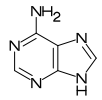
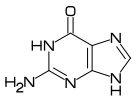
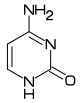
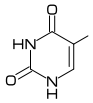
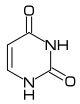
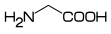
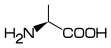
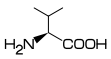
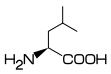
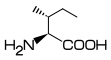
Molecular Coding Format examples

Author : Akira Yamaji Date : February 16, 2025 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,?6,3=?5,1'3'5'9=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
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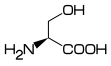
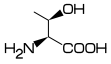
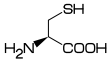
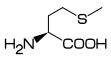
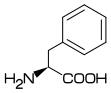
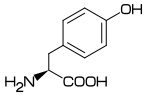
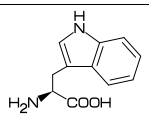
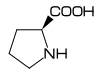
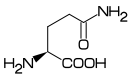
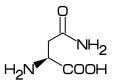
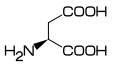
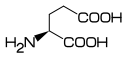
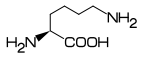
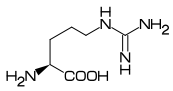
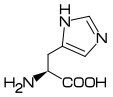
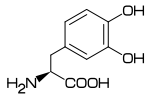
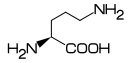
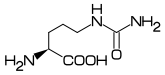
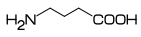
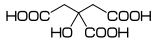
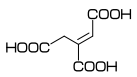
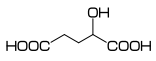
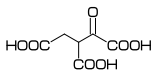
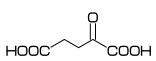
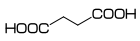
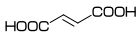
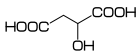
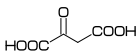
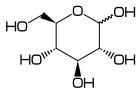
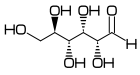
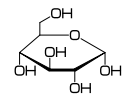
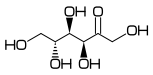
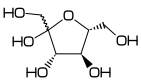
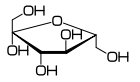
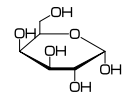
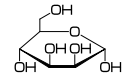
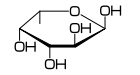
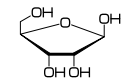
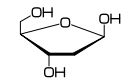
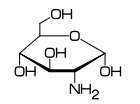
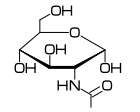
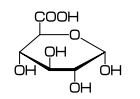
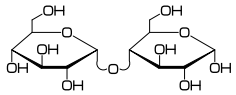
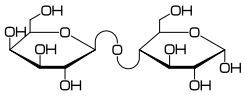
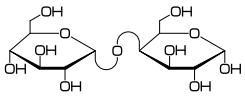
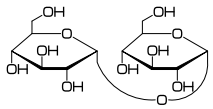
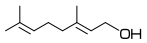
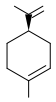
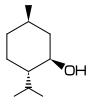
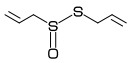
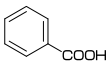
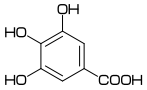
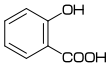
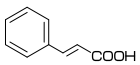
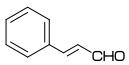
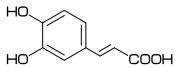
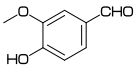
