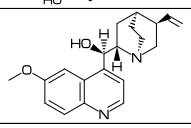
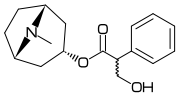
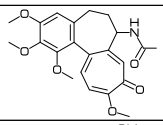
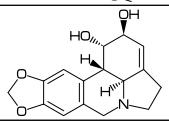
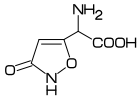
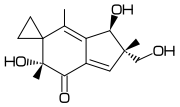
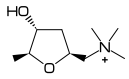
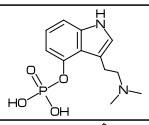
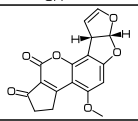
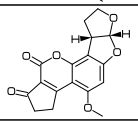
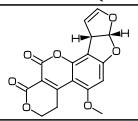
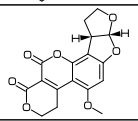
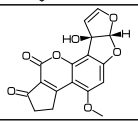
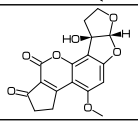
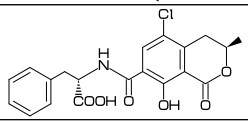
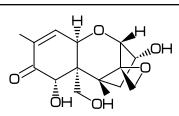
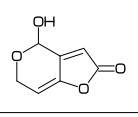
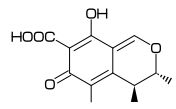
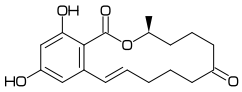
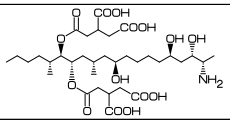
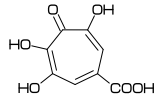
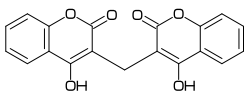
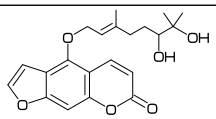
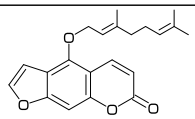
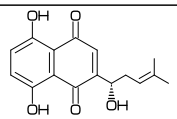
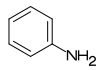
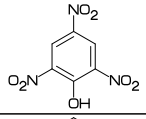
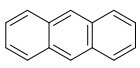
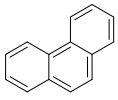
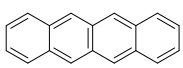
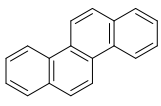
[74] 	Anisaldehyde	biological	136.15	136.1479	C8H8O2
	^30,Ph,4:/CHO,1:/O!				
[75] 	Benzaldehyde	biological	106.12	106.1219	C7H6O
	^30,Ph,4:/CHO				
[76] 	gamma-Nonalactone	biological	156.23	156.2221	C9H16O2
	^18,?5,2:O,1:?O,3^-12:/!4				
[77] 	gamma-Undecalactone	biological	184.27	184.2752	C11H20O2
	^18,?5,2:O,1:?O,3^-12:/!6				
[78] 	Muscone	biological	238.40	238.4088	C16H30O
	^-72,‘1,60,-48,60,60,-48,60,60,-48,60,60,-48,60,60,-48,‘,:1,9:?O,7:?				
[79]	alfa-Pinene	biological	136.24	136.2340	C10H16
	^30,?6,3:??,5:?,5=db,2:,180~zf‘1,:4~zb				
[80]	beta-Pinene	biological	136.24	136.2340	C10H16
	^30,?6,3:??,5:?d,2:,180~zf‘1,:4~zb				
[81] 	Neral	biological	152.24	152.2334	C10H16O
	^30,!?,!d,!3,?,!d,-60,CHO				
[82] 	Geranial	biological	152.24	152.2334	C10H16O
	^30,!?,!d,!3,?,!d,!,CHO				
[83]	p-Cymene	biological	134.21	134.2181	C10H14
	^30,Ph,4:/?!,1:?				
[84] 	Benzyl-acetate	biological	150.18	150.1744	C9H10O2
	^30,Ph,4:,!2,O!,?O!				
[85] 	Benzyl-benzoate	biological	212.25	212.2438	C14H12O2
	^30,Ph,4:,!?O!,O!,!,Ph				
[86] 	Stearic acid	biological	284.48	284.4772	C18H36O2
	^30,!17,COOH				
[87] 	Linoleic acid	biological	280.45	280.4454	C18H32O2
	^30,!5,-30,-30,!,-30,-30,!7,COOH,6’9=dr				
[88] 	Sphingosine	biological	299.50	299.4918	C18H37NO2
	^30,!18,OH,14=dr,-3:*/OH,-2:/*NH2				

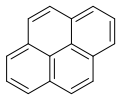
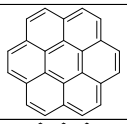
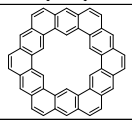
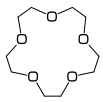
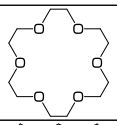
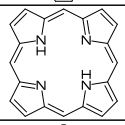
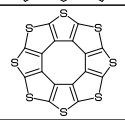
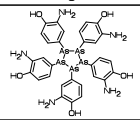
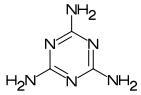
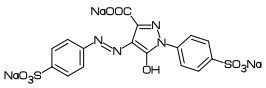
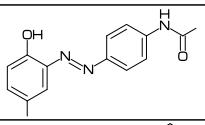
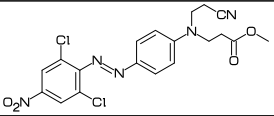
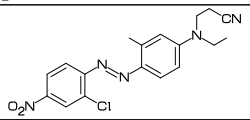
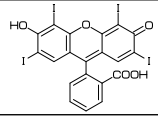
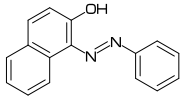
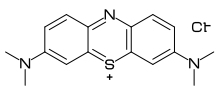
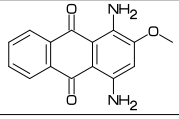
[89] 	Tocopherol	biological	430.717	430.7060	C29H50O2
	^30,Ph,3=?6,7:O,1'2'5:?,8:?z^60,6:/OH,8:,!,<!12,4'8:?z,12:?				
[90] 	Thiamine	biological	265.35	265.3545	C12H17N4OS
	^30,Ph,4:/NH2,3:,!'1,!,^-12,?5,-1'-4=dl,1'5'8:N,11:S,6'9:?, -3^-12:/!2'OH,8:p^72				
[91] 	Riboflavin	biological	376.37	376.3638	C17H20N4O6
	^30,Ph,3'9=?6,8'16=dl,7'10'14:N,12:NH,11'13:?O,1'6:?, 10:,!'1.5,!,*/OH,!,/*OH,!,*/OH,!2,OH				
[92] 	Nicotinic acid	biological	123.11	123.1093	C6H5NO2
	^30,Ph,2:N,4:/COOH				
[93] 	Nicotinamide	biological	122.12	122.1246	C6H6N2O
	^30,Ph,2:N,4:/?O'!NH2				
[94] 	Pantothenic acid	biological	219.23	219.2349	C9H17NO5
	^30,OH,!8,COOH,3:??,4^35:/*H,4^-20:*/OH,5:?O,6:NH				
[95] 	Pyridoxine	biological	169.18	169.1778	C8H11NO3
	^30,Ph,2:N,3:?,4:/OH,5'6:/!OH				
[96] 	Biotin	biological	244.31	244.3106	C10H16N2O3S
	^18,?5,4=?5,2:S,6'8:NH,7:?O,4^-54'5^54:*/H,3^-12:/*!4'COOH				
[97] 	Folic acid	biological	441.3975	441.3974	C19H19N7O6
	^30,?6,3=Ph2,1=dl,2'7'10:N,6:NH,5:?O,1:/NH2, 9:,!,!NH!,Ph,-3:,!?O,!NH!,/*COOH,!3,COOH				
[98] 	Carotene	biological	536.8726	536.8726	C40H56
	^30,?6,4:,!19,?6,8'10'12'14'16'18'20'22'24=dr,5'9'13'18'22'-5:?,4'-6=dl,3'-1:??				
[99] 	Adrenalin	biological	183.21	183.2044	C9H13NO3
	^30,Ph,1'6:/OH,4:,!,*/OH,!2,NH!				
[100] 	Caffeine	biological	194.194	194.1905	C8H10N4O2
	^30,?6,3=dl,1'5:?O,3=?5,8=dl,7:N,2'6'9:N?				
[101] 	Nicotine	biological	162.23	162.2315	C10H14N2
	^30,Ph,2:N,4:/?5'2:N?				
[102] 	Capsaicin	biological	305.418	305.4118	C18H27NO3
	^30,Ph,1:/OH,6:/O!,4:,!,!NH!,?O,!7,?!,-3=dl				
[103] 	Gibberellin A3	biological	346.379	346.3743	C19H22O6
	^18,?5,3=?7,5='1.2'?6,8:,160'1.3,:3,13=dl,6=wf,8=wb, 5:,40~zf'1,O,50,?O^180,:14~zb,2:/COOH,7:?d,*8'13:*/OH,14:?w,1'4:*/H^60				
[104] 	Cholesterol	biological	386.664	386.6535	C27H46O
	^30,?6,-4'-2=?6,-4=?5,7=dl, 1:*/OH,4'12:?w^60,*9^60'10^180'11^-60'-1^-60:/*H,-1:,17,?z,!4,?!				
[105] 	Resveratrol	biological	228.24	228.2432	C14H12O3
	^30,Ph,4:,!,!d!,Ph,2'6'-3:/OH				
[106] 	Glutathione	biological	307.33	307.3234	C10H17N3O6S
	^-30,COOH,!,/*NH2,!3,?O,!NH!,*/!SH,!?O!,NH,!2,COOH				

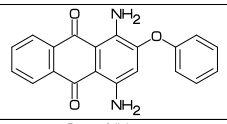
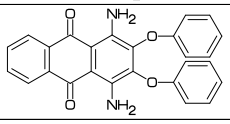
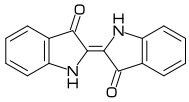
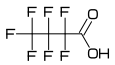
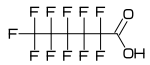
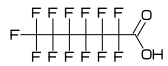
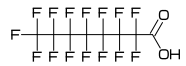
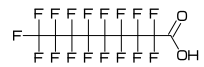
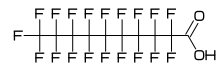
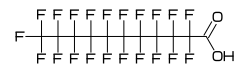
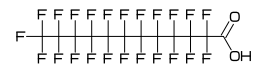
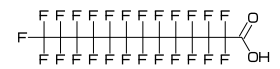
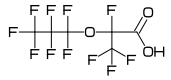
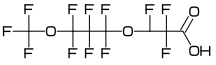
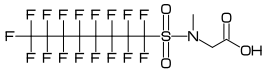
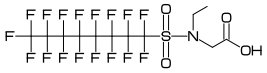
[107] 	Trenbolone	biological	270.37	270.3660	C18H22O2
	^30,?6,3’10=?6,13=?5,2’11’15=dl,1:?O,12:?w^60,-1:/*OH,9^60’*11^-60:*/H				
[108] 	Luciferin	biological	280.33	280.3228	C11H8N2O3S2
	^30,Ph,3=?5,8:,!,?5,9’16=dl,9’14:N,7’11:S,1:/OH,-2:*/COOH				
[109] 	Alizarin	biological	240.21	240.2109	C14H8O4
	^30,Ph,3=?6,-3=Ph2,7’10:?O,13’14:/OH				
[110] 	Indigo	biological	262.26	262.2627	C16H10N2O2
	^30,Ph,3=?5,-2:,!d,?5,-3=Ph2,7’14:NH,9’11:?O				
[111] 	6,6’-dibromoindigo	biological	420.0549	420.0549	C16H8Br2N2O2
	^30,Ph,3=?5,-2:,!d,?5,-3=Ph2,7’14:NH,9’11:?O,1’-2:/Br				
[112] 	Carminic Acid	biological	492.39	492.3863	C22H20O13
	^30,Ph,3=?6,-3=Ph2,7’10:?O,2’5’6’13:/OH,11:?,12:/COOH, 1:,!~wb‘1,?6,-5:O,-1’*-2’-3:/*OH,-4:*/!OH				
[113] 	Curcumin	biological	368.38	368.3798	C21H20O6
	^30,Ph,3:,!8,Ph,8’13=dr,9’11:?O,6’-3:/OH,5’-4:/O!				
[114] 	Berberine	biological	336.36	336.3612	C20H18NO4
	^30,Ph,3=Ph,-3=?6,-2=Ph2,-3=?5,8:N,8:p^60,-1’-3:O,1^vt’2:/!OH				
[115] 	Apigenin	biological	270.24	270.2368	C15H10O5
	^30,Ph,2’6:/OH,3=?6,9=dl,10:O,7:?O,9:,!Ph,-3:/OH				
[116] 	Luteolin	biological	286.24	286.2363	C15H10O6
	^30,Ph,2’6:/OH,3=?6,9=dl,10:O,7:?O,9:,!Ph,-2’-3:/OH				
[117] 	Flavone	biological	222.24	222.2386	C15H10O2
	^30,Ph,3=?6,9=dl,10:O,7:?O,9:/Ph				
[118] 	Isoflavone	biological	222.24	222.2386	C15H10O2
	^30,Ph,3=?6,9=dl,10:O,7:?O,8:/Ph				
[119] 	Flavanone	biological	224.25	224.2545	C15H12O2
	^30,Ph,3=?6,10:O,7:?O,9:/Ph				
[120] 	Flavonol	biological	238.24	238.2381	C15H10O3
	^30,Ph,3=?6,9=dl,10:O,7:?O,8:/OH,9:/Ph				
[121] 	Cianidanol	biological	290.27	290.2680	C15H14O6
	^30,Ph,3=?6,8:,!w,Ph,7:O,1’5’9~zf’13’14:/OH				
[122] 	Quercetin	biological	302.24	302.2357	C15H10O7
	^30,Ph,3=?6,9:,!Ph,9=dl,10:O,7:?O,2’6’8’13’14:/OH				
[123] 	Limonin	biological	470.518	470.5115	C26H30O8
	^30,?6,-3’-4=?6,-5=?3,-2=wf,-1=wb,6=?5,-4=?6,-5=wf,13’15’17’20:O, 3’12’21:?O,4’*8:?w^60,18:??,1^60’5^180’16^60:/*H, 14:,!z,<?5,1’4=dl,3:O				
[124] 	Cromolyn	biological	468.37	468.3665	C23H16O11
	^30,Ph,6=?6,9=dl,7:O,10:?O,8:/COOH, $2:,!,O!2,/OH,!2,O,60,<Ph,2=?6,9=dl,10:O,7:?O,9:/COOH				

[125] 	Emetine	biological	480.649	480.6388	C29H40N2O4
	^30,Ph,-4'-4=?6,8:N,1'6:/O!,-2:/*!,7'12:/*H^-60, -3:,!,!zb,^-60,<?6,5=dl,2:NH,1^-60:*/H,<-2=?6,2'4=dl,2'3:/O!				
[126] 	Acronycine	biological	321.376	321.3697	C20H19NO3
	^30,Ph,<-4=?6,1:N?,4:?O,-3=Ph2,-1:/O!,<-4=?6,2=dl,4:O,3:??				
[127] 	Piperine	biological	285.343	285.3376	C17H19NO3
	^30,Ph,-1=?5,-1'-3:O,4:,!!d,!!d,!?O!,?6,-6:N				
[128] 	Febrifugine	biological	301.34	301.3403	C16H19N3O3
	^30,Ph,3=?6,8=dl,9:,!3,!zb,?6,7'9:N,-5:NH,10'12:?O,-1:*/OH				
[129] 	Hypericin	biological	504.44	504.4432	C30H16O8
	^30,Ph,-4'-3'11--4'16---17'19'23---24'22--29=?6, 12'14'16'17'*22'24'26'28'33'35=dl,7'25:?O,13'26:?,2'6'11'21'23'28:/OH				
[130]	Camphor	biological	152.23	152.2334	C10H16O
	‘1,15,-30,90,90,30,‘,:1,2:,0~si_‘1.6,:5,-1^45'-1^-65'5^-45:?,4:?O				
[131] 	Sparteine	biological	234.3803	234.3803	C15H26N2
	^30,?6,3=?6,9=wf,10=wb,8:,‘1,60,60,N,60,‘,:10,-3=?6,3:N,4^60'*11^-60:*/H				
[132] 	Mitomycine C	biological	334.332	334.3272	C15H18N4O5
	^30,?6,3'6=dl,2'5:?O,1:?,-4=?5,-3:N, 6:/NH2,-3=?5,-2=?3,-1=wb,-2=wf,-1:NH,8:/*O!^35,$9:,!2,O,60,?O!,NH2				
[133] 	Podophyllotoxin	biological	414.41	414.4052	C22H22O8
	^0,?5,2'5:O,3=Ph2,8=?6,-3=?5,-2:O,-1=wb,-3:?O, 10:/*Ph'(3'4'5:/O!),13:/*OH,11^-60'*12^60:*/H				
[134] 	Warfarin	biological	308.333	308.3279	C19H16O4
	^30,Ph,3=?6,8=dl,10:O,7:/OH,9:?O,8:,!,/Ph‘1,!2,?O!				
[135] 	Genistein	biological	270.24	270.2368	C15H10O5
	^30,Ph,3=?6,9=dl,10:O,2'6:/OH,7:?O,8:/Ph'4:/OH				
[136] 	Baicalein	biological	270.24	270.2368	C15H10O5
	^30,Ph,3=?6,9=dl,10:O,1'2'6:/OH,7:?O,8:/Ph				
[137] 	Reserpine	biological	608.688	608.6786	C33H40N2O9
	^54,Ph,3=?5,-2'-4'-3=?6,9=dl,11:N,7:NH,*10^-60'15^-60'16^60:/*H, 20:,!w,O!,?O,!Ph,-2'-3'-4'1'19~zf^rl:/O!,18:*/?O!'O!^lr				
[138] 	Rotenone	biological	394.423	394.4171	C23H22O6
	^-60,?5,-3'-2'-3'-4=?6,*3'7'9'*17'-2'-4=dl, 2'13'16:O,10:?O,11^-60'12^60:*/H,-2'-3:/O!,1:*/?!d				
[139] 	Pyrethrin I	biological	328.452	328.4452	C21H28O3
	^30,?3,3^35'*3^-35:?w,1:,!w,!d,?!, 2:,!z,?O!O,-36~zb,<?5,4=dl,5:?,3:?O,4:,<!5,3'5=dl				
[140] 	Oseltamivir	biological	312.40	312.4045	C16H28N2O4
	^30,?6,3=dl,6:*/NH2,1:,!z,NH!,?O!,2:,!w,O!,/!,!2,4:/?O!'O!2				
[141] 	Mevastatin	biological	390.52	390.5130	C23H34O5
	^30,?6,2=dl,4^60:*/H,-4=?6,-4=dl,9:?w, 10:,!w,!,60~wb,?6,6:O,-2:?O,-4:/*OH,5:,!z,O,60,?O!,?w,!2				
[142] 	Sesamine	biological	354.35	354.3533	C20H18O6
	^54,?5,1=?5,4'7:O,1^-54'2^54:*/H,5'8:*/Ph'4=?5'(7'9:O)^-12				