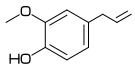
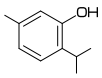
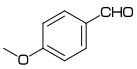
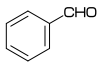
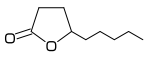
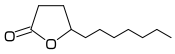
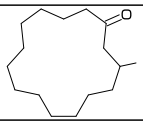
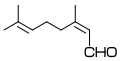
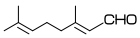
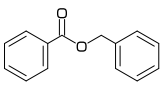
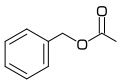
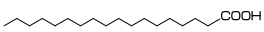
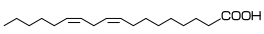
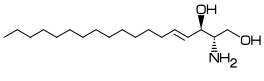
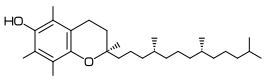
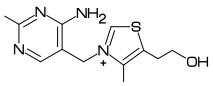
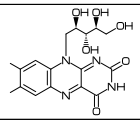
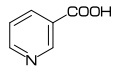
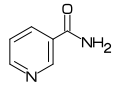
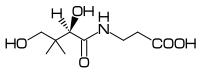
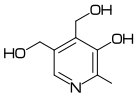
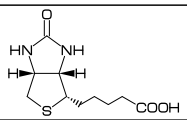
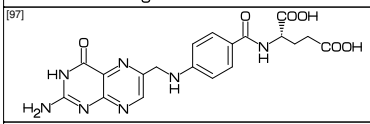
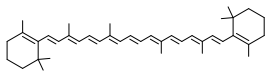
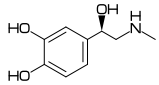
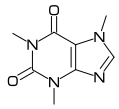
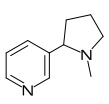
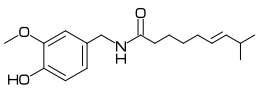
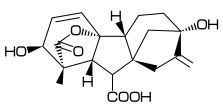
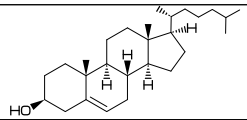
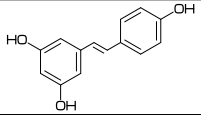
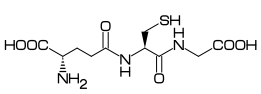
[11] 	L-Serine	amino acid	105.09	105.0925	C3H7NO3
	<30,NH2,!wb,/!OH,!COOH				
[12] 	L-Threonine	amino acid	119.12	119.1191	C4H9NO3
	<30,NH2,!wb,/?'!w'OH,!COOH				
[13] 	L-Cysteine	amino acid	121.16	121.1581	C3H7NO2S
	<30,NH2,!wb,/!SH,!COOH				
[14] 	L-Methionine	amino acid	149.21	149.2113	C5H11NO2S
	<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				

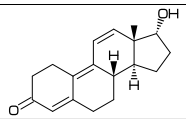
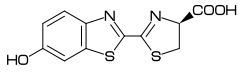
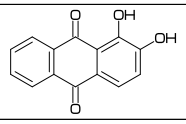
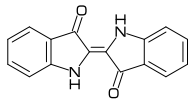
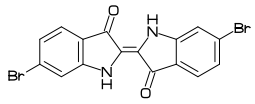
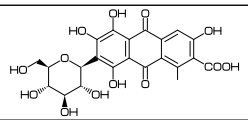
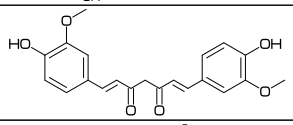
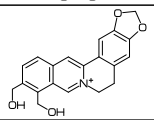
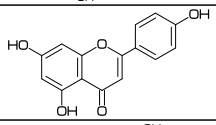
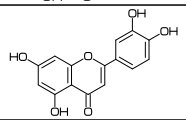
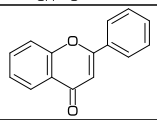
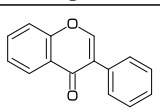
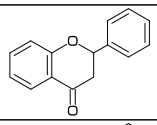
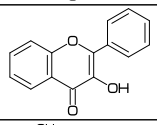
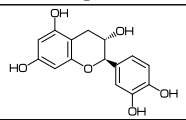
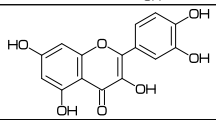
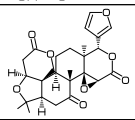
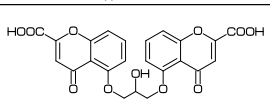
[17] 	L-Triptophan	biological	204.21	204.2251	C11H12N2O2
	<30,NH2,!wb,!COOH,@2,!2,<24,|,?5,2=dr,5=dl,2=Ph,4:NH				
[18] 	L-Proline	amino acid	115.13	115.1304	C5H9NO2
	<18,?5,3:NH,4:*/COOH				
[19] 	L-Glutamine	amino acid	146.15	146.1444	C5H10N2O3
	<30,NH2,!wb,!COOH,@2,!2‘1,!?O!,NH2				
[20] 	L-Asparagine	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	148.1140	C5H8O5
	<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				

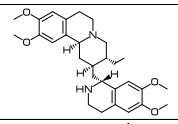
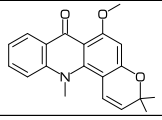
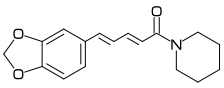
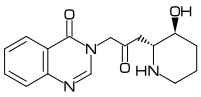