[143] 	Morphine	biological	285.343	285.3376	C17H19NO3
	^30,Ph,2'-4=?6,1---12=?5,-1:O,-1=zb, 7:,60~wf'0.75,70~si_'1.3,45,N?,:9~wb,15=dl,6:/OH,8^180:*/H,12:/*OH				
[144] 	Quinine	biological	324.424	324.4167	C20H24N2O2
	^30,Ph,3=Ph,7:N,6:/O!, 10:,!,*/OH,/*H^-60,!,<?6,2:N,1^60:*/H,4:*/!d,2:,165~zf,60,:5~zb				
[145] 	Atoropin	biological	289.375	289.3694	C17H23NO3
	^30,O!,?O!2,Ph,1:,-60~zb,?7'1.1,-2:,190~wf'1.25,N?,:-5~wb,$3:/!OH~wv				
[146] 	Colchicine	biological	399.443	399.4370	C22H25NO6
	^30,Ph,1'2'6:/O!,-4'-5=?7,-1'-4'-6=dl,-2:?O,-3:/O!,9:/NH!'?O!				
[147] 	Lycorine	biological	287.315	287.3104	C16H17NO4
	^30,Ph,-4'-2=?6,6'9--12=?5,13=dl,8:N,15'17:O,*9^180'10^60:*/H,13'*14:*/OH				
[148] 	Ibotenic acid	biological	158.113	158.1121	C5H6N2O4
	^18,?5,4=dl,3:O,2:NH,1:?O,4^-24:/?NH2'!COOH				
[149] 	Illudin S	biological	264.3	264.3168	C15H20O4
	^30,?6,3=?5,6:,?3,4'7=dl,2:?O,5:?,1'8:?w^35,*1^-35'9:*/OH,8^-35:/*!OH				
[150] 	Muscarine	biological	174.26	174.2605	C9H20NO2
	^18,?5,2:O,1:?w,5:/*OH,3:,!w,48,N,??,p^180,!				
[151] 	Psilocybin	biological	284.248	284.2481	C12H17N2O4P
	^30,Ph,3=?5,8=dl,9:NH,2:,!O,-60,P,?O^-45,/OH^45,90,OH,7:/!2'N?!^lr				
[152] 	Aflatoxin B1	mycotoxin	312.27	312.2735	C17H12O6
	^30,Ph,6=?6,-2'4'-2=?5,-2'10=dl,7'14'17:O,2:/O!,8'11:?O,15^-54'16^54:*/H				
[153] 	Aflatoxin B2	mycotoxin	314.3	314.2894	C17H14O6
	^30,Ph,6=?6,-2'4'-2=?5,10=dl,7'14'17:O,2:/O!,8'11:?O,15^-54'16^54:*/H				
[154] 	Aflatoxin G1	mycotoxin	328.27	328.2729	C17H12O7
	^30,Ph,6'-2=?6,4'-2=?5,-2'10=dl,7'12'15'18:O,2:/O!,8'11:?O,16^-54'17^54:*/H				
[155] 	Aflatoxin G2	mycotoxin	330.29	330.2888	C17H14O7
	^30,Ph,6'-2=?6,4'-2=?5,10=dl,7'12'15'18:O,2:/O!,8'11:?O,16^-54'17^54:*/H				
[156] 	Aflatoxin M1	mycotoxin	328.3	328.2729	C17H12O7
	^30,Ph,6=?6,-2'4'-2=?5,-2'10=dl,7'14'17:O,2:/O!,8'11:?O,15^-54:*/H,16^54:*/OH				
[157] 	Aflatoxin M2	mycotoxin	330.29	330.2888	C17H14O7
	^30,Ph,6=?6,-2'4'-2=?5,10=dl,7'14'17:O,2:/O!,8'11:?O,15^-54:*/H,16^54:*/OH				
[158] 	Ochratoxin A	mycotoxin	403.813	403.8130	C20H18ClNO6
	^30,Ph,4:,!2,/*COOH,!'1.2,NH,!'1.2,?O!,<Ph,5:/Cl,2:/OH,3=?6,8:O,9:?w,7:?O				
[159] 	Deoxynivalenol	mycotoxin	296.32	296.3156	C15H20O6
	^30,?6,3=?6,5=dl,1:?O,6:?,-1:O,*4^60'-2:*/H,7^30:?w,7:,72'.9,80'1.3,:9, 8:,?3,-3=wf_,-1=si_,-1:O,2'12^18:/*OH,3^-60'1:/*!OH				
[160] 	Patulin	mycotoxin	154.12	154.1201	C7H6O4
	^30,?6,3=?5,2'10=dl,6'7:O,5:/OH,8:?O				

[161] 	Citrinin	mycotoxin	250.247	250.2472	C13H14O5
	^30,?6,3=?6,2’5’11=dl,9:O,1:?O,2:?,7’*8:?w,5:/OH,6:/COOH				
[162] 	Zearalenone	mycotoxin	318.364	318.3642	C18H22O5
	^30,Ph,3:,‘1,!6,60,60,!4,:4,‘,8=dl,17:O,16:?w,1’5:/OH,12’18:?O				
[163] 	Fumonisin B1	mycotoxin	721.83	721.8299	C34H59NO15
	^30,!19,6:,!w,O!,?O!2,/COOH,!2,COOH,7:,!z‘1.2,O!,?O!2,/COOH,!2,COOH, 5’9:?z,11’16’*18:*/OH,19:/*NH2				
[164] 	Puberulic acid	mycotoxin	198.13	198.1296	C8H6O6
	^38.5,?7,2’4’7=db,3:/COOH,1’5’7:/OH,6:?O				
[165] 	Dicumarol	biological	336.295	336.2949	C19H12O6
	^30,Ph,3=?6,8:,!‘1.5,!‘1.5,?6,-4=Ph2,8’14=db,10’16:O,9’17:?O,7’13:/OH				
[166] 	Dihydroxybergamotin	biological	372.4	372.4116	C21H24O6
	^30,Ph,3=?6,6=?5,10’13=db,7’13:O,8:?O,5:,!O,!2,!d,?,!3,/OH,!??,!OH				
[167] 	Bergamotin	biological	338.40	338.3969	C21H22O4
	^30,Ph,3=?6,6=?5,10’13=db,7’13:O,8:?O,5:,!O,!2,!d,?,!3,!d,?!				
[168] 	Alkannin	biological	288.29	288.2952	C16H16O5
	^30,Ph,3=?6,9=db,2’5:/OH,7’10:?O,8:,!,/*OH,!2,!d,?!				
[169]	Benzene	synthetic	78.11	78.11184	C6H6
	^30,Ph				
[170]	Phenol	synthetic	94.11	94.11123	C6H6O
	^30,Ph,3:/OH				
[171] 	Aniline	synthetic	93.13	93.12648	C6H7N
	^30,Ph,3:/NH2				
[172] 	Picric acid	synthetic	229.10	229.1039	C6H3N3O7
	^30,Ph,1’3’5:/NO2,2:/OH				
[173]	Hexaphenylbenzene	synthetic	534.6876	534.6875	C42H30
	^30,Ph,1’2’3’4’5’6:/Ph				
[174]	Naphthalene	aromatic	128.17	128.1705	C10H8
	^30,Ph,3=Ph				
[175] 	Anthracene	aromatic	178.23	178.2291	C14H10
	^30,Ph,3’6=Ph				
[176] 	Phenanthrene	aromatic	178.23	178.2291	C14H10
	^30,Ph,4’6=Ph				
[177] 	Naphthacene	aromatic	228.3	228.2878	C18H12
	^30,Ph,6’3’-3=Ph				
[178] 	Chrysene	aromatic	228.3	228.2878	C18H12
	^30,Ph2,6’4’-4=Ph				

[179] 	Pyrene	aromatic	202.25	202.2505	C16H10
	^30,Ph2,6'4=Ph,16---7=?6,-2=dl				
[180] 	Coronene	aromatic	300.35	300.3520	C24H12
	^30,Ph,1'11--2'15--3'19--4'23--5'27---7=?6,9'12'14'17'20'22'25'28'30=dl				
[181] 	Kekulene	aromatic	600.7	600.7041	C48H24
	^30,?6,3'-3'-2'-3'-2'-3'-2'-3'-2'-3'-2----5'5----␣-4=?6, 1'*5'7'9'11'13'17'19'21'23'27'29'31'33'37'39'41'43'47'49'51'53'57'60=dl				
[182]	12-Crown-4	synthetic	176.21	176.2102	C8H16O4
	^-180,O,30,60,60,O,-30,60,60,O,-30,60,60,O,-30,60,:1				
[183] 	15-Crown-5	synthetic	220.26	220.2628	C10H20O5
	^-180,O,48,60,60,O,-48,60,60,O,-48,60,60,O,-48,60,60,O,-48,60,:1				
[184] 	18-Crown-6	synthetic	264.32	264.3153	C12H24O6
	^-180,O,60,60,60,O,-60,60,60,O,-60,60,60,O,-60,60,60,O,-60,60,60,O,-60,60,:1				
[185] 	Porphyrin	synthetic	310.4	310.3519	C20H14N4
	^9,'1,?5,3:,!,54,?5,-2:,!,54,?5,-2:,!,54,?5,-2:,!,:5,', 1'4'6'8'10'14'16'18'21'23'27=dl,4'17:N,11'23:NH				
[186] 	Sulflower	synthetic	448.69	448.6911	C16S8
	^67.5,?8,1'3'5'7=?5,11:,30'1.15,:12,14:,30'1.15,:15, 17:,30'1.15,:18,20:,30'1.15,:9,9'12'13'16'17'20'21'24=dl, 10'13'16'19'21'22'23'24:S				
[187] 	Arsphenamine x5	synthetic	915.2	915.1977	C30H30As5N5O5
	^18,?5,1'2'3'4'5:As,1'2'3'4'5:/Ph'3:/NH2'4:/OH				
[188] 	Melamine	synthetic	126.12	126.1199	C3H6N6
	^30,Ph,2'4'6:N,1'3'5:/NH2				
[189] 	Tartrazine	pigment	534.3	534.3633	C16H9N4Na3O9S2
	^30,Ph,1:/SO3Na,4:,!N,!d,N!,^-12,<?5,1'4=dl,3'4:N,5:/COONa,2:/OH, 3:/Ph'4:/SO3Na				
[190] 	Disperse yellow 3	pigment	269.30	269.2985	C15H15N3O2
	^30,Ph,2:?,5:/OH,4:,!N,!d,N,!Ph,-3:/NH!'?O!				
[191] 	Disperse orenge 30	pigment	450.27	450.2753	C19H17Cl2N5O4
	^30,Ph,1:/NO2,3'5:/Cl,4:,!N,!d,N,!Ph,-3:,!N,/!2'CN,!3,?O,!O!				
[192] 	Disperse red 65	pigment	371.82	371.8208	C18H18ClN5O2
	^30,Ph,1:/NO2,3:/Cl,4:,!N,!d,N,!Ph,-1:?,-3:,!N,/!2'CN,!2				
[193] 	Erythrosine	synthetic	835.9	835.8923	C20H8I4O5
	^30,Ph,3'9=?6,8'13'16=dl,10:O,-2:?O,1'5'12'14:/I,7:,!Ph,-1:/COOH,6:/OH				
[194] 	Sudan red 1	pigment	248.28	248.2792	C16H12N2O
	^30,Ph,1=Ph,4:/OH,3:,!N,!d,N,!Ph				
[195] 	Basic blue 1	pigment	319.86	319.8522	C16H18ClN3S
	^30,Ph,3=Ph,6=Ph,2:S,5:N,8'13:/N?!,2:p,2:,(3.5'1.5):,Cl,n_^15				
[196] 	Disperse red 11	pigment	268.274	268.2673	C15H12N2O3
	^30,Ph,3=?6,9=dr,9=Ph,7'10:?O,-1'-4:/NH2,-2:/O!				

[197] 	Disperse red 60	pigment	331.326	330.3367	C20H14N2O3
	^30,Ph,3=?6,9=dr,9=Ph,7'10:?O,-1'-4:/NH2,-2:/O!'Ph				
[198] 	Disperse violet 26	pigment	422.438	422.4321	C26H18N2O4
	^30,Ph,3=?6,9=dr,7'10:?O,<-3=Ph,1'4:/NH2,2^*30'3^*-30:/O!'Ph				
[199] 	Vat blue 1	pigment	262.27	262.2627	C16H10N2O2
	^30,Ph,3=?5,8:,!d,?5,-3=dr,-3=Ph,7'14:NH,9'11:?O				
[200] 	PFBA	pfas	214.04	214.0383	C4HF7O2
	!3^*0,?O,-60,OH,1_3'1^-90:/F,1_3:/F^180				
[201]	PFPeA	pfas	264.05	264.0458	C5HF9O2
	!4^*0,?O,-60,OH,1_4'1^-90:/F,1_4:/F^180				
[202] 	PFHxA	pfas	314.05	314.0533	C6HF11O2
	!5^*0,?O,-60,OH,1_5'1^-90:/F,1_5:/F^180				
[203] 	PFHpA	pfas	364.06	364.0608	C7HF13O2
	!6^*0,?O,-60,OH,1_6'1^-90:/F,1_6:/F^180				
[204] 	PFOA	pfas	414.07	414.0683	C8HF15O2
	!7^*0,?O,-60,OH,1_7'1^-90:/F,1_7:/F^180				
[205] 	PFNA	pfas	464.08	464.0758	C9HF17O2
	!8^*0,?O,-60,OH,1_8'1^-90:/F,1_8:/F^180				
[206] 	PFDA	pfas	514.08	514.0833	C10HF19O2
	!9^*0,?O,-60,OH,1_9'1^-90:/F,1_9:/F^180				
[207] 	PFUdA	pfas	564.09	564.0908	C11HF21O2
	!10^*0,?O,-60,OH,1_10'1^-90:/F,1_10:/F^180				
[208] 	PFDoA	pfas	614.1	614.0983	C12HF23O2
	!11^*0,?O,-60,OH,1_11'1^-90:/F,1_11:/F^180				
[209] 	PFTrDA	pfas	664.1	664.1058	C13HF25O2
	!12^*0,?O,-60,OH,1_12'1^-90:/F,1_12:/F^180				
[210]	PFTeDA	pfas	714.11	714.1133	C14HF27O2
	!13^*0,?O,-60,OH,1_13'1^-90:/F,1_13:/F^180				
[211] 	HFPO-DA(GenX)	pfas	330.05	330.0527	C6HF11O3
	!4^*0,0'1,?O,-60,OH,-3:O,1_3'1^-90:/F,1_3'5:/F^180,5:/?F?F!F				
[212] 	DONA	pfas	378.07	378.0691	C7H2F12O4
	!8^*0,?O,-60,OH,2'6:O,1'3_5'8'1^-90:/F,3_5'1'7'8:/F^180				
[213] 	NMeFOSAA	pfas	571.21	571.2074	C11H6F17NO4S
	!8^*0,S,?O,?O^180,-.1,^30,N,?,!2,?O,!,OH,1_8'1^-90:/F,1_8:/F^180				
[214] 	NEtFOSAA	pfas	585.24	585.2340	C12H8F17NO4S
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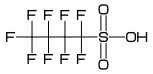
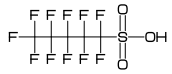
[215] 	PFBS	pfas	300.10	300.0995	C4HF9O3S
	!4^*0,S,?O,?O^180,-.1,OH,1_4'1^-90:/F,1_4:/F^180				
[216] 	PFPeS	pfas	350.11	350.1070	C5HF11O3S
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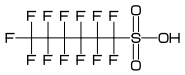
[217] 	PFHxS	pfas	400.12	400.1145	C6HF13O3S
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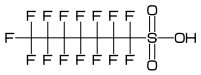
[218] 	PFHpS	pfas	450.12	450.1220	C7HF15O3S
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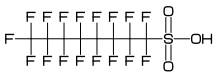
[219] 	PFOS	pfas	500.13	500.1295	C8HF17O3S
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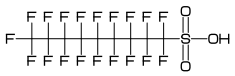
[220] 	PFNS	pfas	550.14	550.1370	C9HF19O3S
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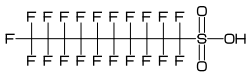
[221] 	PFDS	pfas	600.15	600.1445	C10HF21O3S
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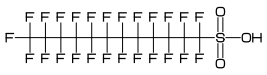
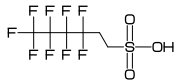
[222] 	PFDoS	pfas	700.16	700.1595	C12HF25O3S
	!12^*0,S,?O,?O^180,-.1,OH,1^-90'1_12:/F,1_12:/F^180				
[223] 	4,2-FTS	pfas	328.15	328.1526	C6H5F9O3S
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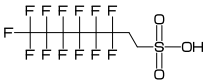
[224] 	6,2-FTS	pfas	428.16	428.1676	C8H5F13O3S
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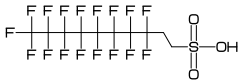
[225] 	8,2-FTS	pfas	528.18	528.1827	C10H5F17O3S
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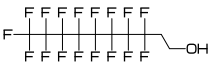
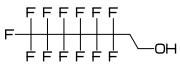
[226] 	8,2-FTOH	pfas	464.12	464.1189	C10H5F17O
	!8^*0,-60,60,OH,1^-90'1_8:/F,1_8:/F^180				
[227] 	6,2-FTOH	pfas	364.10	364.1038	C8H5F13O
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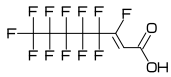
[228] 	6,2 FTUCA	pfas	358.08	358.0810	C8H2F12O2
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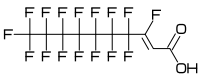
[229] 	8,2 FTUCA	pfas	458.10	458.0960	C10H2F16O2
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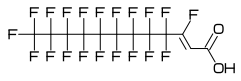
[230] 	10,2 FTUCA	pfas	558.11	558.1110	C12H2F20O2
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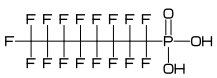
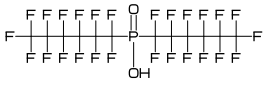
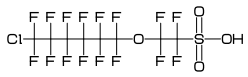
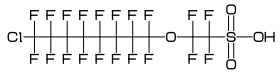
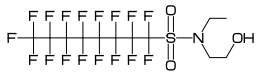
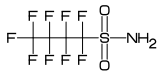
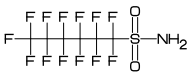
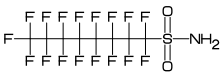
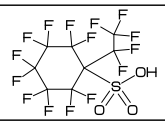
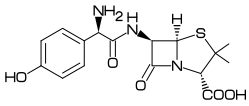
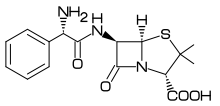
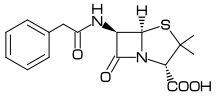
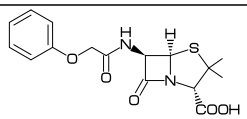
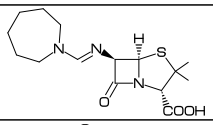
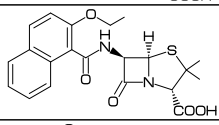
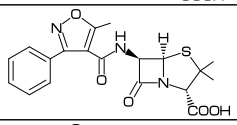
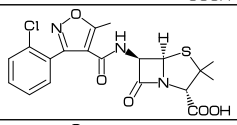
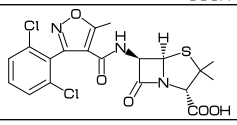
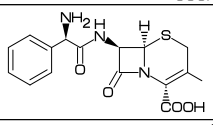
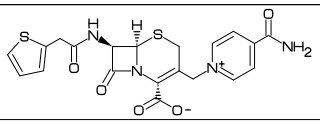
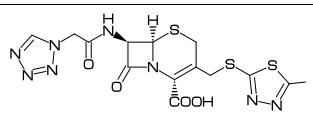
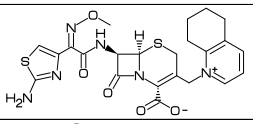
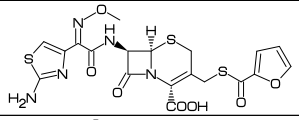
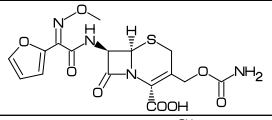
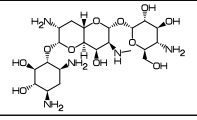
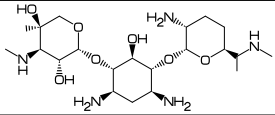
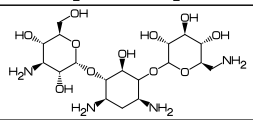
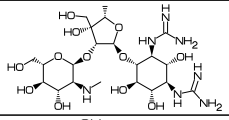
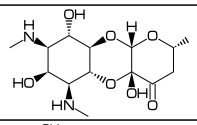
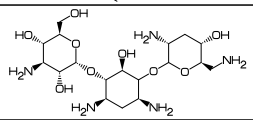
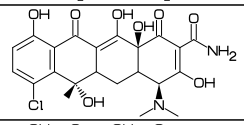
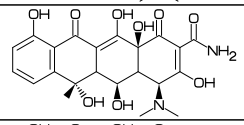
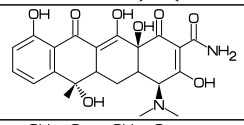
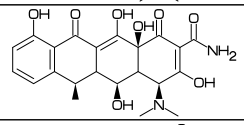
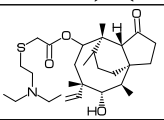
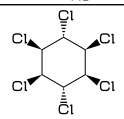
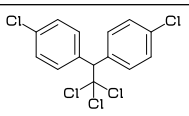
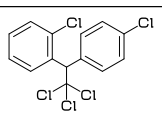
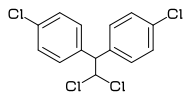
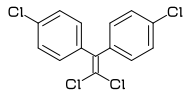
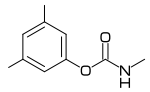
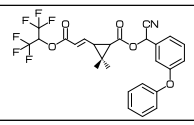
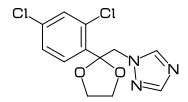
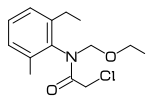
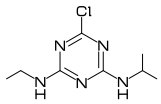
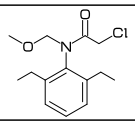
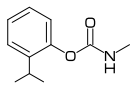
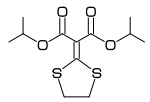
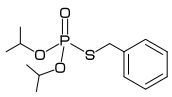
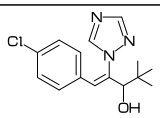
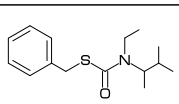
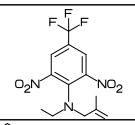
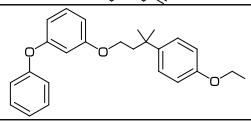
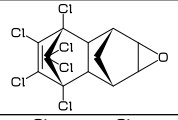
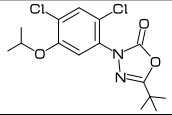
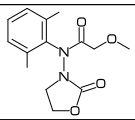
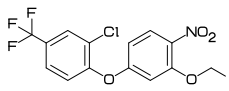
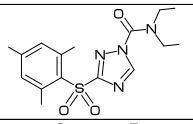
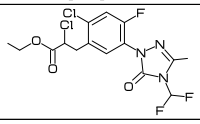
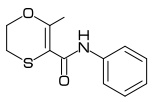
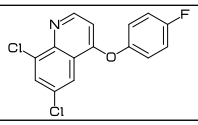
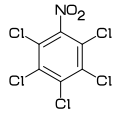
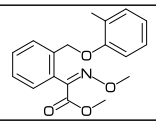
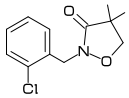
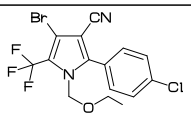
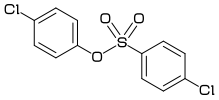
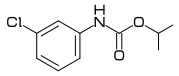
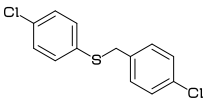
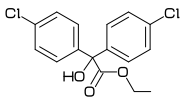
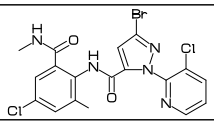
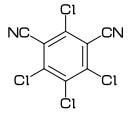
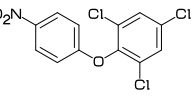
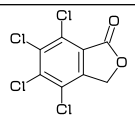
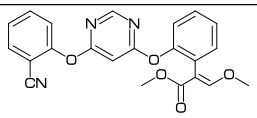
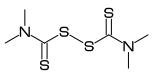
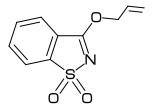
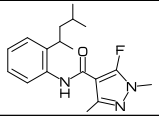
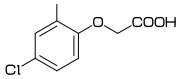
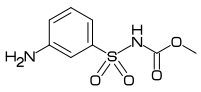
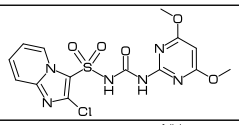
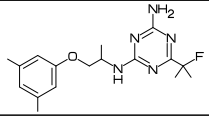
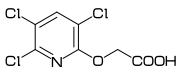
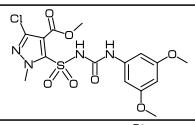
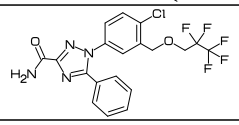
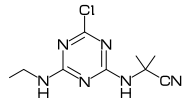
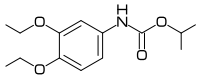
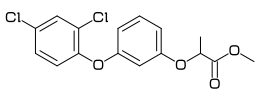
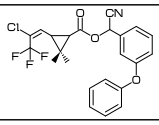
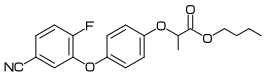
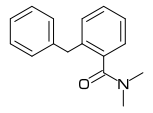
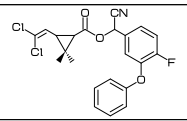
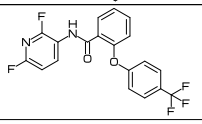
[231] 	PFOPA	pfas	500.13	500.0462	C8H2F17O3P
	!8^*0,P,?O,/OH^-179.8,-.1,OH,1^-90'1_8:/F,1_8:/F^180				
[232] 	6,6-FPi	pfas	702.06	702.0673	C12HF26O2P
	!6^*0,P,!6^*0,7^180:?O,7'1.5:/OH,1^-90'1_6'8_13'13^90'13^-90:/F,1_6'8_12:/F^180				

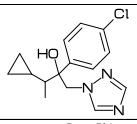
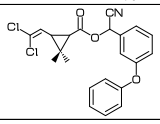
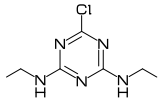
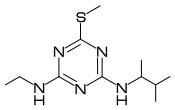
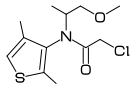
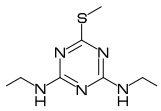
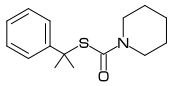
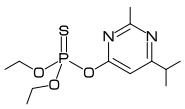
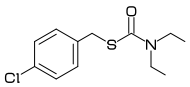
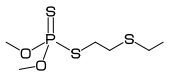
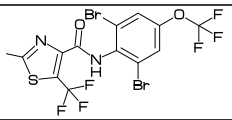
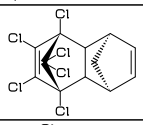
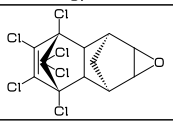
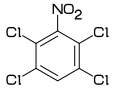
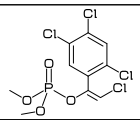
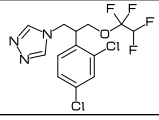
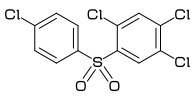
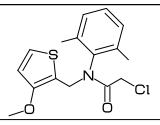
[233] 	9Cl-PF3ONS	pfas	532.58	532.5835	C8HClF16O4S
	Cl,!10^*0,S,?O,?O^180,.1,OH,-4:O,2_7'9'10:/F,2_7'9'10:/F^180				
[234] 	11Cl-PF3OUDS	pfas	632.60	632.5985	C10HClF20O4S
	Cl,!12^*0,S,?O,?O^180,.1,OH,-4:O,2_9'11'12:/F,2_9'11'12:/F^180				
[235] 	NEtFOSE	pfas	571.25	571.2505	C12H10F17NO3S
	!8^*0,S,?O,?O^180,-.1,N,/!,-60,!2,OH,1^-90'1_8:/F,1_8:/F^180				
[236] 	FBSA	pfas	299.12	299.1147	C4H2F9NO2S
	!4^*0,S,?O,?O^180,-.1,NH2,1^-90'1_4:/F,1_4:/F^180				
[237] 	FHxSA	pfas	399.13	399.1297	C6H2F13NO2S
	!6^*0,S,?O,?O^180,-.1,NH2,1^-90'1_6:/F,1_6:/F^180				
[238] 	FOSA	pfas	499.15	499.1447	C8H2F17NO2S
	!8^*0,S,?O,?O^180,-.1,NH2,1^-90'1_8:/F,1_8:/F^180				
[239] 	FMeCHS	pfas	462.13	462.1327	C8HF15O3S
	?6,4:,30'1.4,60,60,F,1'2'3'5'6'7'8:/F^35,1'2'3'5'6'7'8:/F^-35, 4:,-30'1.5,S?O?O,!OH				
[240] 	Amoxicillin	antibiotics	365.4042	365.4041	C16H19N3O5S
	^45,?4,2=?5,2:N,7:S,3^45:/*H,1:?O^15,5:/*COOH,6:??, 4:,15~wf,NH!,?O!,*/NH2,!Ph,-3:/OH				
[241] 	Ampicillin	antibiotics	349.405	349.4047	C16H19N3O4S
	^45,?4,2=?5,2:N,7:S,3^45:/*H,1:?O^15,5:/*COOH,6:??,4:,15~wf,NH!,?O!,/*NH2,!Ph				
[242] 	Penicillin G	antibiotics	334.4	334.3901	C16H18N2O4S
	^45,?4,2=?5,2:N,7:S,3^45:/*H,1:?O^15,5:/*COOH,6:??,4:,15~wf,NH!,?O!2,Ph				
[243] 	Penicillin V	antibiotics	350.3895	350.3895	C16H18N2O5S
	^45,?4,2=?5,2:N,7:S,3^45:/*H,1:?O^15,5:/*COOH,6:??,4:,15~wf,NH!,?O!2,O,!Ph				
[244] 	Mecillinam	antibiotics	325.4264	325.4264	C15H23N3O3S
	^45,?4,2=?5,2:N,7:S,3^45:/*H,1:?O^15,5:/*COOH,6:??,4:,15~wf,N,!d,!,?7,-7:N				
[245] 	Nafcillin	antibiotics	414.4748	414.4747	C21H22N2O5S
	^45,?4,2=?5,2:N,7:S,3^45:/*H,1:?O^15,5:/*COOH,6:??, 4:,15~wf,NH!,?O,!Ph,-2=Ph,-9:/O!2				
[246] 	Oxacillin	antibiotics	401.4363	401.4362	C19H19N3O5S
	^45,?4,2=?5,2:N,7:S,3^45:/*H,1:?O^15,5:/*COOH,6:??, 4:,15~wf,NH!,?O!,^-24,<?5,1'4=dl,4:N,3:O,2:?,5:,-24,Ph				
[247] 	Cloxacillin	antibiotics	435.8813	435.8813	C19H18ClN3O5S
	^45,?4,2=?5,2:N,7:S,3^45:/*H,1:?O^15,5:/*COOH,6:??, 4:,15~wf,NH!,?O!,^-24,<?5,1'4=dl,4:N,3:O,2:?,5:,-24,Ph,-5:/Cl				
[248] 	Dicloxacillin	antibiotics	470.3264	470.3263	C19H17Cl2N3O5S
	^45,?4,2=?5,2:N,7:S,3^45:/*H,1:?O^15,5:/*COOH,6:??, 4:,15~wf,NH!,?O!,^-24,<?5,1'4=dl,4:N,3:O,2:?,5^-24:/Ph'(2'6:/Cl)				
[249] 	Cefalexin	antibiotics	347.3889	347.3888	C16H17N3O4S
	^45,?4,2=?6,6=db,2:N,8:S,3^45:/*H,1:?O^15,5:/*COOH,6:?, 4:,15~wf,NH!,?O!,*/NH2,!Ph				
[250] 	Cefalonium	antibiotics	458.5107	458.5107	C20H18N4O5S2
	^45,?4,2=?6,6=db,2:N,8:S,3^45:/*H,1:?O^15,5:,!z,?O!O,n^40, 4:,15~wf,NH!,?O!2,?5,-1'-3=dl,-4:S,6:,!2,<Ph,1:N,1:p^180,4:/?O!'NH2				

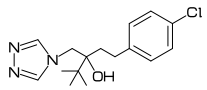
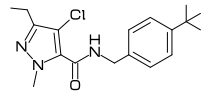
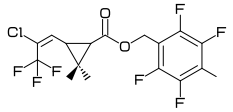
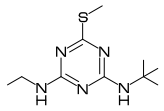
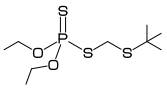
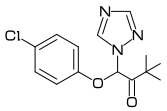
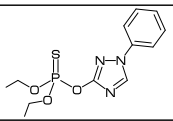
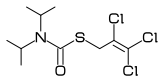
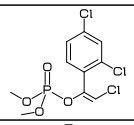
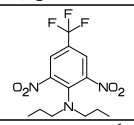
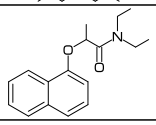
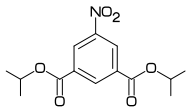
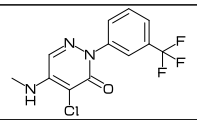
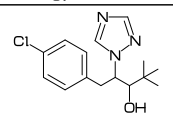
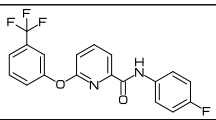
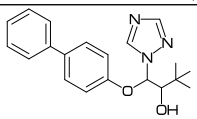
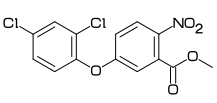
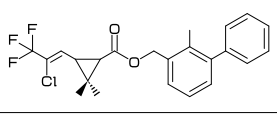
[251] 	Cefazorin	antibiotics	454.51	454.5071	C14H14N8O4S3
	^45,?4,2=?6,6=db,2:N,8:S,3^45:/*H,1^15:?O,5:/*COOH, 4:,15~wf,NH!,?O!2,<?5,2'4=dl,1'3'4'5:N>, 6:,!2,S!,<?5,1'3=dl,5:S,4:?,2'3:N				
[252] 	Cefquinome	antibiotics	528.6	528.6038	C23H24N6O5S2
	^45,?4,2=?6,6=db,2:N,8:S,3^45:/*H,1:?O^15,5:,!z,?O!O,n_^40, 4:,15~wf,NH!,?O!,//N!'O!,!,<?5,1'4=dl,3:S,5:N,4:/NH2>, 6:,!2,<Ph,5=?6,1:N,1:p^180				
[253] 	Ceftiofur	antibiotics	523.5626	523.5625	C19H17N5O7S3
	^45,?4,2=?6,6=db,2:N,8:S,3^45:/*H,1:?O^15,5:/*COOH, 4:,15~wf,NH!,?O!,//N!'O!,!,<?5,1'4=dl,3:S,5:N,4:/NH2>, 6:,!2,S,!?O!,<?5,3'5=dl,2:O				
[254] 	Cefuroxime	antibiotics	424.3852	424.3852	C16H16N4O8S
	^45,?4,2=?6,6=db,2:N,8:S,3^45:/*H,1:?O^15,5:/*COOH, 4:,15~wf,NH!,?O!,//N!'O!,!,<?5,3'5=dl,2:O>, 6:,!2,O!,?O!,NH2				
[255] 	Apramycin	antibiotics	539.58	539.5771	C21H41N5O11
	^30,?6,3=?6,2'10:O,1:,!z,O,60~zb,?6,9:,!z,O,-60~zb,?6,-5:O, 7'13'*14'*-1'-2:*/OH,*6'15'17'*-3:*/NH2,8:*/NH!^-20,-4:*/!OH,*3^-60'4^60:*/H				
[256] 	Gentamycin	antibiotics	477.596	477.5954	C21H43N5O7
	^-30,?6,1:,!z,O,0~zb,?6,-5:O,5:,!z,O,0~zb,?6,-5:O,2'4'*20:*/NH2,6:*/OH, 11:*/OH^-35,11:?z^35,12:*/NH!,13:/*OH,17:*/?!'NH!				
[257] 	Kanamycin	antibiotics	484.499	484.4986	C18H36N4O11
	^-30,?6,1:,!z,O,0~zb,?6,-5:O,5:,!O,0,?6,-5:O, 2'4'12:*/NH2,*6'11'13'18'*19'20:/*OH,10:*/!OH,17:*/!NH2				
[258] 	dihydro-Streptmycin	antibiotics	583.574	583.5899	C21H41N7O12
	^54,?5,3:O,4:?z,5:/!OH^-48,5:/*OH^35,1:,!z,O,-24~wb,?6,-5:O,2:,!w,O,24~zb,?6, 10'*11'15'*16'*18:*/OH,9:/*!OH,12:*/NH!,17^-18'19:*/NH!'?NH'!NH2				
[259] 	Spectinomycin	antibiotics	332.35	332.3495	C14H24N2O7
	^30,?6,3'9=?6,7=zf,11=wb,7'10'14:O,9^60:*/H,11:?O,1'*5'8^-60:*/OH, 13:?z,2'6:*/NH!				
[260] 	Tobramycin	antibiotics	467.51	467.5144	C18H37N5O9
	^-30,?6,1:,!z,O,0~zb,?6,-5:O,5:,!O,0,?6,-5:O, 2'4'12'*20:*/NH2,*6'11'13'18:/*OH,10:*/!OH,17:*/!NH2				
[261] 	Chlortetracyclin	antibiotics	478.88	478.8796	C22H23ClN2O8
	^30,Ph,-4'-3'-3=?6,16'19=dl,10'18:?O,7:?w^-35,2:/Cl, 5'7~zf^35'13~wf^60'14'16:/OH,15:*/N?!,17:/?O!'NH2				
[262] 	Oxytetracyclin	antibiotics	460.434	460.4339	C22H24N2O9
	^30,Ph,-4'-3'-3=?6,16'19=dl,10'18:?O,7:?w^-35,11:*/OH, 5'7~zf^35'13~wf^60'14'16:/OH,15:*/N?!,17:/?O!'NH2				
[263] 	Tetracyclin	antibiotics	444.435	444.4345	C22H24N2O8
	^30,Ph,-4'-3'-3=?6,16'19=dl,10'18:?O,7:?w^-35, 5'7~zf^35'13~wf^60'14'16:/OH,15:*/N?!,17:/?O!'NH2				
[264] 	Doxycyclin	antibiotics	444.43	444.4345	C22H24N2O8
	^30,Ph,-4'-3'-3=?6,16'19=dl,10'18:?O,7:?w, 5'13~wf^60'11~wf'14'16:/OH,15:*/N?!,17:/?O!'NH2				
[265] 	Tiamulin	antibiotics	493.74	493.7420	C28H47NO4S
	^-45.5,?8,-3=?5,8:,'.8,-210~zf,?^60,45,56,',:6~zb, 3^-45'5'8:?w,3:,30~zf,!d,4:/*OH,11:?O,7:*/H^60, 1:,15,O!,?O!2,S,60,60,-60,N?2,!2				
[266] 	BHC	pesticide	290.83	290.8298	C6H6Cl6
	^30,?6,1'*2'3'4'*5'6:*/Cl				
[267] 	pp-DDT	pesticide	354.49	354.4862	C14H9Cl5
	^30,Ph,6:/Cl,3:,!,/?Cl?Cl!Cl,!Ph,-3:/Cl				
[268] 	op-DDT	pesticide	354.49	354.4862	C14H9Cl5
	^30,Ph,4:/Cl,3:,!,/?Cl?Cl!Cl,!Ph,-3:/Cl				