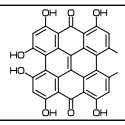
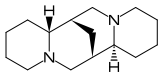
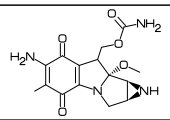
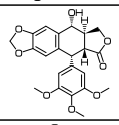
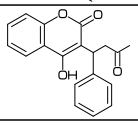
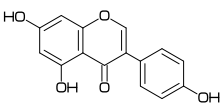
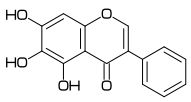
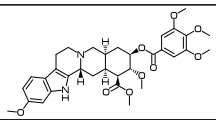
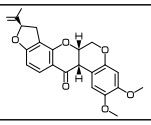
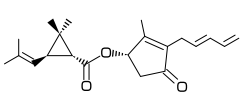
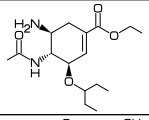
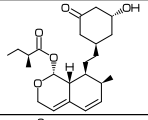
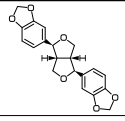
[35] 	Succinate	biological	118.09	118.0880	C4H6O4
	<30,COOH,!3,COOH				
[36] 	Fumarate	biological	116.07	116.0721	C4H4O4
	<30,COOH,!!d,!COOH				
[37] 	Malate	biological	134.09	134.0874	C4H6O5
	<30,COOH,!3,COOH,3:/OH				
[38] 	Oxaloacetate	biological	132.07	132.0715	C4H4O5
	<30,COOH,!,?O!2,COOH				
[39] 	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				

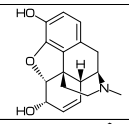
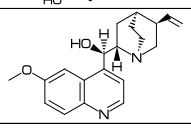
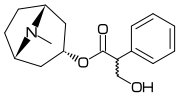
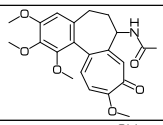
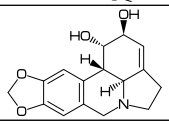
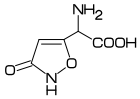
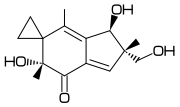
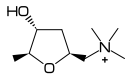
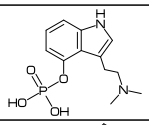
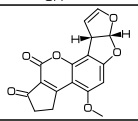
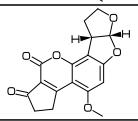
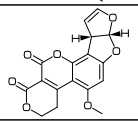
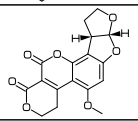
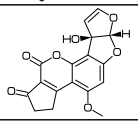
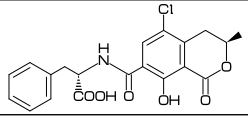
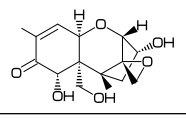
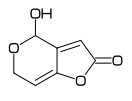
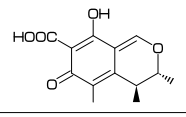
[53] 	Maltose	sugar	342.3	342.2964	C12H22O11
	`hexose_hp,#.5,{1^$270'2^$90'3^$270}:/OH,6^$90:/!OH,##, @4,$310~arc_lb‘1,O,$50~arc_br‘1,<$0, |,hexose_hp,#.5,{2^$90'3^$270'4^$270}:/OH,6^$90:/!OH`				
[54] 	Lactose	sugar	342.3	342.2964	C12H22O11
	`hexose_hp,#.5,{1^$90'2^$90'3^$270}:/OH,6^$90:/!OH,##, @4,$0~arc_ltr,O,$0~arc_lbr, |,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,O,$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,O,&10~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`				

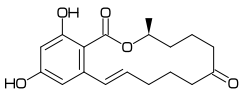
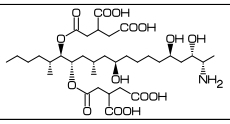
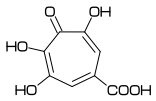
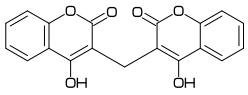
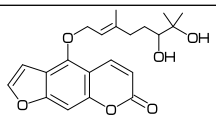
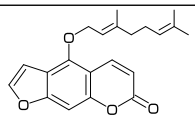
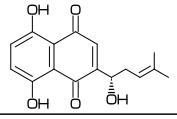
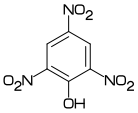
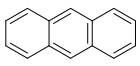
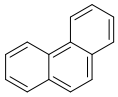
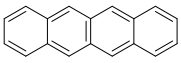
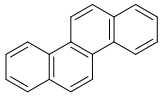
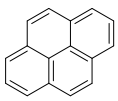
[71] 	delta-Terpinene	biological	136.24	136.2340	C10H16
	<30,?6,3://?!,6:?,5=db				
[72] 	Eugenol	biological	164.20	164.2010	C10H12O2
	<30,Ph,1:/OH,6:/O!,4:/!'!d				
[73] 	Thymol	biological	150.22	150.2175	C10H14O
	<30,Ph,4:/OH,3:/?!,6:?				
[74] 	Anisaldehyde	biological	136.15	136.1479	C8H8O2
	<30,Ph,4:/CHO,1:/O!				
[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	212.2438	C14H12O2
	<30,Ph,@4,!?O!,O!,!,Ph				
[85] 	Benzyl-benzoate	biological	212.25	150.1744	C9H10O2
	<30,Ph,4:/!O!'?O!				
[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				

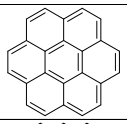
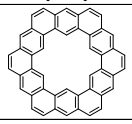
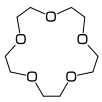
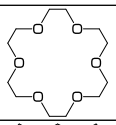
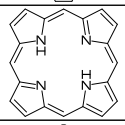
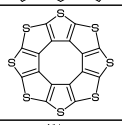
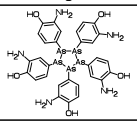
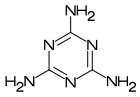
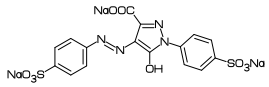
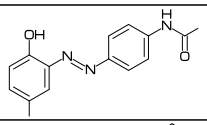
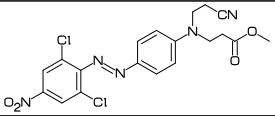
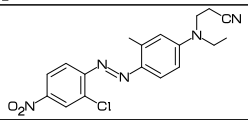
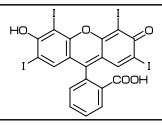
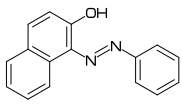
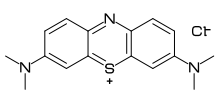
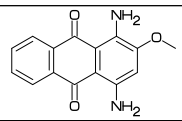
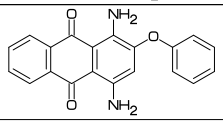
[89] 	Tocopherol	biological	430.717	430.7060	C29H50O2
	<30,Ph,3=?6,7:O,1'2'5:?,8:?z^60,6:/OH,@8,!,|,!12,4'8:?z,12:?				
[90] 	Thiamine	biological	265.35	265.3545	C12H17N4OS
	<30,Ph,4:/NH2,@3,!'1,!,<-12,?5,-1'-4=dl,1'5'8:N,11:S,6'9:?, -3^-12:/!2'OH,8:p_^72				
[91] 	Riboflavin	biological	376.37	376.3638	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,-4=?5,-3=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				

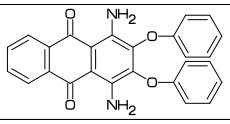
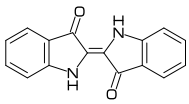
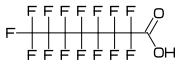
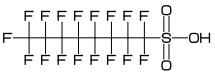
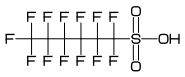
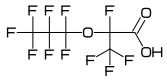
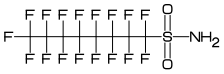
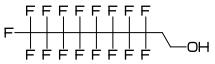
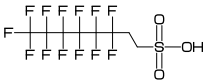
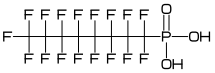
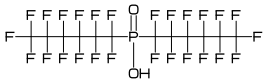
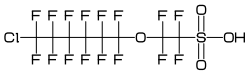
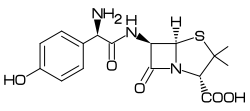
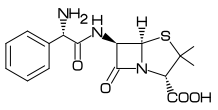
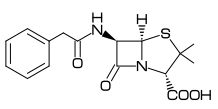
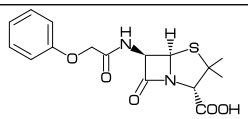
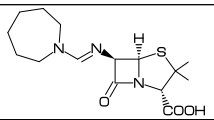
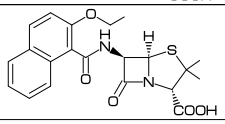
[107] 	Trenbolone	biological	270.37	270.3660	C18H22O2
	<30,?6,3'10=?6,13=?5,2'11'15=dl,1:?O,12:?w^60,-1:/*OH,{9^60'*11^-60}:*/H				
[108] 	Luciferin	biological	280.33	280.3228	C11H8N2O3S2
	<30,Ph,3=?5,@8,!,?5,9'16=dl,9'14:N,7'11:S,1:/OH,-2:*/COOH				