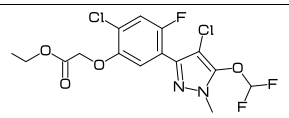
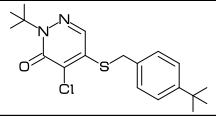
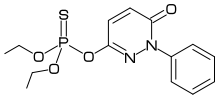
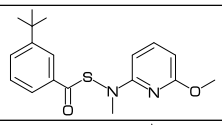
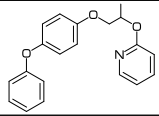
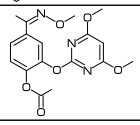
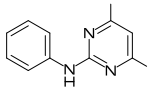
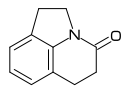
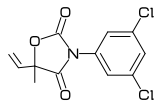
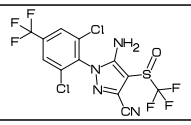
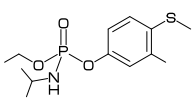
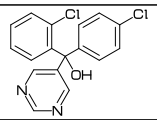
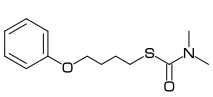
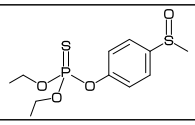
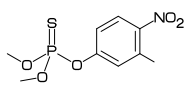
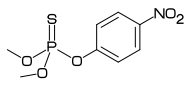
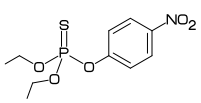
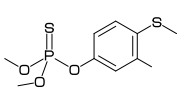
[269] 	pp-DDD	pesticide	320	320.0412	C14H10Cl4
	^30,Ph,6:/Cl,3:,!,/?Cl!Cl,!Ph,-3:/Cl				
[270] 	pp-DDE	pesticide	318	318.0253	C14H8Cl4
	^30,Ph,6:/Cl,3:,!,//?Cl!Cl,!Ph,-3:/Cl				
[271] 	XMC	pesticide	179.2	179.2157	C10H13NO2
	^30,Ph,1'5:?,3:,!O!,?O!,NH!				
[272] 	Acrinathrin	pesticide	541.45	541.4390	C26H21F6NO5
	^-30,?3,2^-35'*2^35:?w, 1:,!!d,!?O,!O!,/?F?F!F,!,?F?F!F,3:,!?O,!O!,/CN,!Ph,-4:/O!'Ph^rl				
[273] 	Azaconazole	pesticide	300.139	300.1406	C12H11Cl2N3O2
	^30,Ph,4'6:/Cl,3:,!3,<?5,2'4=dl,1'2'4:N>,7:,?5,-1'-4:O				
[274] 	Acetochlor	pesticide	269.769	269.7671	C14H20ClNO2
	^30,Ph,2:?,4:/!,3:,!N,/?O!2'Cl,!2,O!2				
[275] 	Atrazine	pesticide	215.7	215.6832	C8H14ClN5
	^30,Ph,2'4'6:N,5:/Cl,1:/NH!2,3:/NH'!?!				
[276] 	Alachrol	pesticide	269.8	269.7671	C14H20ClNO2
	^-30,!,O!2,N,/Ph'(2'6:/!),!,?O!2,Cl				
[277] 	Isoprcarb	pesticide	193.246	193.2423	C11H15NO2
	^30,Ph,2:/?!,3:/O!'?O!'NH!				
[278] 	Isoprothiolane	pesticide	290.4	290.3989	C12H18O4S2
	^30,!?!,O!,?O!,//?5'(2'5:S),!?O,!O,!?!				
[279] 	Iprobenfos	pesticide	288.34	288.3428	C13H21O3PS
	^30,!?!,O!,P,?O,/O'!?!^170,!S,!2,Ph				
[280] 	Uninnazole-P	pesticide	291.779	291.7759	C15H18ClN3O
	^30,Ph,6:/Cl,3:,!!d,!,/OH,!,??!,8:,!,<?5,2'4=dl,1'2'4:N				
[281] 	Esprocarb	pesticide	265.4	265.4142	C15H23NOS
	^30,Ph,3:,!2,S!,?O!,N?2,!,?!,?!				
[282] 	Ethalfluralin	pesticide	333.3	333.2631	C13H14F3N3O4
	^30,Ph,1'3:/NO2,5:/?F?F!F,2:,!'1.1,/!,N,!2,?,!d				
[283] 	Ethofenprox	pesticide	376.5	376.4880	C25H28O3
	^30,Ph,5:,!O!,Ph,10:,!,O!3,??,!Ph,-3:/O!2				
[284] 	Endrin	pesticide	380.91	380.9093	C12H8Cl6O
	^30,?6'1.3,3=?6,6=dl,9=?3,-1:O, 2:,210~wf'1.5,:5~wb,7:,210~wf'1.5,:10~wb,1'2'5'6'12^-210'12^-150:/Cl				
[285] 	Oxadiazon	pesticide	345.2	345.2210	C15H18Cl2N2O3
	^30,Ph,4'6:/Cl,1:/O'!?!,3:,!,<?5,2=dl,1'2:N,4:O,5:?O,3:/??!				
[286] 	Oxadixyl	pesticide	278.3	278.3037	C14H18N2O4
	^30,Ph,2'4:?,3:,!N,!,?O!2,O!,7:,!,<?5,1:N,4:O,5:?O				

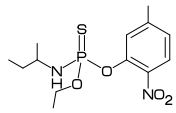
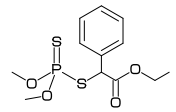
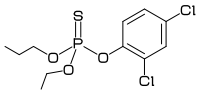
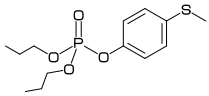
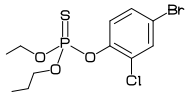
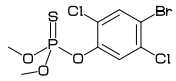
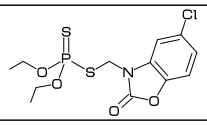
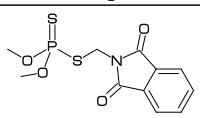
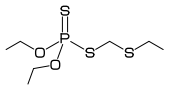
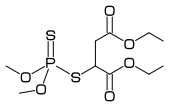
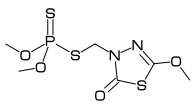
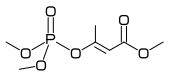
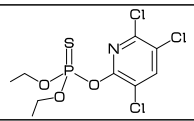
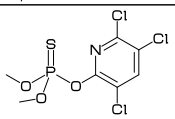
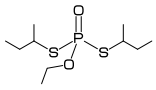
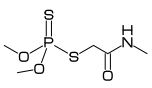
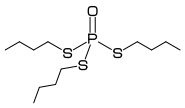
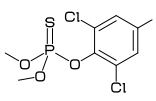
[287] 	Oxyfluorfen	pesticide	361.701	361.7003	C15H11ClF3NO4
	^30,Ph,6:/?F?F!F,4:/Cl,3:,!O!,Ph,-3:/NO2,-4:/O!2				
[288] 	Cafenstrole	pesticide	350.4	350.4358	C16H22N4O3S
	^30,Ph,2'4'6:?,3:,!,S?O?O,!,<?5,2'5=dl,2'4'5:N,4:/?O!'N?2'!2				
[289] 	Carfentrazone-ethyl	pesticide	412.19	412.1911	C15H14Cl2F3N3O3
	^30,Ph,4:/F,6:/Cl,1:,!2,/Cl,!?O!,O!2,3:,!,<?5,4=dl,1'3'5:N,2:?O,3:/?F!F,4:?				
[290] 	Carboxin	pesticide	235.301	235.3021	C12H13NO2S
	^30,?6,3=dl,2:S,5:O,4:?,3:,!?O,!NH!,Ph				
[291] 	Quinoxyfen	pesticide	308.13	308.1345	C15H8Cl2FNO
	^30,Ph,4=Ph,10:N,2'6:/Cl,7:,!O!,Ph,-3:/F				
[292] 	Quitozene	pesticide	295.3	295.3347	C6Cl5NO2
	^30,Ph,1'2'3'4'6:/Cl,5:/NO2				
[293] 	Kresoxim-Methyl	pesticide	313.348	313.3477	C18H19NO4
	^30,Ph,3:,!,/?O!'O!,!d,N,!O!,4:,!2,O,!Ph,-1:?				
[294] 	Clomazone	pesticide	239.7	239.6980	C12H14ClNO2
	^30,Ph,2:/Cl,3:,!2,<?5,1:N,2:O,4:??,5:?O				
[295] 	Chlorfenapyr	pesticide	407.62	407.6128	C15H11BrClF3N2O
	^18,?5,3=dl,5=dl,2:N,4:/CN,5:/Br,1:/?F?F!F,2:/!O'!2,3:/Ph'4:/Cl				
[296] 	Chlorfenson	pesticide	303.153	303.1611	C12H8Cl2O3S
	^30,Ph,3:,!O!,S?O?O,!Ph,6'12:/Cl				
[297] 	Chlorpropham	pesticide	213.7	213.6607	C10H12ClNO2
	^30,Ph,6:/Cl,4:,!NH!,?O!O,!?!				
[298] 	Chlorbenside	pesticide	269.183	269.1894	C13H10Cl2S
	^30,Ph,3:,!S,!2,Ph,6'12:/Cl				
[299] 	Chlorobenzilate	pesticide	325.2	325.1865	C16H14Cl2O3
	^30,Ph,3:,!,/OH^-35,/?O!'O!2^30^lr,!Ph,6'11:/Cl				
[300] 	Chlorantraniliprole	pesticide	483.15	483.1460	C18H14BrCl2N5O2
	^30,Ph,1:/Cl,3:?,5:,!?O,60,NH!,4:,!NH!,?O!,^24,<?5,3'5=db,2'3:N,4:/Br, 2:,24,Ph,-5:N,-1:/Cl				
[301] 	Chlorothalonil	pesticide	265.9	265.911	C8Cl4N2
	^30,Ph,4'6:/CN,1'2'3'5:/Cl				
[302] 	Chlornitrofen	pesticide	318.5	318.5399	C12H6Cl3NO3
	^30,Ph,6:/NO2,3:,!O!,<Ph,2'4'6:/Cl				
[303] 	Fthalide	pesticide	271.9	271.9122	C8H2Cl4O2
	^30,Ph,3=?5,8:O,9:?O,1'2'5'6:/Cl				
[304] 	Azoxystrobin	pesticide	403.4	403.3874	C22H17N3O5
	^30,Ph,2:/CN,3:,!O!,<Ph,4'6:N,3:,!O!,Ph,-5:,!,/?O!'O!,!d,!O!				

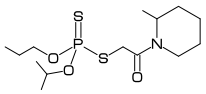
[305] 	Thiuram	pesticide	240.43	240.4328	C6H12N2S4
	^30,!,N?!,?S,!S,!,S!,?S,!,N?!				
[306] 	Probenazole	pesticide	223.25	223.2483	C10H9NO3S
	^12,Ph,3=?5,9=dl,7:S,8:N,7^35’7^-35:?O,9:/O!2’!d				
[307] 	Penflufen	pesticide	317.41	317.4010	C18H24FN3O
	^30,Ph,3:,!NH!,?O!,<?5,2’5=db,3’4:N,2’4:?,5:/F>,4:,!?,60,!?!				
[308] 	MCPA	pesticide	200.62	200.6189	C9H9ClO3
	^30,Ph,1:/Cl,5:?,4:/O!2’COOH				
[309] 	Asulam	pesticide	230.2	230.2409	C8H10N2O4S
	^30,Ph,1:/NH2,3:,!,S?O?O,!NH!,?O!,O!				
[310] 	Imazosulfuron	pesticide	412.81	412.8082	C14H13ClN6O5S
	^-11.8,?6,3=?5,1’5’7’9=db,4’7:N,8:/Cl, -1:,!,S?O?O,!NH!,?O,!NH!,<Ph,2’6:N,3’5:/O!				
[311] 	Triaziflam	pesticide	333.4	333.4037	C17H24FN5O
	^30,Ph,2’6:?,4:,!,O!2,?!,NH!,<Ph,2’4’6:N,5:/NH2,3:/??’!F				
[312] 	Trichlopyr	pesticide	256.47	256.4705	C7H4Cl3NO3
	^30,Ph,2:N,1’4’6:/Cl,3:/O!2’COOH				
[313] 	Halosulfuron-methyl	pesticide	434.82	432.8360	C15H17ClN4O7S
	^6,?5,3’5=db,1’2:N,2:?,5:/Cl,3:,!,S?O?O,!NH!,?O,!NH!,Ph,-2’-4:/O!,4:/?O!’O!				
[314] 	Flupoxam	pesticide	460.8	460.7850	C19H14ClF5N4O2
	^30,Ph,4:/Cl,1:,!,<?5,2’4=db,1’2’4:N,5:/Ph,3:/?O!’NH2>, 3:,!2,O!2,/F^35,/F^-35,!,?F?F!F				
[315] 	Cyanazine	pesticide	240.7	240.6927	C9H13ClN6
	^30,Ph,2’4’6:N,5:/Cl,1:/NH!2,3:/NH!’??’!CN				
[316] 	Diethofencarb	pesticide	267.3	267.3208	C14H21NO4
	^30,Ph,4:,!NH!,?O!O,!?!,1’6:/O!2				
[317] 	Diclofop-methyl	pesticide	341.2	341.1859	C16H14Cl2O4
	^30,Ph,4’6:/Cl,3:,!O!,Ph,-4:,!O,!?!,?O,!O!				
[318] 	Cyhalothrin	pesticide	449.86	449.8500	C23H19ClF3NO3
	^-30,?3,2^-35’*2^35:?w,1:,!!d,/?F?F!F,!Cl,3:,!?O,!O!,/CN,!Ph,-4:/O!’Ph^rl				
[319] 	Cyhalofop-Buthyl	pesticide	357.381	357.3754	C20H20FNO4
	^30,Ph,1:/CN,4:/F,3:,!O!,Ph,-3:,!O,!?!,?O!O,!4				
[320] 	Diphenamid	pesticide	239.3	239.3122	C16H17NO
	^30,Ph,3:,!2,Ph,-5:/?O!’N?!				
[321] 	Cyfluthrin	pesticide	434.3	434.2876	C22H18Cl2FNO3
	^-30,?3,2^-35’*2^35:?w, 1:,!!d,?Cl!Cl,3:,!?O,!O!,/CN,!Ph,-3:/F,-4:/O!’Ph^rl				
[322] 	Diflufenican	pesticide	394.29	394.2948	C19H11F5N2O2
	^30,Ph,1’5:/F,4:,!NH!,?O,!Ph,6:N,-5:,!O!,Ph,-3:/?F?F!F				

[323] 	Cyproconazole	pesticide	291.8	291.7759	C15H18ClN3O
	^30,?3,2:,!,?!,/OH^30,-90,!,^-18,<?5,2'4=dl,1'3'5:N,$5:,-30,Ph,-3:/Cl				
[324] 	Cypermethrin	pesticide	416.3	416.2971	C22H19Cl2NO3
	^-30,?3,2^-35'*2^35:?w,1:,!!d,?Cl!Cl,3:,!?O,!O!,/CN,!Ph,-4:/O!'Ph^rl				
[325] 	Simazine	pesticide	201.7	201.6566	C7H12ClN5
	^30,Ph,2'4'6:N,5:/Cl,1:/NH!2,3:/NH!2				
[326] 	Dimethametryn	pesticide	255.4	255.3829	C11H21N5S
	^30,Ph,2'4'6:N,5:/S!,1:/NH!2,3:/NH'!?!'?!				
[327] 	Dimethenamid	pesticide	275.8	275.7948	C12H18ClNO2S
	^-6,?5,3'5=dl,2:S,3'5:?,4:,!,N!,?O!2,Cl,6:/?!2'O!				
[328] 	Simetryn	pesticide	213.3	213.3032	C8H15N5S
	^30,Ph,2'4'6:N,5:/S!,1'3:/NH!2				
[329] 	Dimepiperate	pesticide	263.4	263.3983	C15H21NOS
	^30,Ph,3:,!??,!S!,?O!,?6,-6:N				
[330] 	Diazinon	pesticide	304.35	304.3455	C12H21N2O3PS
	^30,!2,O!,P,?S,/O!2^160^rl,!O!,<Ph,4'6:N,5:?,3:/?!				
[331] 	Thiobencarb	pesticide	257.776	257.7795	C12H16ClNOS
	^30,Ph,1:/Cl,4:,!2,S!,?O!,N?2,!2				
[332] 	Thiometon	pesticide	246.34	246.3508	C6H15O2PS3
	^-30,!O!,P,?S,/O!^160,!,S!3,S!2				
[333] 	Thifluzamide	pesticide	528.08	528.0623	C13H6Br2F6N2O2S
	^-12,?5,3'5=dl,2:S,5:N,3:/?F?F!F,1:?, 4:,!?O,!NH!,^6,<Ph,2'6:/Br,4:/O!'?F?F!F				
[334] 	Aldrin	pesticide	364.908	364.9099	C12H8Cl6
	^30,?6'1.3,3=?6,6'9=dl,2:,210~wf'1.5,:5~wb,7:,210~zf'1.5,:10~zb, 1'2'5'6'11^-210'11^-150:/Cl				
[335] 	Dieldrin	pesticide	380.895	380.9093	C12H8Cl6O
	^30,?6'1.3,3=?6,9=?3,6=dl,2:,210~wf'1.5,:5~wb,7:,210~zf'1.5,:10~zb, 11:O,1'2'5'6'12^-210'12^-150:/Cl				
[336] 	Tecnazene	pesticide	260.879	260.8896	C6HCl4NO2
	^30,Ph,1'3'4'6:/Cl,5:/NO2				
[337] 	Tetrachlorvinfos	pesticide	365.97	365.9618	C10H9Cl4O4P
	^-30,!O!,P,?O,/O!^160,!O!,/Ph'(2'4'5:/Cl),!d,!Cl				
[338] 	Tetraconazole	pesticide	372.14	372.1455	C13H11Cl2F4N3O
	^-6,?5,2'5=dl,1'2'4:N,4:,!4,O!,/F^35,/F^-35,!,?F!F,7:/Ph'(4'6:/Cl)				
[339] 	Tetradifon	pesticide	356.038	356.0518	C12H6Cl4O2S
	^30,Ph,3:,!,S?O?O,!Ph,6'10'11'13:/Cl				
[340] 	Thenylchlor	pesticide	323.835	323.8376	C16H18ClNO2S
	^6,?5,2'5=dl,4:S,2:/O!,3:,!2,N,7^-15:/Ph'(6'2:?),!,?O!2,Cl				

[341] 	Tebuconazole	pesticide	307.8	307.8183	C16H22ClN3O
	^36,?5,1’4=dl,1’3’5:N,3:,30,!4,Ph,-3:/Cl,7^-30:/??!,7^30:/OH				
[342] 	Tebufenpyrad	pesticide	333.86	333.8556	C18H24ClN3O
	^6,?5,3’5=dl,1’2:N,4:/Cl,5:/!,2:?,3:,!?O!,NH,!2,Ph,-3:/??!				
[343] 	Tefluthrin	pesticide	418.736	418.7336	C17H14ClF7O2
	^-30,?3,2^-35’*2^35:?w,1:,!!d,/?F?F!F,!Cl,3:,!?O!,O!2,<Ph,2’3’5’6:/F,4:?				
[344] 	Terbutryn	pesticide	241.4	241.3563	C10H19N5S
	^30,Ph,2’4’6:N,5:/S!,1:/NH!2,3:/NH!’??!				
[345] 	Terbufos	pesticide	288.42	288.4306	C9H21O2PS3
	^30,!2,O!,P,?S,/O!2^160^rl,!,S!2,S!,??!				
[346] 	Triadimefon	pesticide	293.8	293.7487	C14H16ClN3O2
	^30,Ph,6:/Cl,3:,!,O!2,?O!,??!,8:,!,<?5,2’4=dl,1’2’4:N				
[347] 	Triazophos	pesticide	313.31	313.3125	C12H16N3O3PS
	^30,!2,O!,P,?S,/O!2^160^rl,!O!,^-12,<?5,2’5=dl,2’4’5:N,4:/Ph				
[348] 	Triallate	pesticide	304.7	304.6641	C10H16Cl3NOS
	^-30,!?!,N,/?!,!?O!,S!2,/Cl,!d,?Cl!Cl				
[349] 	Dimethylvinphos	pesticide	331.52	331.5167	C10H10Cl3O4P
	^-30,!O!,P,?O,/O!^160,!O!,/Ph’(2’4:/Cl)‘1,!d,!Cl				
[350] 	Trifluralin	pesticide	335.3	335.2790	C13H16F3N3O4
	^30,Ph,1’3:/NO2,5:/?F?F!F,2:,!N,/!2,!3				
[351] 	Napropamide	pesticide	271.4	271.3541	C17H21NO2
	^-30,Ph,4=Ph,10:,!O!,?!,?O!,N?2,!2				
[352] 	Nitrothal-isopropyl	pesticide	295.3	295.2878	C14H17NO6
	^30,Ph,5:/NO2,1’3:/?O!’O!’?!				
[353] 	Norflurazon	pesticide	303.7	303.6675	C12H9ClF3N3O
	^30,?6,1’5=dl,4’5:N,1:/NH!,3:?O,2:/Cl,4:/Ph’3:/?F?F!F				
[354] 	Paclobutrazole	pesticide	293.795	293.7917	C15H20ClN3O
	^30,Ph,6:/Cl,3:,!3,/OH,!,??!,8:,!,<?5,2’4=dl,1’2’4:N				
[355] 	Picolinafen	pesticide	376.331	376.3043	C19H12F4N2O2
	^30,Ph,5:/?F?F!F,3:,!O!,Ph,-5:N,-4:,!?O,!NH!,Ph,-3:/F				
[356] 	Bitertanol	pesticide	337.4	337.4155	C20H23N3O2
	^30,Ph,3:,!Ph,-3:,!,O!2,/OH,!,??!,14:,!,<?5,2’4=dl,1’2’4:N				
[357] 	Bifenox	pesticide	342.14	342.1309	C14H9Cl2NO5
	^30,Ph,4’6:/Cl,3:,!O!,Ph,-4:/?O!’O!,-3:/NO2				
[358] 	Bifenthrin	pesticide	422.88	422.8677	C23H22ClF3O2
	^-30,?3,2^-35’*2^35:?w,1:,!!d,/Cl,!,?F?F!F,3:,!?O,!O!,-60,Ph,-1:?,-2:/Ph				