[109] 	Alizarin	biological	240.21	240.2109	C14H8O4
	<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,|,-1=?6,3=dl,1:O,4:?O,2:/COOH, @$2,!,O!2,/OH,!2,O,60,Ph,|,-5=?6,3=dl,4:O,1:?O,3:/COOH				

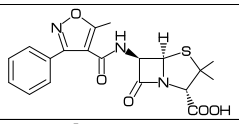
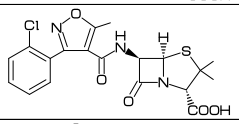
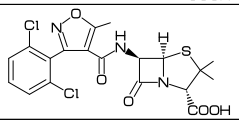
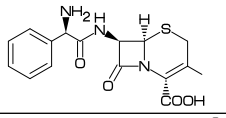
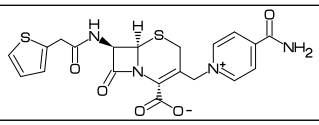
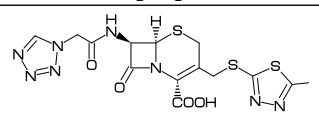
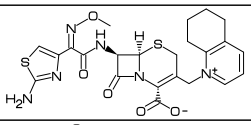
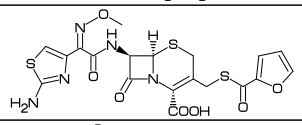
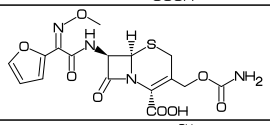
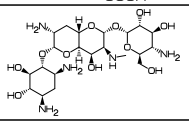
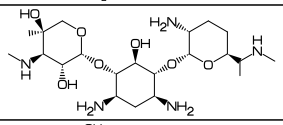
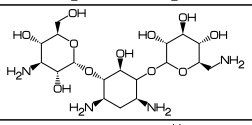
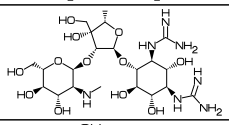
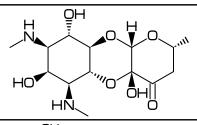
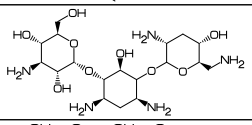
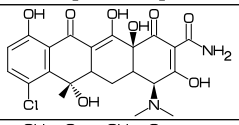
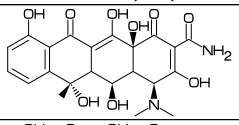
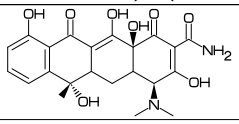
[125] 	Emetine	biological	480.649	480.6388	C29H40N2O4
	<30,Ph,-4'-4=?6,8:N,1'6:/O!,-2:/*!,7'12:/*H^-60, @-3,!,!zb,<-60,|,?6,5=dl,2:NH,-6^-60:*/H,|,-2=?6,2'4=dl,-2'-3:/O!				
[126] 	Acronycine	biological	321.376	321.3697	C20H19NO3
	<30,Ph,|,-4=?6,1:N?,4:?O,-3=Ph2,-1:/O!,|,-4=?6,2=dl,4:O,3:??				
[127] 	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,-3=?6,-3=?5,-2:O,-1=wb,-3:?O, @10,!z,Ph,-2'-3'-4:/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'1,60,!,?O!				
[135] 	Genistein	biological	270.24	270.2368	C15H10O5
	<30,Ph,3=?6,9=dl,10:O,2'6:/OH,7:?O,8:/Ph'(-3:/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,-2=dl,-1:?,-3:?O,@-2,!5,-1'-3=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^-12:*/Ph'(4=?5)'(7'9:O),8^-12:*/Ph'(4=?5)'(7'9:O)				

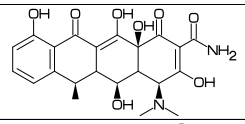
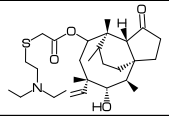
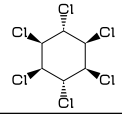
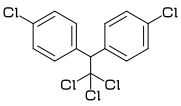
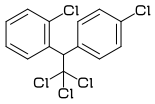
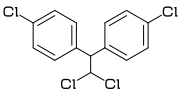
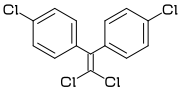
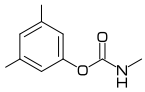
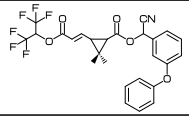
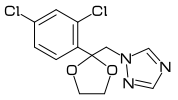
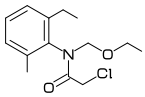
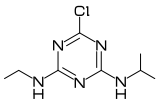
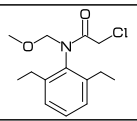
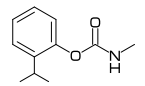
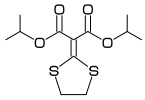