[359] 	Pyraflufen-ethyl	pesticide	413.174	413.1759	C15H13Cl2F3N2O4
	^30,Ph,6:/Cl,4:/F,3:,!,<?5,1'4=dl,2'3:N,-3:?,5:/Cl, -2:,!O!,/F,!F,$1:,!,O!2,?O!,O!2				
[360] 	Pyridaben	pesticide	364.9	364.9325	C19H25ClN2OS
	^30,?6,2'4=dl,5'6:N,6:/??!,1:?O,2:/Cl,-4:,!S,!2,Ph,-3:/??!				
[361] 	Pyridaphenthion	pesticide	340.34	340.3345	C14H17N2O4PS
	^30,!2,O!,P,?S,/O!2^160^rl,!O!,<?6,1'5=dl,2'3:N,4:?O,3:/Ph				
[362] 	Pyributicarb	pesticide	330.4	330.4444	C18H22N2O2S
	^30,Ph,5:/??!,3:,!?O!,S!,N?!,Ph,-5:N,-4:/O!				
[363] 	Pyriproxyfen	pesticide	321.5	321.3697	C20H19NO3
	^30,Ph,5:,!O!,Ph,-3:,!,O!2,?!,O,-60,Ph,-5:N				
[364] 	Pyriminobac-Methyl	pesticide	361.354	361.3492	C17H19N3O6
	^30,Ph,2:/O!'?O!,5:,!?,!d,N,!O!,3:,!O!,<Ph,2'6:N,3'5:/O!				
[365] 	Pyrimethanil	pesticide	199.257	199.2517	C12H13N3
	^30,Ph,3:,!NH!,<Ph,2'6:N,3'5:?				
[366] 	Pyroquilon	pesticide	173.2	173.2111	C11H11NO
	^30,Ph,3=?6,10:N,9:?O,11--4=?5				
[367] 	Vinclozolin	pesticide	286.108	286.1107	C12H9Cl2NO3
	^36,?5,3:N,5:O,2'4:?O,1:?^54,1:/!d^-30,3:/Ph'(3'5:/Cl)				
[368] 	Fipronil	pesticide	437.2	437.1477	C12H4Cl2F6N4OS
	^30,Ph,2'4:/Cl,6:/?F?F!F,3:,!,<?5,2'4=dl,1'2:N,3:/CN,5:/NH2,-2:/S?O'!'?F?F!F				
[369] 	Fenomiphos	pesticide	303.36	303.3574	C13H22NO3PS
	^30,!2,O!,P,?O,/NH'!?!^160,!O!,<Ph,3:?,4:/S!				
[370] 	Fenarimol	pesticide	331.2	331.1959	C17H12Cl2N2O
	^30,Ph,3:,!2,Ph,4'11:/Cl,7:/OH^30,7^-30:/Ph'(3'5:N)				
[371] 	Fenothiocarb	pesticide	253.4	253.3604	C13H19NO2S
	^30,Ph,3:,!O,!5,S,!?O!,N?!				
[372] 	Fensulfothion	pesticide	308.35	308.3540	C11H17O4PS2
	^30,!2,O!,P,?S,/O!2^160^rl,!O!,Ph,-3:/S'?O!				
[373] 	Fenitrothion	pesticide	277.23	277.2340	C9H12NO5PS
	^-30,!O!,P,?S,/O!^160,!O!,<Ph,3:?,4:/NO2				
[374] 	Parathion-methyl	pesticide	263.2	263.2074	C8H10NO5PS
	^-30,!O!,P,?S,/O!^160,!O!,Ph,-3:/NO2				
[375] 	Parathion	pesticide	291.3	291.2606	C10H14NO5PS
	^30,!2,O!,P,?S,/O!2^160^rl,!O!,Ph,-3:/NO2				
[376] 	Fenthion	pesticide	278.33	278.3280	C10H15O3PS2
	^-30,!O!,P,?S,/O!^160,!O!,<Ph,3:?,4:/S!				

[377] 	Butamifos	pesticide	332.36	332.3556	C13H21N2O4PS
	^-30,!2,?!,NH!,P,?S,/O!2^170^rl,!O!,<Ph,2:/NO2,5:?				
[378] 	Phenthoate	pesticide	320.358	320.3647	C12H17O4PS2
	^-30,!O!,P,?S,/O!^160,!S,!,/Ph,!?O!,O!2				
[379] 	Prothyophos	pesticide	329.18	329.1797	C11H15Cl2O3PS
	^-30,!3,O!,P,?S,/O!2^160^rl,!O!,<Ph,2'4:/Cl				
[380] 	Propaphos	pesticide	304.343	304.3422	C13H21O4PS
	^-30,!3,O!,P,?O,/O!3^160^rl,!O!,Ph,-3:/S!				
[381] 	Profenofos	pesticide	373.6	373.6307	C11H15BrClO3PS
	^30,!2,O!,P,?S,/O!3^160^rl,!O!,<Ph,2:/Cl,4:/Br				
[382] 	Bromophos	pesticide	365.99	365.9960	C8H8BrCl2O3PS
	^-30,!O!,P,?S,/O!^160,!O!,<Ph,3'6:/Cl,4:/Br				
[383] 	Phosalone	pesticide	367.80	367.8085	C12H15ClNO4PS2
	^30,!2,O!,P,?S,/O!2^160^rl,!,S!2,<?5,4=Ph,4=dr,1:N,2:?O,3:O,8:/Cl				
[384] 	Phosmet	pesticide	317.32	317.3210	C11H12NO4PS2
	^-30,!O!,P,?S,/O!^160,!S,!2,<?5,3=Ph2,1:N,2'5:?O				
[385] 	Phorate	pesticide	260.4	260.3774	C7H17O2PS3
	^30,!2,O!,P,?S,!,S!2,S!2,4:/O!2^160^rl				
[386] 	Malathion	pesticide	330.35	330.3580	C10H19O6PS2
	^-30,!O!,P,?S,/O!^160,!S!,/!?O!'O!2'1,!?O!,O!2				
[387] 	Methidathion	pesticide	302.32	302.3313	C6H11N2O4PS3
	^-30,!O!,P,?S,/O!^160,!,S!2,<?5,4=dl,1'5:N,3:S,2:?O,4:/O!				
[388] 	Mevinphos	pesticide	224.15	224.1482	C7H13O6P
	^-30,!O!,P,?O,/O!^160,!O,!?,!d,!?O!,O!				
[389] 	Chlorpyrifos	pesticide	350.59	350.5863	C9H11Cl3NO3PS
	^30,!2,O!,P,?S,/O!2^160^rl,!O!,<Ph,6:N,2'4'5:/Cl				
[390] 	Chlorpyrifos-methyl	pesticide	322.53	322.5331	C7H7Cl3NO3PS
	^-30,!O!,P,?S,/O!^160^rl,!O!,<Ph,6:N,2'4'5:/Cl				
[391] 	Cadusafos	pesticide	270.386	270.3921	C10H23O2PS2
	^-30,!2,?!,S!,P,?O,/O!2^160^rl,!S,!?,!2				
[392] 	Dimethoate	pesticide	229.25	229.2574	C5H12NO3PS2
	^-30,!O!,P,?S,/O!^160,!,S!2,?O,!NH!				
[393] 	Tribufos	pesticide	314.50	314.5109	C12H27OPS3
	^30,!4,S!,P,?O,/S'!4^160^rl,!S,!4				
[394] 	Tolclofos-methyl	pesticide	301.13	301.1266	C9H11Cl2O3PS
	^-30,!O!,P,?S,/O!^160,!O!,<Ph,2'6:/Cl,4:?				

[395] 	Piperophos	pesticide	353.48	353.4807	C14H28NO3PS2
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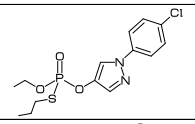
[396] 	Pyraclofos	pesticide	360.80	360.7960	C14H18ClN2O3PS
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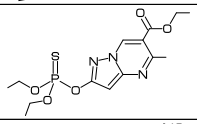
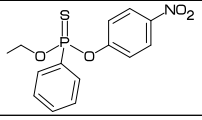
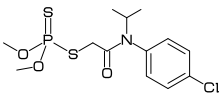
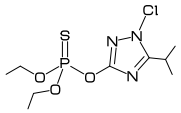
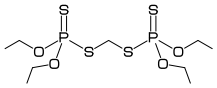
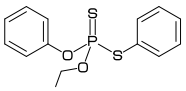
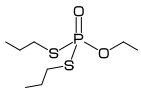
[397] 	Pyrazophos	pesticide	373.37	373.3644	C14H20N3O5PS
	^30,!2,O!,P,?S,/O!2^160^rl,!O!,<?5,3=?6,2'5'7'9=dl,4'5'6:N,7:?,-2:/?O!'O!2				
[398] 	EPN	pesticide	323.303	323.3040	C14H14NO4PS
	^30,!2,O!,P,?S,/Ph^170,!O!,Ph,-3:/NO2				
[399] 	Anilofos	pesticide	367.9	367.8516	C13H19ClNO3PS2
	^-30,!O!,P,?S,/O!^160,!S,!2,?O!,N,/?!,!Ph,-3:/Cl				
[400] 	Isazofos	pesticide	313.74	313.7413	C9H17ClN3O3PS
	^30,!2,O!,P,?S,/O!2^160^rl,!O!,<?5,2'5=dl,2'4'5:N,4:/Cl,3:/?!				
[401] 	Ethion	pesticide	384.46	384.4761	C9H22O4P2S4
	^30,!2,O!,P,?S,/O!2^160^rl,!S,!2,S!,P,?S,/O!2^200^lr,!,O!2				
[402] 	Edifenphos	pesticide	310.37	310.3714	C14H15O2PS2
	^30,Ph,3:,!O!,P,?S,/O!2^rl^160,!S,!Ph				
[403] 	Ethoprophos	pesticide	242.33	242.3390	C8H19O2PS2
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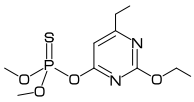
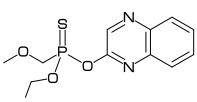
[404] 	Ethrimfos	pesticide	292.29	292.2917	C10H17N2O4PS
	^-30,!O!,P,?S,/O!^160,!O!,<Ph,2'4:N,5:/!,3:/O!2				
[405] 	Quinalphos	pesticide	298.30	298.2978	C12H15N2O3PS
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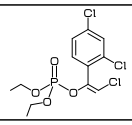
[406] 	Chlorfenvinphos	pesticide	359.58	359.5699	C12H14Cl3O4P
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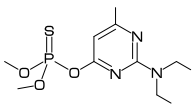
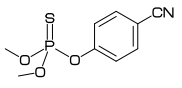
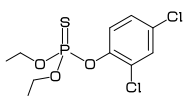
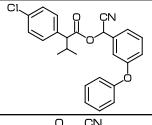
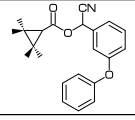
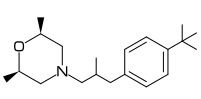
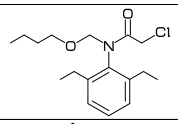
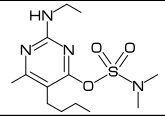
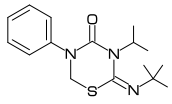
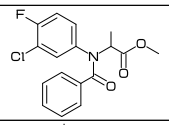
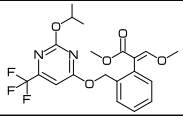
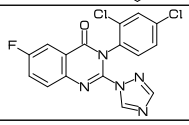
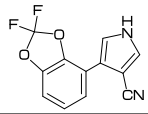
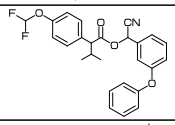
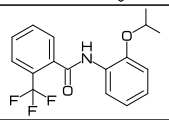
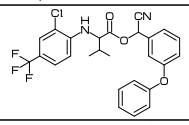
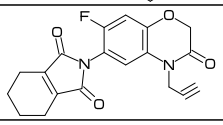
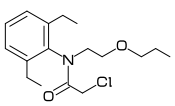
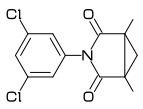
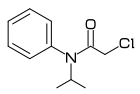
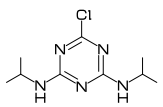
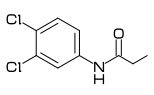
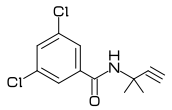
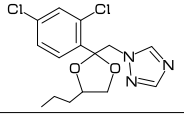
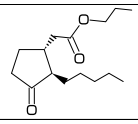
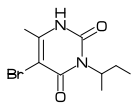
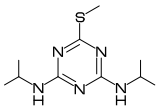
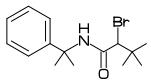
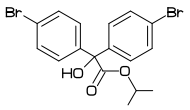
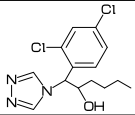
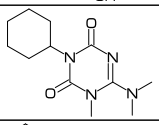
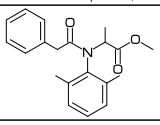
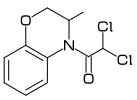
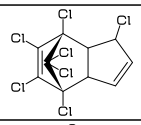
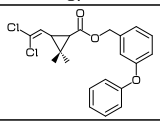
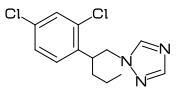
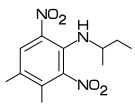
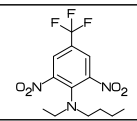
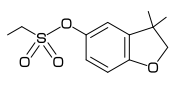
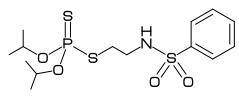
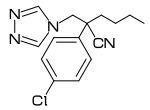
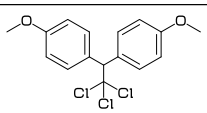
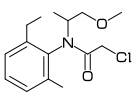
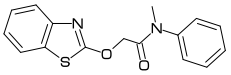
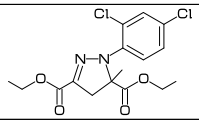
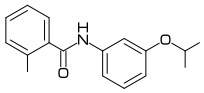
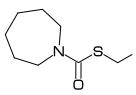
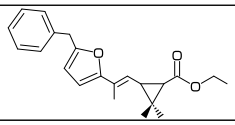
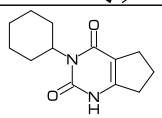
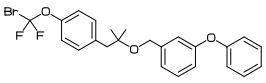
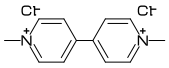
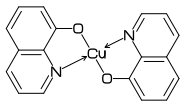
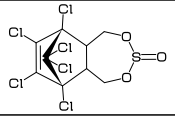
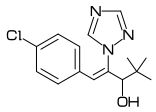
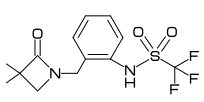
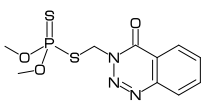
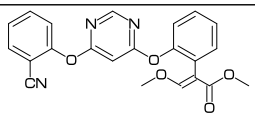
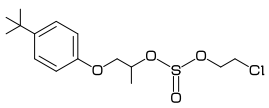
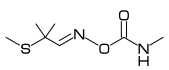
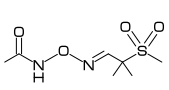
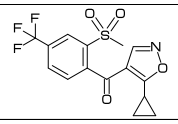
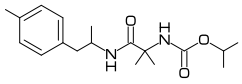
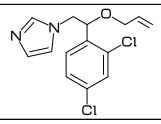
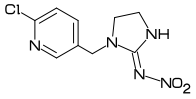
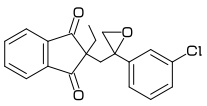
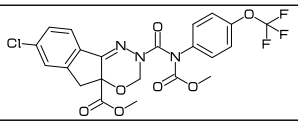
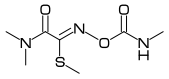
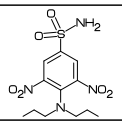
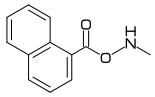
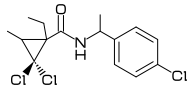
[407] 	Pirimiphos-methyl	pesticide	305.333	305.3335	C11H20N3O3PS
	^-30,!O!,P,?S,/O!^160,!O!,<Ph,2'4:N,5:?,3:/N?2'!2				
[408] 	Cyanophos	pesticide	243.22	243.2193	C9H10NO3PS
	^-30,!O!,P,?S,/O!^160,!O!,Ph,-3:/CN				
[409] 	Dichlofenthion	pesticide	315.2	315.1531	C10H13Cl2O3PS
	^30,!2,O!,P,?S,/O!2^160^rl,!O!,Ph,-5'-3:/Cl				
[410] 	Fenvalerate	pesticide	419.91	419.9000	C25H22ClNO3
	^30,Ph,6:/Cl,3:,!,/?!,!?O,!O!,/CN,!Ph,-4:/O'!Ph^rl				
[411] 	Fenpropathrin	pesticide	349.4	349.4229	C22H23NO3
	^-30,?3,1^35'2^-35:?w,1^-35'2^35:?z,3:,!?O,!O!,/CN,!Ph,-4:/O!'Ph^rl				
[412] 	Fenpropimorph	pesticide	303.49	303.4821	C20H33NO
	^30,?6,3:N,6:O,1'5:?w,3:,!,!?,!2,Ph,-3:/??!				