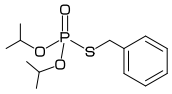
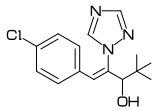
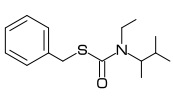
[143] 	Morphine	biological	285.343	285.3376	C17H19NO3
	<30,Ph,2'-4=?6,1---12=?5,-1:O,-1=zb, @7,60~wf'0.75,70~si_'1.3,45,N?,&9~wb,15=dl,6:/OH,8^180:*/H,12:/*OH				
[144] 	Quinine	biological	324.424	324.4167	C20H24N2O2
	<30,Ph,3=Ph,7:N,6:/O!, @10,!,*/OH,/*H^-60,!,|,?6,2:N,1^60:*/H,4:*/!d,@2,165~zf,60,&5~zb				
[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] 	Ochratoxin A	mycotoxin	403.813	403.8130	C20H18ClNO6
	<30,Ph,@4,!2,/*COOH,!'1.2,NH,!'1.2,?O!,Ph,-2:/Cl,-5:/OH,-4=?6,-3:O,-2:?w,-4:?O				
[158] 	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				
[159] 	Patulin	mycotoxin	154.12	154.1201	C7H6O4
	<30,?6,3=?5,2'10=dl,6'7:O,5:/OH,8:?O				
[160] 	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				

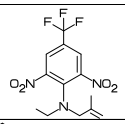
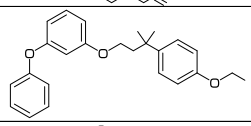
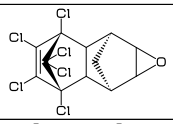
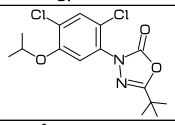
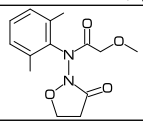
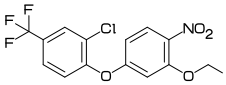
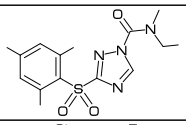
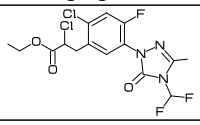
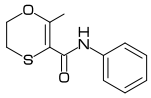
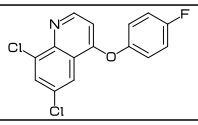
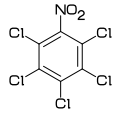
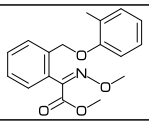
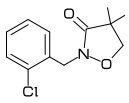
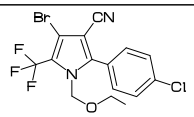
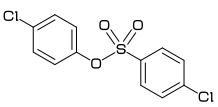
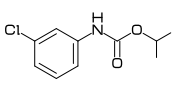
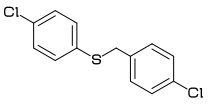
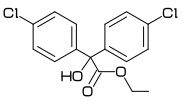
[161] 	Zearalenone	mycotoxin	318.364	318.3642	C18H22O5
	<30,Ph,@3,#1,!6,60,60,!4,&4,##,1’5’8=dl,17:O,16:?w,1’5:/OH,12’18:?O				
[162] 	Fumonisin B1	mycotoxin	721.83	721.8299	C34H59NO15
	<30,!19,@6,!w,O!,?O!2,/COOH,!2,COOH,@7,!z‘1.2,O!,?O!2,/COOH,!2,COOH, 5’9:?z,11’16’*18:*/OH,19:/*NH2				
[163] 	Puberulic acid	mycotoxin	198.13	198.1296	C8H6O6
	<38.5,?7,2’4’7=db,3:/COOH,1’5’7:/OH,6:?O				
[164] 	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				
[165] 	Dihydroxybergamotin	biological	338.40	372.4116	C21H24O6
	<30,Ph,3=?6,6=?5,10’13=db,7’13:O,8:?O,@5,!O,!2,!d,?,!3,/OH,!??,!OH				
[166] 	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,?!				
[167] 	Alkannin	biological	288.29	288.2952	C16H16O5
	<30,Ph,3=?6,9=db,2’5:/OH,7’10:?O,@8,!,/*OH,!2,!d,?!				