[413] 	Butachlor	pesticide	311.85	311.8468	C17H26ClNO2
	^30,!4,O!2,N,/Ph'(-1'-5:/!),!,?O!2,Cl				
[414] 	Bupirimate	pesticide	316.42	316.4196	C13H24N4O3S
	^30,Ph,4'6:N,1:?,3:,!O!,S?O?O,!,N?!,2:/!3,5:/NH!2				
[415] 	Buprofezin	pesticide	305.4	305.4383	C16H23N3OS
	^-30,?6,1'5:N,1:/Ph,3:S,6:?O,5:/?!,4://N'!??!				
[416] 	Flamprop-methyl	pesticide	335.8	335.7572	C17H15ClFNO3
	^30,Ph,1:/Cl,6:/F,3:,!N,/?O!'Ph^rl,!?!,?O,!O!				
[417] 	Fluacrypyrim	pesticide	426.392	426.3863	C20H21F3N2O5
	^30,Ph,4'6:N,1:/?F?F!F,5:/O'!?!,3:,!,O!2,Ph,-1:,!,<!d,!O!,1:/?O!'O!				
[418] 	Fluquinconazole	pesticide	376.2	376.1720	C16H8Cl2FN5O
	^30,Ph,3=?6,8=dl,7'9:N,6:/F,10:?O,8:,!,<?5,2'4=dl,1'3'5:N,$9:/Ph'(4'6:/Cl)				
[419] 	Fludioxonil	pesticide	248.2	248.1850	C12H6F2N2O2
	^30,Ph,5=?5,7'9:O,8^-40'8^40:/F,4:,!,<?5,2'5=dl,4:NH,2:/CN				
[420] 	Flucythrinate	pesticide	451.5	451.4619	C26H23F2NO4
	^30,Ph,6:,!O!,/F,!,F,3:,!,/?!,!?O,!O!,/CN,!Ph,-4:/O!'Ph^rl				
[421] 	Flutolanil	pesticide	323.3	323.3096	C17H16F3NO2
	^30,Ph,2:/?F?F!F,3:,!?O,!NH!,Ph,-1:/O'!?!				
[422] 	Fluvalinate	pesticide	502.92	502.9126	C26H22ClF3N2O3
	^30,Ph,5:/Cl,1:/?F?F!F,4:,!NH!,/?!,!?O,!O!,/CN,!Ph,-4:/O!'Ph^rl				
[423] 	Flumioxazin	pesticide	354.337	354.3317	C19H15FN2O4
	^30,Ph,6:/F,3=?6,-1:O,-4:N,-3:?O,-4:,!2,!t,1:,!,<?5,3=?6,3=dr,1:N,2'5:?O				
[424] 	Pretilachlor	pesticide	311.85	311.8468	C17H26ClNO2
	^30,Ph,2'4:/!,3:,!N,/?O!2'Cl'1,!3,O!3				
[425] 	Procymidone	pesticide	284.136	284.1379	C13H11Cl2NO2
	?6,1:N,3:,:5,2'6:?O,3'5:?,1:/Ph'(3'5:/Cl)				
[426] 	Propachlor	pesticide	211.689	211.6879	C11H14ClNO
	^30,Ph,3:,!N,/?!,!,?O!2,Cl				
[427] 	Propazine	pesticide	229.7	229.7098	C9H16ClN5
	^30,Ph,2'4'6:N,5:/Cl,1'3:/NH'!?!				
[428] 	Propanil	pesticide	218.077	218.0798	C9H9Cl2NO
	^30,Ph,1'6:/Cl,3:/NH!'?O!2				
[429] 	Propyzamide	pesticide	256.1	256.1278	C12H11Cl2NO
	^30,Ph,1'5:/Cl,3:,!?O,!NH,!??!,!t				
[430] 	Propiconazole	pesticide	342.22	342.2203	C15H17Cl2N3O2
	^30,Ph,4'6:/Cl,3:,!3,<?5,2'4=dl,1'2'4:N>,7:,<?5,1'4:O,2:/!2^-15				

[431] 	Prohydrojasmon	pesticide	254.37	254.3651	C15H26O3
	^18,?5,2:?O,3:*/!4^-12,4:/*!?O!'O!3				
[432] 	Bromacil	pesticide	261.119	261.1157	C9H13BrN2O2
	^30,?6,6=dl,3:N,1:/Br,2'4:?O,5:NH,6:?,3:/?!2				
[433] 	Prometryn	pesticide	241.4	241.3563	C10H19N5S
	^30,Ph,2'4'6:N,5:/S!,1'3:/NH'!?!				
[434] 	Bromobutide	pesticide	312.2	312.2452	C15H22BrNO
	^30,Ph,3:,!??,!NH!,?O!,/Br,!??!				
[435] 	Bromopropylate	pesticide	428.12	428.1151	C17H16Br2O3
	^30,Ph,3:,!2,Ph,6'11:/Br,7:/OH^-45,7:,30,?O!O,-60,?!				
[436] 	Hexaconazole	pesticide	314.2	314.2102	C14H17Cl2N3O
	^36,?5,1'4=dl,1'3'5:N,3:,30,!5,-4^30:/OH,-5:,-30,Ph,-3'-1:/Cl				
[437] 	Hexazinone	pesticide	252.31	252.3127	C12H20N4O2
	^30,?6,3=dl,2'4'6:N,2:?,1'5:?O,6:/?6,3:/N?!				
[438] 	Benalaxyl	pesticide	325.4	325.4015	C20H23NO3
	^30,Ph,3:,!2,?O!,N,/Ph'(-5'-1:?),!?!,?O,!O!				
[439] 	Benoxacor	pesticide	260.1	260.1165	C11H11Cl2NO2
	^90,Ph,3=?6,7:N,10:O,8:?,7:,!?O!,?Cl!Cl				
[440] 	Heptachlor	pesticide	373.35	373.3177	C10H5Cl7
	^30,?6'1.3,3=?5,6'8=dl,2:,210~wf'1.5,:5~wb,1'2'5'6'9'10^-210'10^-150:/Cl				
[441] 	Permethrin	pesticide	391.30	391.2876	C21H20Cl2O3
	^-30,?3,2^-35'*2^35:?w,1:,!!d,?Cl!Cl,3:,!?O!,O!2,Ph,-4:/O!'Ph^rl				
[442] 	Penconazole	pesticide	284.184	284.1843	C13H15Cl2N3
	^30,Ph,4'6:/Cl,3:,!,/!2,!2,^30,<?5,2'4=dl,1'2'4:N				
[443] 	Pendimethalin	pesticide	281.3	267.2810	C12H17N3O4
	^30,Ph,3'5:/NO2,1'2:?,4:,!,NH,!?,!2				
[444] 	Benfluralin	pesticide	335.3	335.2790	C13H16F3N3O4
	^30,Ph,1'3:/NO2,5:/?F?F!F,2:/N?2'!4				
[445] 	Benfuresate	pesticide	256.3	256.3180	C12H16O4S
	^30,Ph,3=?5,7:O,9:??,6:,!O!,S?O?O,!2				
[446] 	Bensulide	pesticide	397.5	397.5134	C14H24NO4PS3
	^30,!?!,O!,P,?S,/O'!?!^160^rl,!,S!3,NH!,S?O?O,!Ph				
[447] 	Myclobutanil	pesticide	288.8	288.7752	C15H17ClN4
	^36,?5,1'4=dl,1'3'5:N,3:,30,!,/CN^30,/Ph'(4:/Cl)^-30,!4				
[448] 	Methoxychlor	pesticide	345.644	345.6481	C16H15Cl3O2
	^30,Ph,3:,!2,Ph,6'11:/O!,7:/?Cl?Cl!Cl				

[449] 	Metolachlor	pesticide	283.8	283.7936	C15H22ClNO2
	^30,Ph,5:/!,3:?,4:,!N,/?!2'O!,!,?O!2,Cl				
[450] 	Mefenacet	pesticide	298.4	298.3595	C16H14N2O2S
	^12,Ph,3=?5,9=dl,9:N,7:S,8:,!,O!2,?O!,N?!,Ph				
[451] 	Mefenpyr-diethyl	pesticide	373.23	373.2311	C16H18Cl2N2O4
	^18,?5,5=dl,4'5:N,3^65:?,1^12'3^-12:/?O!'O!2,4:,-24,Ph,-3'-1:/Cl				
[452] 	Mepronil	pesticide	269.3	269.3382	C17H19NO2
	^30,Ph,2:?,3:,!?O,!NH!,Ph,-2:/O'!?!				
[453] 	Molinate	pesticide	187.3	187.3023	C9H17NOS
	^47,?7,3:N,3:,!?O!,S!2				
[454] 	Resmethrin	pesticide	338.4	338.4400	C22H26O3
	^-30,?3,2^-35'*2^35:?w,1:,!!d,?!,3:/?O!'O!2,<?5,3'5=dl,2:O,3:/!Ph				
[455] 	Lenacil	pesticide	234.3	234.2942	C13H18N2O2
	^30,?6,3=?5,3=dl,6:N,2:NH,1'5:?O,6:/?6				
[456] 	Halfenprox	pesticide	477.4	477.3384	C24H23BrF2O3
	^30,Ph,6:,!O!,/F^35,/F^-35,!,Br,3:,!,!??!,O!2,Ph,-2:/O!'Ph^rl				
[457] 	Paraquat	pesticide	257.16	257.1589	C12H14Cl2N2
	Ph,4:,!Ph,1'10:N?,1^-90'10^90:p,1:,(0'1.2):,Cl,n_^15,10:,(0'1.2):,Cl,n_^15				
[458] 	Oxine-Copper	pesticide	351.852	351.8460	C18H12CuN2O2
	Ph,4:N,5=Ph,-4:,!O,-60,^90,Cu,-90,O,60,Ph,-2=Ph,-1:N,4:,:12~vf,23:,:12~vf				
[459] 	Endosulfan	pesticide	406.904	406.9251	C9H6Cl6O3S
	^26,?7,7='1.3'?6,11:,208~wf'1.45,:8~wb,10=dl,3'5:O,4:S,4:?O, 8'9'10'11'12^-210'12^-150:/Cl				
[460] 	Uniconazole-P	pesticide	291.779	291.7759	C15H18ClN3O
	^30,Ph,6:/Cl,3:,!!d,!,/OH,!??!,8:,!,<?5,2'4=dl,1'2'4:N				
[461] 	Dimesulfazet	pesticide	336.33	336.3299	C13H15F3N2O3S
	^-60,Ph,3:,!2,?4,-4:N,-2:??,-3:?O,4:,30,NH!,S?O?O,!,?F?F!F				
[462] 	Azinphos-methyl	pesticide	317.318	317.3243	C10H12N3O3PS2
	^-30,!O!,P,?S,/O!^160,!,S!2,<?6,-3=?6,2'4'8'10=dl,1'2'3:N,6:?O				
[463] 	Azoxystorbin	pesticide	403.394	403.3874	C22H17N3O5
	^30,Ph,2:/CN,3:,!O!,Ph,-1'-3:N,-4:,!O!,Ph,-5:,!,//!O!,!?O!,O!				
[464] 	Aramite	pesticide	334.859	334.8587	C15H23ClO4S
	^30,Ph,6:/??!,3:,!,O!2,?!,O!,S,?O,!,O!3,Cl				
[465] 	Aldicarb	pesticide	190.3	190.2632	C7H14N2O2S
	^-30,!S,!??,!!d,N,!O!,?O,!NH!				
[466] 	Aldoxycarb	pesticide	222.3	222.2620	C7H14N2O4S
	^30,!?O,!NH!,O!,N,!d,!??,!,S?O?O,!				

[467] 	Isoxaflutole	pesticide	359.319	359.3202	C15H12F3NO4S
	^30,Ph,6:/?F?F!F,4:,!,S?O?O,!,3:,!‘1,?O,!‘1,^-12,<?5,1’4=dl,3:O,4:N,2:/?3				
[468] 	Iprovalicarb	pesticide	320.4	320.4265	C18H28N2O3
	^30,Ph,6:?,3:,!,!?!,NH!,?O!,??,!NH!,?O!O,!?!				
[469] 	Imazalil	pesticide	297.2	297.1797	C14H14Cl2N2O
	^-30,!,/Ph’(4’6:/Cl),!,O!2,!d,1:,60,<?5,2’4=dl,1’3:N				
[470] 	Imidacloprid	pesticide	255.662	255.661	C9H10ClN5O2
	^30,Ph,1:N,6:/Cl,3:,!2,<?5,1:N,3:NH,2://N’!NO2				
[471] 	Indanofan	pesticide	340.80	340.8001	C20H17ClO3
	^30,Ph,3=?5,7’9:?O,8^55^lr:/!,8:,-30,!2,Ph,-2:/Cl,11:,?3,-2:O				
[472] 	Indoxacarb	pesticide	527.837	527.8344	C22H17ClF3N3O7
	^-6,Ph,3=?5,9=?6,15=dl,10:O,12’13:N,1:/Cl, 12:,!?O!,N,!Ph,-3:/O!’?F?F!F,8^-54‘1’15:/?O!’O!				
[473] 	Oxamyl	pesticide	219.3	219.2614	C7H13N3O3S
	^-30,!,N?!,?O!,/S!,!d,N,!O!,?O!,NH!				
[474] 	Oryzalin	pesticide	346.4	346.3595	C12H18N4O6S
	^30,Ph,1’3:/NO2,5:/S?O?O’!NH2,2:,!,/!2,N,!3				
[475] 	Carbaryl	pesticide	201.22	201.2212	C12H11NO2
	^30,Ph,5=Ph,4:,!?O,!O!,NH!				
[476] 	Carpropamid	pesticide	334.665	334.6685	C15H18Cl3NO
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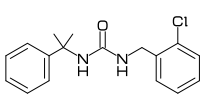
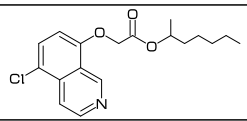
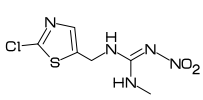
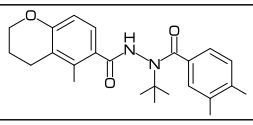
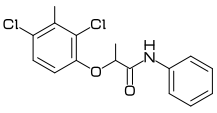
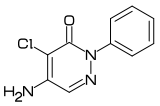
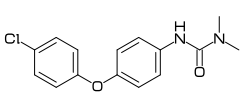
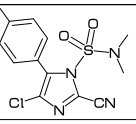
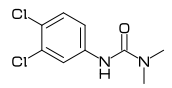
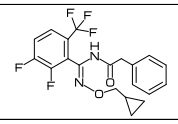
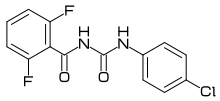
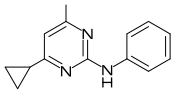
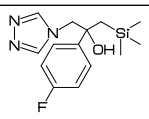
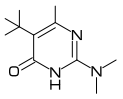
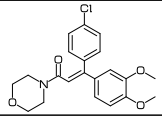
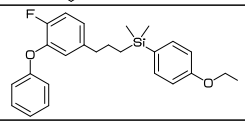
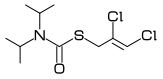
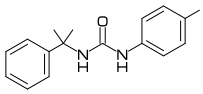
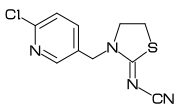
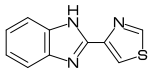
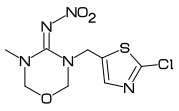
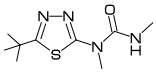
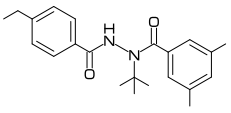
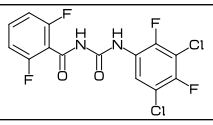
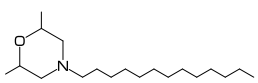
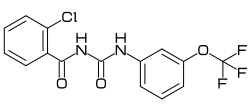
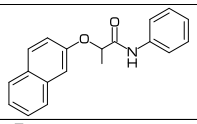
[477] 	Cumyluron	pesticide	302.802	302.7985	C17H19ClN2O
	^30,Ph,4:,!??,!NH!,?O!,NH,!2,Ph,-1:/Cl				
[478] 	Cloquintocet-methyl	pesticide	335.83	335.8251	C18H22ClNO3
	^90,Ph,4=Ph,2:N,10:/Cl,7:,!,O!2,?O!O,!?,!5				
[479] 	Clotianidin	pesticide	249.673	249.6780	C6H8ClN5O2S
	^6,?5,3’5=dl,2:S,5:N,1:/Cl,3:,!2,NH!,/NH!,!d,N,!NO2				
[480] 	Chromafenozide	pesticide	394.515	394.5065	C24H30N2O3
	^30,?6,3=?6,5:O,7’9’11=dl,7:?,8:,!?O,!NH!,N,/??!,!?O,!Ph,-4’-3:?				
[481] 	Clomeprop	pesticide	324.2	324.2018	C16H15Cl2NO2
	^30,Ph,4’6:/Cl,5:?,3:,!O,!?!,?O,!NH!,Ph				
[482] 	Chloridazon	pesticide	221.6	221.6430	C10H8ClN3O
	^30,?6,3’4:N,2’6=dl,5:?O,1:/NH2,6:/Cl,4:/Ph				
[483] 	Chloroxuron	pesticide	290.745	290.7448	C15H15ClN2O2
	^30,Ph,6:/Cl,3:,!O!,Ph,-3:,!NH!,?O!,N?!				
[484] 	Cyazofamid	pesticide	324.783	324.7859	C13H13ClN4O2S
	^18,?5,2’5=dl,2’4:N,1:/Cl,3:/CN,4:,!,S?O?O,!,N?!,5:,!Ph,-3:?				

[485] 	Diuron	pesticide	233.1	233.0945	C9H10Cl2N2O
	^30,Ph,1'6:/Cl,3:,!NH!,?O!,N?!				
[486] 	Cyflufenamid	pesticide	412.36	412.3531	C20H17F5N2O2
	^30,Ph,4^20:/?F?F!F,1'2:/F,3:,!2,NH!,?O!2,Ph,-10:,!d,N!,^-12,O!2,?3				
[487] 	Diflubenzuron	pesticide	310.7	310.6832	C14H9ClF2N2O2
	^30,Ph,2'4:/F,3:,!?O,!NH!,?O,!NH!,Ph,-3:/Cl				
[488] 	Cyprodinil	pesticide	225.295	225.2889	C14H15N3
	^30,Ph,2'4:N,5:?,1:/?3,3:/NH!'Ph				
[489] 	Simeconazole	pesticide	293.417	293.4120	C14H20FN3OSi
	^36,?5,1'3'5:N,1'4=dl,3:,30,!,/OH^30,!2,Si,??!,7^-30:/Ph'4:/F				
[490] 	Dimethirimol	pesticide	209.29	209.2880	C11H19N3O
	^30,?6,3'5=dl,1:?O,2:NH,3:/N?!,4:N,5:?,6:/??!				
[491] 	Dimethomorph	pesticide	387.86	387.8566	C21H22ClNO4
	^30,?6,1:O,4:N,4:,!?O!,!d'1,/Ph'4:/Cl,!,<Ph,4'5:/O!				
[492] 	Silafluofen	pesticide	408.588	408.5804	C25H29FO2Si
	^30,Ph,5:,!O!,Ph,-1:/F,10:,!4,Si,??,!Ph,-3:/O!2				
[493] 	Di-allate	pesticide	270.212	270.2190	C10H17Cl2NOS
	^-30,!?!,N!,?O!,S,!2,!d,!Cl,3:/?!,7:/Cl				
[494] 	Daimuron	pesticide	268.4	268.3534	C17H20N2O
	^30,Ph,4:,!??,!NH!,?O,!NH!,Ph,-3:?				
[495] 	Thiacloprid	pesticide	252.72	252.7232	C10H9ClN4S
	^30,Ph,1:N,6:/Cl,3:,!2,^-12,<?5,1:N,3:S,-4://N'!CN				
[496] 	Thiabendazole	pesticide	201.247	201.2476	C10H7N3S
	^30,Ph,3=?5,8=dl,9:NH,7:N,8:,!,<?5,1'4=dl,3:S,5:N				
[497] 	Thiamethoxam	pesticide	291.71	291.7146	C8H10ClN5O3S
	^30,?6,2:O,4'6:N,6:?,5:,!dm,N,!NO2,4:,!2,<?5,1'3=dl,3:N,5:S,4:/Cl				
[498] 	Tebuthiuron	pesticide	228.3	228.3145	C9H16N4OS
	^18,?5,3'5=dl,4'5:N,2:S,1:/??!,3:,!,N?!,?O,!NH!				
[499] 	Tebufenozide	pesticide	352.5	352.4699	C22H28N2O2
	^30,Ph,6:/!,3:,!?O,!NH!,N,/??!,!?O,!Ph,-4'-2:?				
[500] 	Teflubenzuron	pesticide	381.1	381.1092	C14H6Cl2F4N2O2
	^30,Ph,2'4:/F,3:,!?O,!NH!,?O,!NH!,<Ph,3'5:/Cl,4'6:/F				
[501] 	Tridemorph	pesticide	297.5	297.5190	C19H39NO
	^30,?6,3:N,6:O,1'5:?,3:/!12				
[502] 	Triflumuron	pesticide	358.701	358.6997	C15H10ClF3N2O3
	^30,Ph,4:/Cl,3:,!?O,!NH!,?O,!NH!,Ph,-2:/O!'?F?F!F				