[168] 	Benzene	synthetic	78.11	78.11184	C6H6
	<30,Ph				
[169] 	Phenol	synthetic	94.11	94.11123	C6H6O
	<30,Ph,3:/OH				
[170] 	Aniline	synthetic	93.13	93.12648	C6H7N
	<30,Ph,3:/NH2				
[171] 	Picric acid	synthetic	229.10	229.1039	C6H3N3O7
	<30,Ph,1’3’5:/NO2,2:/OH				
[172] 	Hexaphenylbenzene	synthetic	534.6876	534.6875	C42H30
	<30,Ph,1’2’3’4’5’6:/Ph				
[173] 	Naphthalene	aromatic	128.17	128.1705	C10H8
	<30,Ph,3=Ph				
[174] 	Anthracene	aromatic	178.23	178.2291	C14H10
	<30,Ph,3’6=Ph				
[175] 	Phenanthrene	aromatic	178.23	178.2291	C14H10
	<30,Ph,4’6=Ph				
[176] 	Naphthacene	aromatic	228.3	228.2878	C18H12
	<30,Ph,6’3’-3=Ph				
[177] 	Chrysene	aromatic	228.3	228.2878	C18H12
	<30,Ph2,6’4’-4=Ph				
[178] 	Pyrene	aromatic	202.25	202.2505	C16H10
	<30,Ph2,6’4=Ph,16---7=?6,-2=dl				

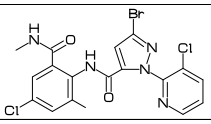
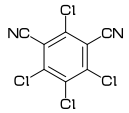
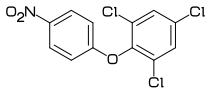
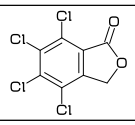
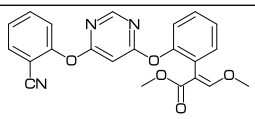
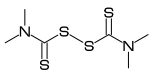
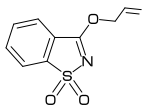
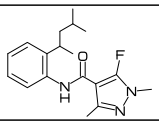
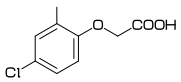
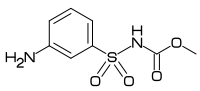
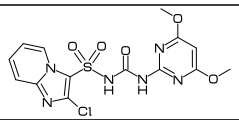
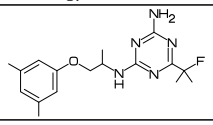
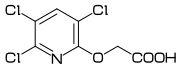
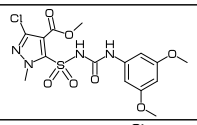
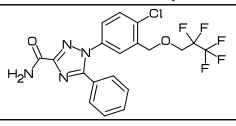
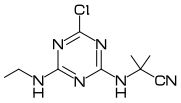
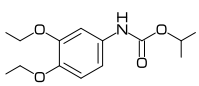
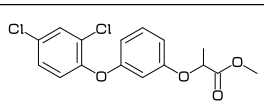
[179] 	Coronene	aromatic	300.35	300.3520	C24H12
	<30,Ph,{1’11--2’15--3’19--4’23--5’27---7}=?6,9’12’14’17’20’22’25’28’30=dl				
[180] 	Kekulene	aromatic	600.7	600.7041	C48H24
	<30,?6,3’-3’-2’-3’-2’-3’-2’-3’-2’-3’(-2----5)’(5----␣-4)=?6, 1’*5’7’9’11’13’17’19’21’23’27’29’31’33’37’39’41’43’47’49’51’53’57’60=dl				
[181] 	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				
[182] 	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				
[183] 	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				
[184] 	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				
[185] 	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				
[186] 	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)				
[187] 	Melamine	synthetic	126.12	126.1199	C3H6N6
	<30,Ph,2’4’6:N,1’3’5:/NH2				
[188] 	Tartrazine	pigment	534.3	534.3633	C16H9N4Na3O9S2
	<30,Ph,1:/SO3Na,@4,!N,!d,N!,<-12,?5,-2’-5=dl,-2’-3:N,-1:/COONa,-4:/OH, -3:/Ph’(4:/SO3Na)				
[189] 	Disperse yellow 3	pigment	269.30	269.2985	C15H15N3O2
	<30,Ph,2:?,5:/OH,@4,!N,!d,N,!Ph,-3:/NH!’?O!				
[190] 	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!				
[191] 	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				
[192] 	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				
[193] 	Sudan red 1	pigment	248.28	248.2792	C16H12N2O
	<30,Ph,1=Ph,4:/OH,@3,!N,!d,N,!Ph				
[194] 	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				
[195] 	Disperse red 11	pigment	268.274	268.2673	C15H12N2O3
	<30,Ph,3=?6,-3=dr,9=Ph,7’10:?O,-1’-4:/NH2,-2:/O!				