[503] 	Naproanilide	pesticide	291.35	291.3437	C19H17NO2
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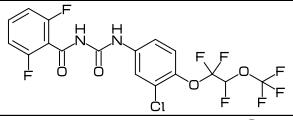
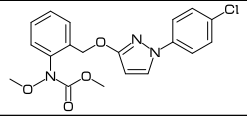
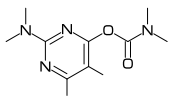
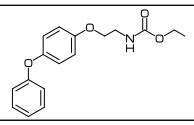
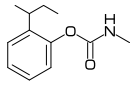
[504] 	Novaluron	pesticide	492.706	492.7045	C17H9ClF8N2O4
	^30,Ph,2'4:/F,3:,!?O,!NH!,?O,!NH!, Ph,-4:/Cl,-3:,!O!,/F^-35,/F^35,!,/F,!O!,?F?F!F				
[505] 	Pyraclostrobin	pesticide	387.817	387.8169	C19H18ClN3O4
	^30,Ph,3:,!2,O!,^12,<?5,2'5=dl,4'5:N,4:,12,Ph,-3:/Cl>,2:,!N,/O!,!?O,!O!				
[506] 	Pirimicarb	pesticide	238.291	238.2862	C11H18N4O2
	^30,Ph,1'5:N,2'3:?,6:/N?!,4:,!O!,?O!,N?!				
[507] 	Fenoxycarb	pesticide	301.35	301.3370	C17H19NO4
	^30,Ph,5:,!O!,Ph,-3:,!,O!3,NH!,?O!,O!2				
[508] 	Fenobucarb	pesticide	207.3	207.2688	C12H17NO2
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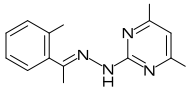
[509] 	Ferimzone	pesticide	254.337	254.3302	C15H18N4
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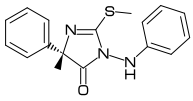
[510] 	Fenamidone	pesticide	311.403	311.4013	C17H17N3OS
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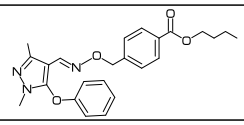
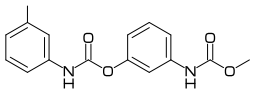
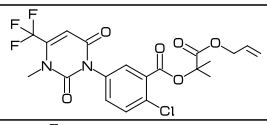
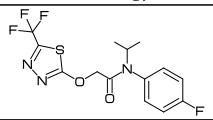
[511] 	Fenpyroximate	pesticide	421.49	421.4888	C24H27N3O4
	^-6,?5,3'5=db,1'2:N,2'5:?,3:,-15,O,!Ph,4:,!!d,N!,O!2,Ph,-3:,!?O,!O,!4				
[512] 	Phenmedipham	pesticide	300.32	300.3092	C16H16N2O4
	^30,Ph,5:?,3:,!NH!,?O!O,!Ph,-4:/NH!'?O!'O!				
[513] 	Butafenacil	pesticide	474.817	474.8149	C20H18ClF3N2O6
	^30,?6,5=dl,1'3:N,1:?,2'4:?O,6:/?F?F!F,3:,!Ph,-3:/Cl, -2:,!?O,!O!,??!,?O!,O!2,!d				
[514] 	Flufenacet	pesticide	363.331	363.3305	C14H13F4N3O2S
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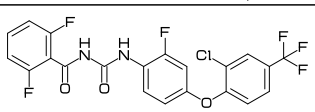
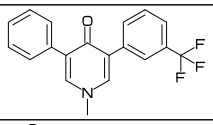
[515] 	Flufenoxuron	pesticide	488.77	488.7670	C21H11ClF6N2O3
	^30,Ph,2'4:/F,3:,!?O,!NH!,?O,!NH!,Ph,-1:/F,-3:,!O!,Ph,-3:/?F?F!F,-1:/Cl				
[516] 	Fluridone	pesticide	329.3	329.3157	C19H14F3NO
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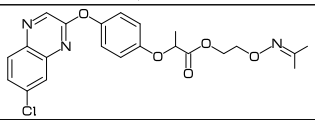
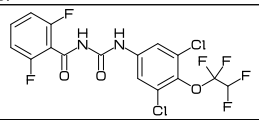
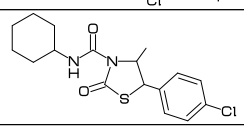
[517] 	Propaquizafop	pesticide	443.884	443.8801	C22H22ClN3O5
	^90,Ph,3=?6,8'10=dl,7'10:N,1:/Cl,8:,!O!,Ph,-3:,!O,!?!,?O,!O,!3,O!,N,!dr,?!				
[518] 	Hexaflumuron	pesticide	461.14	461.1427	C16H8Cl2F6N2O3
	^30,Ph,2'4:/F,3:,!?O,!NH!,?O,!NH!,<Ph,3'5:/Cl,4:,!O!,/F^-35,/F^35,!,/F,!F				
[519] 	Hexathiazox	pesticide	352.877	352.8788	C17H21ClN2O2S
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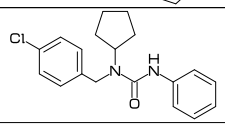
[520] 	Pencycuron	pesticide	328.84	328.8358	C19H21ClN2O
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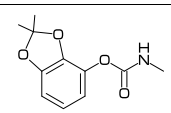
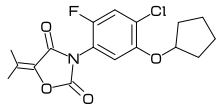
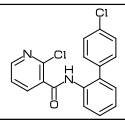
[521] 	Bendiocarb	pesticide	223.228	223.2252	C11H13NO4
	^30,Ph,5=?5,7'9:O,8:??,4:,!O!,?O,!NH!				
[522] 	Pentoxazone	pesticide	353.774	353.7725	C17H17ClFNO4
	^66,?5,5://?!,1:O,3:N,2'4:?O,3:,!,<Ph,4:/Cl,6:/F,3:/O!'?5				
[523] 	Boscalid	pesticide	343.21	343.2066	C18H12Cl2N2O
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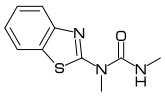
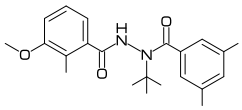
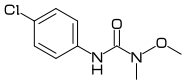
[524] 	Methabenzthiazuron	pesticide	221.3	221.2788	C10H11N3OS
	Ph,3=?5,9=dl,7:S,9:N,8:,!,N?!,?O,!NH!				
[525] 	Methoxyfenozide	pesticide	368.48	368.4693	C22H28N2O3
	^30,Ph,2:?,1:/O!,3:,!?O,!NH!,N,/??!,!?O,!Ph,-4'-2:?				
[526] 	Monolinuron	pesticide	214.6	214.6488	C9H11ClN2O2
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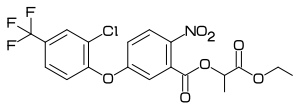
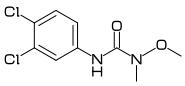
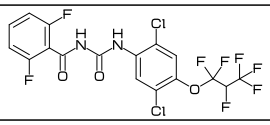
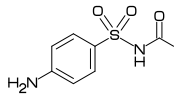
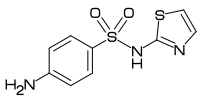
[527] 	Lactofen	pesticide	461.78	461.7731	C19H15ClF3NO7
	^30,Ph,4:/Cl,6:/?F?F!F,3:,!O!,Ph,-3:/NO2,-4:,!?O!,O,!?!,?O!,O!2				
[528] 	Linuron	pesticide	249.1	249.0938	C9H10Cl2N2O2
	^30,Ph,1'6:/Cl,3:,!NH!,?O!,N?!,O!				
[529] 	Lufenuron	pesticide	511.15	511.1502	C17H8Cl2F8N2O3
	^30,Ph,2'4:/F, 3:,!?O,!NH!,?O,!NH!,<Ph,3'6:/Cl,4:,!O!,/F^35,/F^-35,!,/F,!,?F?F!F				
[530] 	Sulfacetamide	antibacterial	214.239	214.2415	C8H10N2O3S
	^30,Ph,1:/NH2,4:,!,S?O?O,!NH!,?O!				
[531] 	Sulfatiazole	antibacterial	255.31	255.3166	C9H9N3O2S2
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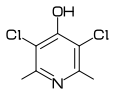
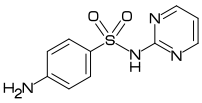
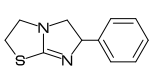
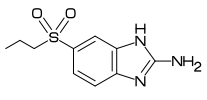
[532] 	Chlopidol	antibacterial	192.039	192.0425	C7H7Cl2NO
	^30,Ph,1'3:?,2:N,4'6:/Cl,5:/OH				
[533] 	Sulfadiadine	antibacterial	250.276	250.2769	C10H10N4O2S
	^30,Ph,1:/NH2,4:,!,S?O?O,!NH!,<Ph,2'6:N				
[534] 	Levamisole	antibacterial	204.29	204.2913	C11H12N2S
	?5,3=?5,6=dl,2:S,4'6:N,7:/Ph				
[535] 	5-(Propylsulphonyl)-1-H-Benzimidazole-2-Amine	antibacterial	239.29	239.2941	C10H13N3O2S
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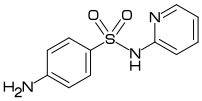
[536] 	Sulfapyrizine	antibacterial	249.288	249.2889	C11H11N3O2S
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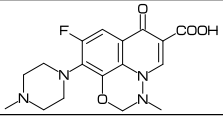
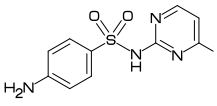
[537] 	Marbofloxacin	antibacterial	362.361	362.3555	C17H19FN4O4
	^30,Ph,3'2--7=?6,9=dl,6:/F,7'13:N,11:O,9:/COOH,10:?O,13:?,1:,!,<?6,1:N,4:N?				
[538] 	Sulfamerazine	antibacterial	264.303	264.3035	C11H12N4O2S
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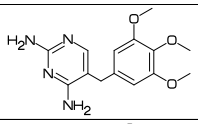
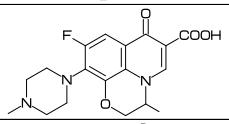
[539] 	Trimethoprim	antibacterial	290.323	290.3177	C14H18N4O3
	^30,Ph,1'5:N,2'6:/NH2,3:/!Ph'(4'5'6:/O!)				
[540] 	Ofloxacin	antibacterial	361.373	361.3675	C18H20FN3O4
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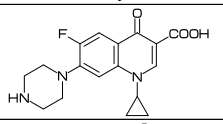
[541] 	Ciprofloxacin	antibacterial	331.347	331.3415	C17H18FN3O3
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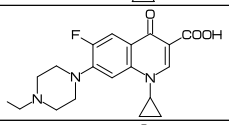
[542] 	Enrofloxacin	antibacterial	359.401	359.3946	C19H22FN3O3
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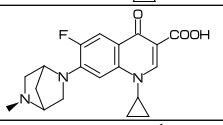
[543] 	Danofloxacin	antibacterial	357.385	357.3788	C19H20FN3O3
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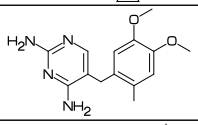
[544] 	Ormetoprim	antibacterial	274.324	274.3183	C14H18N4O2
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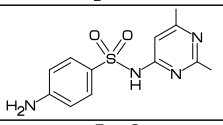
[545] 	Sulfadimidine	antibacterial	278.33	278.3301	C12H14N4O2S
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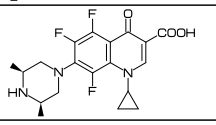
[546] 	Orbifloxacin	antibacterial	395.382	395.3756	C19H20F3N3O3
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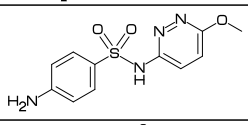
[547] 	Sulfamethoxypyridazine	antibacterial	280.302	280.3029	C11H12N4O3S
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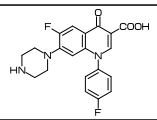
[548] 	Sarafloxacin	antibacterial	385.371	385.3640	C20H17F2N3O3
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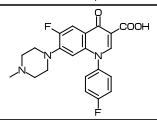
[549] 	Difloxacin	antibacterial	399.398	399.3906	C21H19F2N3O3
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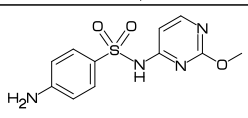
[550] 	Sulfamonomethoxine	antibacterial	280.302	280.3029	C11H12N4O3S
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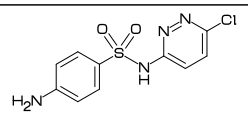
[551] 	Sulfachlorpyridazine	antibacterial	284.723	284.7220	C10H9ClN4O2S
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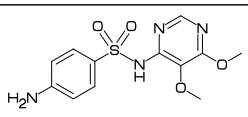
[552] 	Sulfadoxine	antibacterial	310.328	310.3289	C12H14N4O4S
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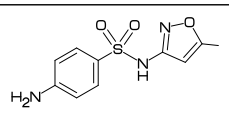
[553] 	Sulfamethoxazole	antibacterial	253.276	253.2776	C10H11N3O3S
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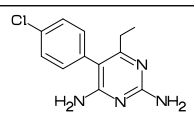
[554] 	Pirimethamin	antibacterial	248.714	248.7114	C12H13ClN4
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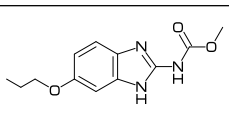
[555] 	Oxibendazole	antibacterial	249.27	249.2658	C12H15N3O3
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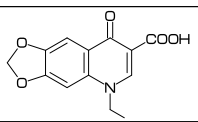
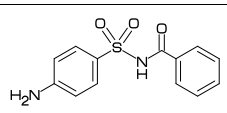
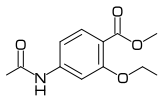
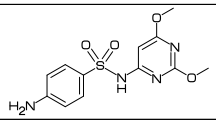
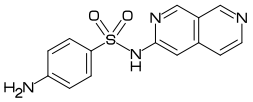
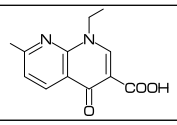
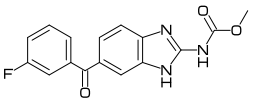
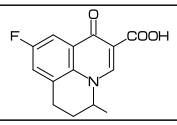
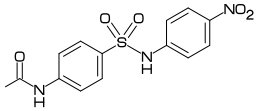
[556] 	Oxolinic acid	antibacterial	261.233	261.2301	C13H11NO5
	^30,Ph,3=?6,6=?5,9=dl,7:N,11'13:O,10:?O,7:/!,9:/COOH				

[557] 	Sulfabenzamide	antibacterial	276.31	276.3109	C13H12N2O3S
	^30,Ph,1:/NH2,4:,!,S?O?O,!NH!,?O,!Ph				
[558] 	Ethopabate	antibacterial	237.255	237.2518	C12H15NO4
	^30,Ph,1:/NH!'?O!,3:/O!2,4:/?O!'O!				
[559] 	Sulfadimethoxine	antibacterial	310.33	310.3289	C12H14N4O4S
	^30,Ph,1:/NH2,4:,!,S?O?O,!NH!,<Ph,2'4:N,3'5:/O!				
[560] 	Sulfaquinoxaline	antibacterial	300.337	300.3356	C14H12N4O2S
	^30,Ph,1:/NH2,4:,!,S?O?O,!NH!,<Ph,3=Ph,6'9:N				
[561] 	Nalidixic acid	antibacterial	232.239	232.2352	C12H12N2O3
	^30,Ph,3=?6,9=dl,5'10:N,6:?,7:?O,8:/COOH,10:/!				
[562] 	Flubendazole	antibacterial	313.288	313.2831	C16H12FN3O3
	^30,Ph,3=?5,9=dl,7:NH,9:N,1:,!?O,!Ph,-2:/F,8:/NH!'?O!'O!				
[563] 	Flumequine	antibacterial	261.225	261.2483	C14H12FNO3
	^30,Ph,3'2--7=?6,9=dl,7:N,6:/F,9:/COOH,10:?O,13:?				
[564] 	Sulfanitran	antibacterial	335.334	335.3351	C14H13N3O5S
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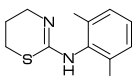
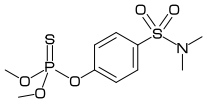
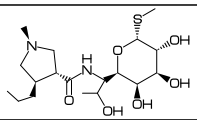
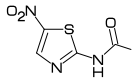
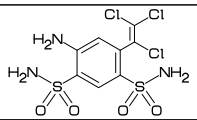
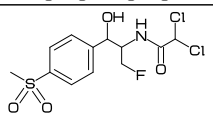
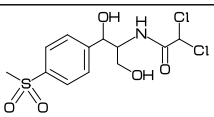
[565] 	Xylazine	antibacterial	220.334	220.3338	C12H16N2S
	^30,?6,3=dl,2:S,4:N,3:,!NH!,Ph,-5'-1:?				
[566] 	Famphur	antibacterial	325.3	325.3415	C10H16NO5PS2
	^-30,!O!,P,?S,/O!^160,!O!,Ph,-3:/S?O?O!'N?!				
[567] 	Lincomycin	antibacterial	406.54	406.5373	C18H34N2O6S
	^6,?5,5:N,5:?w,2:*/!2, 3:,!z,?O,!NH!,!wb,<?6,6:O,2'3'*4:*/OH,5:/*S!>,8:/?!'OH^-30^lr				
[568] 	2-acethylamino-5-nitrothiazole	antibacterial	187.178	187.1764	C5H5N3O3S
	^18,?5,2'5=dl,2:N,4:S,3:/NH!'?O!,5:/NO2				
[569] 	Chlorsulon	antibacterial	380.66	380.6558	C8H8Cl3N3O4S2
	^30,Ph,6:/NH2,1'3:/S?O?O'!NH2,4:,!,/Cl,60~dl,?Cl!Cl				
[570] 	Florfenicol	antibacterial	358.21	358.2132	C12H14Cl2FNO4S
	^30,Ph,1:/S?O?O!,4:,!,/OH,!,/!F,!NH!,?O!,?Cl!Cl				
[571] 	Thiamphenicol	antibacterial	356.22	356.2221	C12H15Cl2NO5S
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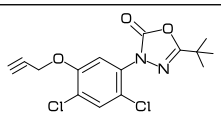
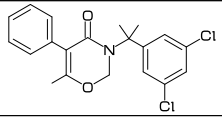
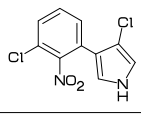
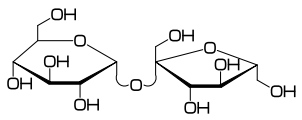
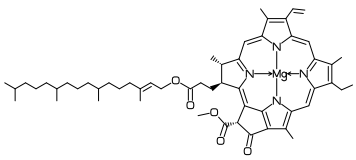
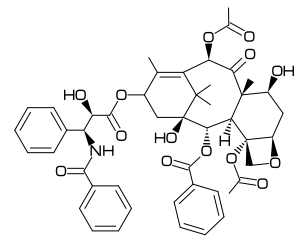
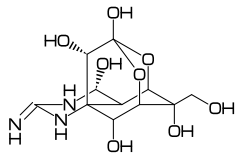
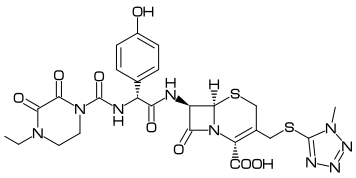
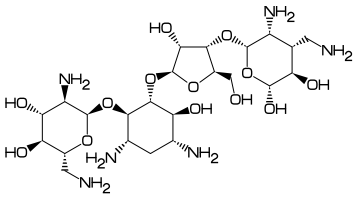
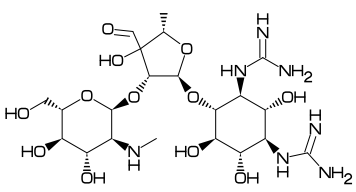
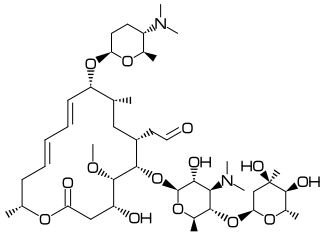
[572] 	Oxadiargyl	antibacterial	341.19	341.1892	C15H14Cl2N2O3
	^30,Ph,1'3:/Cl,6:/O!2'!t,4:,!,<?5,2=dl,1'2:N,4:O,5:?O,3:/??!				
[573] 	Oxaziclomefone	antibacterial	376.277	376.2763	C20H19Cl2NO2
	^30,?6,6=dl,4:N,2:O,1:?,5:?O,6:/Ph,4:,!??,!Ph,-4'-2:/Cl				
[574] 	Pyrrolnitrin	biological	257.07	257.0728	C10H6Cl2N2O2
	^30,Ph,3:,!,?5,8'11=db,1'11:/Cl,9:NH,2:/NO2				

[1] 	Sucrose	sugar	342.3	342.2964	C12H22O11
	hexose_hp,‘.5,1^$270’2^$90’3^$270:/OH,6^$90:/!OH,‘, 4:,$310~arc_lb‘1,O,$50~arc_br‘1,^$0, <Pyranose_hp,‘.5,2^$270’3^$90:/OH,1^$90’4^$270:/!OH				
[2] 	Chlorophyll a	biological	893.509	893.4889	C55H72MgN4O5
	^-36,?5,3:,!‘1,54‘1,?5,-2:,!‘1,54‘1,?5, -2:,!‘1,54‘1,?5,-2:,!‘1,:5,6:,22‘1,70‘1,:8, 4’6’8’10’14’16’18’21’23’27=dl,4:,!‘1.48~vf,Mg,:17~vb,11:,:27,27:,:23, 4’11’17’23:N,1~zf’9’15’21:?,14:/!,20:/!d,25:/*?O!’O!,26:?O, 2:,-6~wf,!2,?O!,O!2,!d,<!13,1’5’9’13:?				
[3] 	Paclitaxel	biological	853.918	853.9061	C47H51NO14
	?6,5=dl,3:,‘1,36,45,45,45,45,‘,:5,-4=?6,-4=?4,-1=wb,-3=wf,-1:O, 4:??,6:?,3^-60’15:*/OH,8^-60:/*H,9^60:?w,10:?O, 1:,!O!,?O!,*/OH,!,/Ph,60~wf,NH,-60,?O,60,Ph, 7:,!z,O,-45,?O,60,Ph,11^rl’*12^-15^lr:*/O!’?O!				
[4] 	Tetrodotoxine	marine toxine	319.27	319.2679	C11H17N3O8
	‘1,^60,-90,60,-30‘1.15,150,60,:1,3:,-135,60,-30‘1.15,150,:4, 10:,!O,60‘1.33,60,:$3~si_,8:,-15~si_,O,:12,‘, 9:,45,-60,OH,1^120:?NH,5~zf^-15’7’9^-75’12’13~zf:/OH,2:NH,6^180:NH				
[5] 	Cefoperazone	antibiotics	645.67	645.6673	C25H27N9O8S2
	^45,?4,2=?6,6=db,2:N,8:S,3^45:/*H,1:?O^15,5:/*COOH, 4:,15~wf,NH!,?O!,/*Ph’4:/OH,!NH!,?O!,<?6,1’4:N,2’3:?O,4:/!>, 6:,!2,S!,<?5,1’3=dl,5:?,2’3’4’5:N				
[6] 	Neomycin	antibiotics	614.644	614.6437	C23H46N6O13
	^30,?6,3:O,2:/*!NH2,1’*6:*/OH,5:*/NH2, 4:,!w,O,!wb,<?6,4’2^15:/*NH2,5:*/OH^-15, 6:,!z,O,-72~wb,<?5,2:O,5:/*OH^vt,3:*/!OH^vt, 4:,-24~zf,O,-60~zb,<?6,2:O,6:/*NH2,4’*3:*/OH,5:/*!NH2				
[7] 	Streptmycin	antibiotics	581.574	581.5740	C21H39N7O12
	^54,?5,3:O,4:?z,5:/OH^45,1:,!z,O,-24~wb,?6,-5:O,2:,!w,O,24~zb,?6, 5:/!dO^-48,10’*11’15’*16’*18:*/OH,9:/*!OH,12:*/NH!,17^-18’19:*/NH!’?NH’!NH2				
[8] 	Spiramycin	antibiotics	843.1	843.0526	C43H74N2O14
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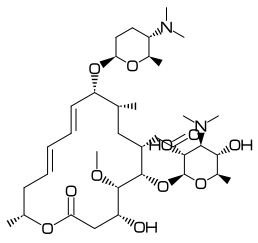
[9]



Neospiramycin	antibiotics	698.9	698.8842	C36H62N2O11

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 -6:,!z^-30,O,!wb,<?6‘.7,2:O,‘.5,4:/*N?!,3:?w,‘,
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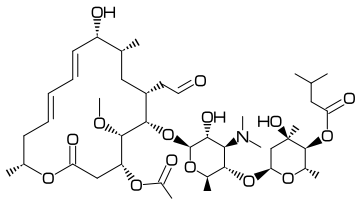
```

[10]



Josamycin	antibiotics	827.995	827.9949	C42H69NO15

```
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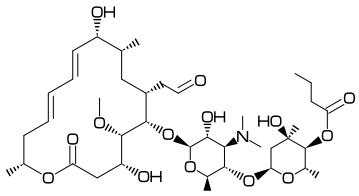
 12’14=dl,2:O,1:?z,3:?O,10:?z,6:/*O!^vt,-6:/*OH,5:/*O!’?O!^-25,8:/*!’!dO,
 7:,!z,O,0~wb,<?6‘.7,2:O,‘.5,5:*/N?!,6:/*OH,3:?w,‘,
   4:,!z‘1,O,!wb,<?6‘.7,2:O,‘.5,5^35:*/OH,5^-35’3:?z,‘,
   4:,!w,O,60,?O,60,-60,?,!
```

[11]



Leucomycin A5	antibiotics	771.942	771.9317	C39H65NO14

```
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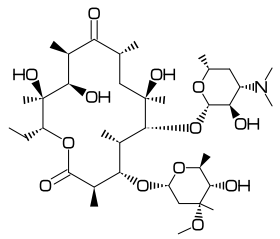
 12’14=dl,2:O,1:?z,3:?O,10:?z,6:/*O!^vt,-6:/*OH,5:/*OH,8:/*!’!dO,
 7:,!z,O,0~wb,<?6‘.7,2:O,‘.5,5:*/N?!,6:/*OH,3:?w,‘,
   4:,!z‘1,O,!wb,<?6‘.7,2:O,‘.5,5^35:*/OH,5^-35’3:?z,‘,
   4:,!w,O,60,?O,60,-60,60
```

[12]



Erythromycin	antibiotics	733.93	733.9267	C37H67NO13

```
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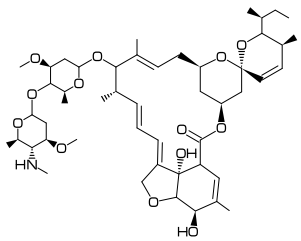
 14:O,13:/*!,1’9:?O,*2’4’6^-35’8’*10’12^35:?z,
 6^35’11’12^-35:*/OH,
 $3:,!z,O,30~zb,<?6‘.7,6:O,‘.5,5~wf’3^35:?,4:/*OH,3^-35:/*O!,‘,
 $5:,30~zf‘1.7,O,!zb,<?6‘.7,6:O,‘.5,5:?z,2:*/OH,3:/*N?!
```

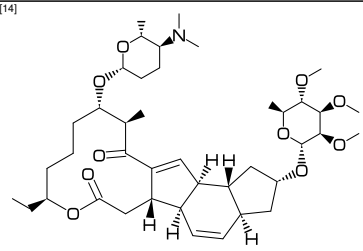
[13]



Emamectine	antibiotics	886.133	886.1187	C49H75NO13

```
^24,?6,6=?5,3=dl,9:O,2:*/OH,3:?,6:/*OH^-60,
 5:,‘1.04,6,-60,O,60~wb,60,-60,60~wf,60,-60,60,60,60,-60,60,‘,:7,
 -1’-3’-7=dl,-11--␣-10=?6,-2:,?6,-6=wf,-1=zb,-5=dl,
 -1’-6:O,-3:?w,-2:,!,?w,!2,10:?O,
 17:?,19:?z,18:,!O!,<?6‘.7,6:O,‘.5,5:?w,3:*/O!,‘,
 -3:,!O,60,<?6‘.7,2:O,‘.5,3:?w,4:/*NH!,5:*/O!
```

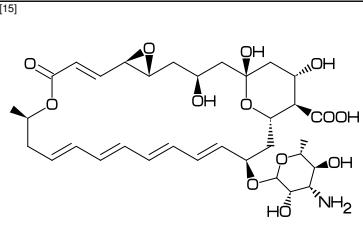
[14]



Spinosad	antibiotics	731.968	731.9555	C41H65NO10

```
^30,‘1,^-120,60,60,-60,60,60,60,-60,60,60,60,-60,:1,‘,
 5=?5,-1=dl,-2^60’-3^-35:/*H,-3=?6,-4=dl,
 -1^35’*-2^-60:*/H,-2=?5,2:O,3^25’7^-25:?O,1:*/!,
 -2:,!z,O,66~zb,<?6‘.7,6:O,‘.5,5:?w,*4’3’2:*/O!>,‘,
 8:?w,5^-65:*/H,9:,!z,O,!zb,<?6‘.7,6:O,‘.5,5:?z,4:*/N?!
```

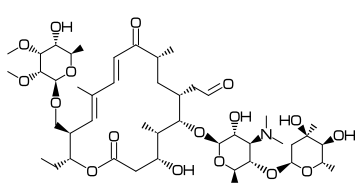
[15]



Natamycin	antibiotics	665.733	665.7251	C33H47NO13

```
^-90,‘1,60,60,-60,60,-60,60,-60,60,-60,60,60,60,60,O,-60,
 60,60,-60,60,-60,60,-60,60,60,60,-60,:1,‘,12--13=?6,
 2’4’6’8’20=dl,11=zb,23:O,-2:/*OH,-3:*/COOH,
 18=?3,-1=wb,-2=wf,-1:O,22:?O,24:?w,14^60’16:*/OH,
 10:,15~wf,O,90,<?6‘.7,6:O,‘.5,4’*2:*/OH,3:/*NH2,5:?z
```

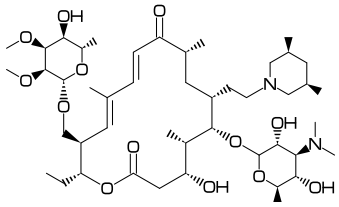
[16]



Tylocin	antibiotics	916.10	916.1000	C46H77NO17

```
^-90,‘1,60,60,-60,60,60,-60,60,60,-60,60,60,60,-60,60,-60,:1,‘,
 12’14=dl,2:O,1:/*!,5:/*OH,3:?O,10:?z,6:?z,-6:?O,-3:?,8:/*!’!dO,
 -1:,!w,-60,O,0~wb,?6‘.7,-5:O,‘.5,-3:/*OH,-4:?w,-1’-2:/*O!,‘,
 7:,!z,O,0~wb,<?6‘.7,2:O,‘.5,5:*/N?!,6:/*OH,3:?w,‘,
   4:,!z‘1,O,!wb,<?6‘.7,2:O,‘.5,5^35:*/OH,5^-35’3:?z,4:*/OH
```

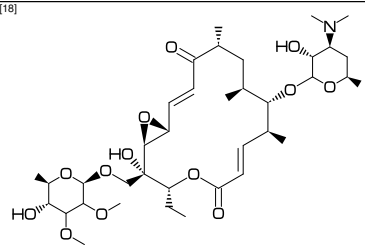
[17]



Tilmicosin	antibiotics	869.133	869.1330	C46H80N2O13

```
^-90,‘1,60,60,-60,60,60,-60,60,60,-60,60,60,60,-60,60,-60,:1,‘,
 12’14=dl,2:O,1:/*!,5:/*OH,3’11:?O,6’10:?z,14:?,
 -1:,!w,-60,O,O~zb,<?6‘.7,2:O,‘.5,6’5:*/O!,4:*/OH,3:?z,‘,
 $7:,!z,O,O,<?6‘.7,2:O,‘.5,5:*/N?!,6’4:/*OH,3:?w,‘,
 $8:,!z,!2,<?6‘.7,1:N,‘.5,5’3:?w
```

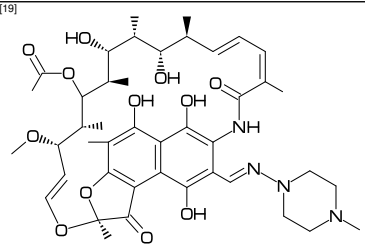
[18]



Mirosamicin	antibiotics	727.8791	727.8791	C37H61NO13

```
^-90,‘1,60,60,-60,60,60,-60,60,60,-60,60,60,60,-60,60,-60,:1,‘,
 5’13=dl,15=?3,-2=wf,-1=wb,-1:O,3:O,2:/*!,4’12:?O,7’9’*11:?w,1:/*OH^-80,
 $1:,!w,!O,!wb,<?6‘.7,2:O,‘.5,4:/*OH,3:?w,5’6:/O!,‘,
 $8:,!z,O,O,<?6‘.7,2:O,‘.5,5:*/N?!,6:/*OH,3:?w
```

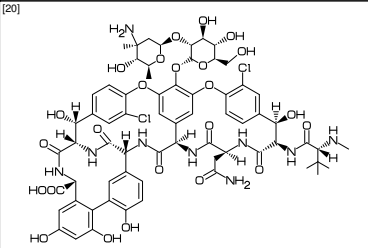
[19]



Rifampicin	antibiotics	822.94	822.9402	C43H58N4O12

```
^30,Ph,6:?^30,5:/OH,-6=?5,-3:O,-8=?6,-2’-4=dl,-1’-4:/OH,
 ‘1,-2:,!,NH,60,-60,60~dl,60,60~dl,-60,
 60,-60,60,60,-60,60,-53,66,-53~dl,66‘1.2,O,‘,:$8,
 9’15:?O,16:?,20’24^30:?w,21’23:/*OH,8^60’22’26^30:?z,
 -4:/*O!,-6:,-30,O!,?O!,$11:,!!d,N!,<?6,1:N,4:N?
```

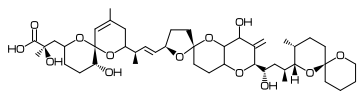
[20]



Vancomycin	antibiotics	1449.25	1449.253	C66H75Cl2N9O24

```
^-30,!12‘1,1’3’12=zf,7=wf,‘1,60,60,Ph,-3:,!O!,Ph,-4:,!O!,Ph,-3:,!,:1,
 7:,:26,$1:,60,60,NH,60,-60,Ph,-1:,!Ph,-2:,:4,‘,
 36’3^40’6’9’12:?O,2’5’8’11:NH,1’4^180’*7^-60’*10^60’*14^60’35^-60:*/H,
 41’43’46:/OH,14’*35:*/OH,17’34^15:/Cl,38^180:*/COOH,
 10:,-60~wf,60,?O!,NH2,13:,!w,NH!,?O!,/??!,*/H^60,!z,NH!,
 23:,!O,!z,‘.7,<?6,2:O,3^10:*/!OH,*4’5:*/OH,‘,
 -1:,!z,O,!wb,‘.7,<?6,6:O,*3^35’5:?w,3^-35:/NH2,4:/*OH
```

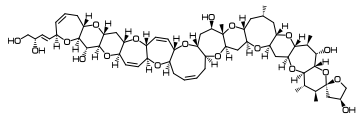
[21]



Okadaic acid	marine toxine	805.00	805.0029	C44H68O13

```
^30,?6,4:,?6,-4:,!4,^-12,?5,-3:,^-12,?6,-3=?6,-3:,!w,!3,
 ?6,-4:,?6,6:,!2,?z^-40,*/OH^20,!?O!,OH,
 3’38=wb,11=dl,15=dr,17’19=wf,5’7’16’24’25’33’42:O,
 32:*/H^60,10:?,12’31’*37:?w,27:?d,28:/OH,3’29:/*OH
```

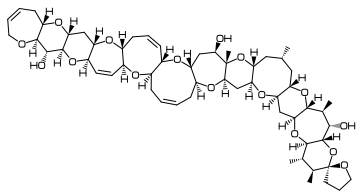
[22]



Ciguatoxine-1B	marine toxine	1111.31	1111.313	C60H86O19

```
^30,?7,-5’-3=?6,-3’-3=?7,-4=?9,-3=?7,-4=?6,-3=?8,-5=?6,-3=?7,-4=?6,-2:,?5,
 -5=zf,-1=wb,6’19’28’32=db,2’11’12’20’21’32’33’41’42’51’52’60’64:O,
 1:/*H^60,3’9’13’18’22’30’34’39’43’49’53:/*H^-60,
 4’10’14’19’23^75’31^55’40’44’50’54:*/H^60,
 35^60’*46’56’*57’58:?w‘.8,*8’36’*55’62:*/OH,
 1:,!,!dl,!,/*OH,!2,OH
```

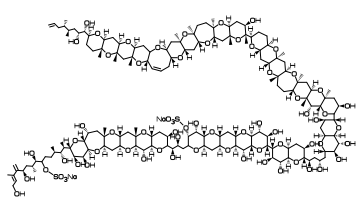
[23]



Ciguatoxine-3C	marine toxine	1023.25	1023.251	C57H82O16

```
^30,?7,-5’-3=?6,-3=?7,-3=?8,-5=?9,-3=?7,-4=?6,-3=?8,-5=?6,-3=?7,-4=?6,-2:,?5,
 -5=zf,-1=wb,6’19’28’33=db,2’11’12’20’21’33’34’42’43’52’53’61’65:O,
 3’9’13’18^-65’22’31^-70’35^-55’40^-65’44’50’54:/*H^-60,
 4’10’14’19’23^75’32^65’41’45’51’55:*/H^60,
 36^60’*47’57’*58’59:?w‘.8,*8’37’*56:*/OH
```

[24]



Maitotoxin	marine toxine	3425.86	3425.856	C164H256Na2O68S2

```
^55.8,?6,-4=?7,-4’-3’-3’-3=?6,-3:,!4,?6,-4’-3’-3’-3=?6,-3:,!,?6,-3=?6,
 -3:,!4,60,^-30,?6,-3=?6,-3:,30,^30,?6,-3’-3=?6,-3=?7,-4’-3’-3=?6,
 -2:,!,?6,-3=?6,-3=?7,-3’-3=?6,-3=?8,-3=dl,-5’-3’-3’-3=?6,
 5’7’15’16’23’24’32’40’41’48’49’58’59’72’73’82’83’90’91’99’
    100’107’113’114’122’123’130’131’140’141’148’149:O,
 1^60’2’26’28’29’51’54’61’63’68’75^60’78’109:*/OH,
 11’20’35’45’52’55’65’69’86:/*OH,
 3’8’13’17’21’33’38’42’56’70’84’92’101’106’111’128’138’142’146’150:/*H^-60,
 4’14’22’34’39’43’*47’*57’*71’81’89’98’102’116’121’125’129’133:*/H^60,
 6’46’50’53’60’67’74:*/H^-60,
 9’18’85’93’112’139’143’147:?w^60‘1,80’88’97’*108’115’120’124:?z^-60‘1,
 $6:,!,<!11,60~dr,-60,60,OH,*2’7’10:*/OH,1’3’*8:?w,11:?d,12:?,6:,!O,30,SO3Na,
 $36:,-45~zf,O,30,SO3Na,
 $150:,!,<!7,1’2:/*OH,4:?w,5:?z,7=dl
```