[196] 	Disperse red 60	pigment	331.326	330.3367	C20H14N2O3
	<30,Ph,3=?6,-3=dr,9=Ph,7’10:?O,-1’-4:/NH2,-2:/O!’Ph				

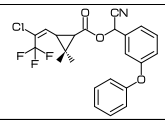
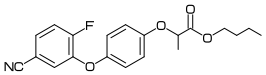
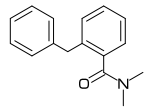
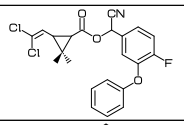
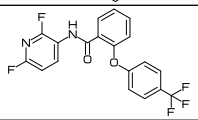
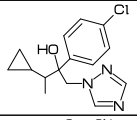
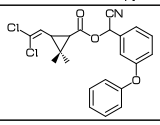
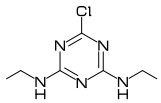
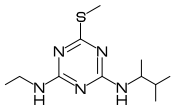
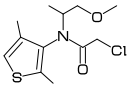
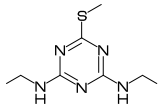
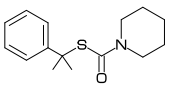
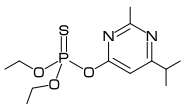
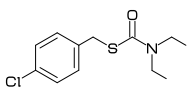
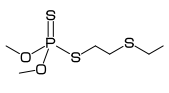
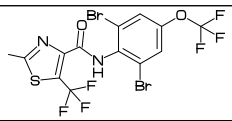
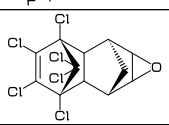
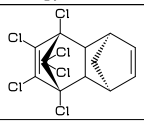
[197] 	Disperse violet 26	pigment	422.438	422.4321	C26H18N2O4
	<30,Ph,3=?6,-3=dr,9=Ph,7'10:?O,-1'-4:/NH2,{-2>-30'-3>30}:/O!'Ph				
[198] 	Vat blue 1	pigment	262.27	262.2627	C16H10N2O2
	<30,Ph,3=?5,@8,!d,?5,-3=dr,-3=Ph,7'14:NH,9'11:?O				
[199] 	PFOA	pfas	414.07	414.0683	C8HF15O2
	0,0,0,0,0,0,0,?O,-60,OH,{1^-90'1:7}:/F,{1:7}:/F^180				
[200] 	PFOS	pfas	500.13	500.1295	C8HF17O3S
	0,0,0,0,0,0,0,0,S,?O,?O^-180,-.1,OH,{1^-90,1:8}:/F,{1:8}:/F^180				
[201] 	PFHxS	pfas	400.12	400.1145	C6HF13O3S
	0,0,0,0,0,0,S,?O,?O^-180,-.1,OH,{1^-90'1:6}:/F,{1:6}:/F^180				
[202] 	GenX	pfas	330.05	330.0527	C6HF11O3
	0,0,0,O,0,0'1,?O,-60,OH,{1^-90,1:3}:/F,{1:3'5}:/F^180,5:/?F?F!F				
[203] 	FOSA	pfas	499.15	499.1447	C8H2F17NO2S
	0,0,0,0,0,0,0,0,S,?O,?O^-180,-.1,NH2,{1^-90'1:8}:/F,{1:8}:/F^180				
[204] 	8,2-FTOH	pfas	464.12	464.1189	C10H5F17O
	0,0,0,0,0,0,0,0,-60,60,OH,{1^-90'1:8}:/F,{1:8}:/F^180				
[205] 	6,2-FTS	pfas	428.16	428.1676	C8H5F13O3S
	0,0,0,0,0,0,-60,60,S,?O,?O^-180,-.1,OH,{1^-90'1:6}:/F,{1:6}:/F^180				
[206] 	PFOPA	pfas	500.13	500.0462	C8H2F17O3P
	0,0,0,0,0,0,0,0,P,?O,/OH^-179.8,-.1,OH,{1^-90'1:8}:/F,{1:8}:/F^180				
[207] 	6,6-FPi	pfas	702.06	702.0673	C12HF26O2P
	0,0,0,0,0,0,P,0,0,0,0,0,0,7^180:?O,7'1.5:/OH, {1^-90,1:6'8:13,13^90,13^-90}:/F,{1:6'8:12}:/F^180				
[208] 	9Cl-PF3ONS	pfas	532.58	532.5835	C8HClF16O4S
	0,0,0,0,0,0,0,0,0,0,S,?O,?O^-180,-.1,OH, {1:6'8'9}:/F,{1:6'8'9}:/F^180,1^-90:/Cl				
[209] 	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				
[210] 	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				
[211] 	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				
[212] 	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				
[213] 	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				
[214] 	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				

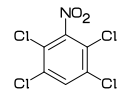
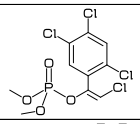
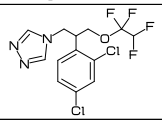
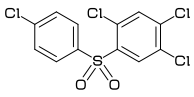
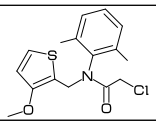
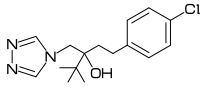
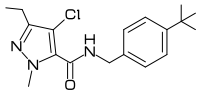
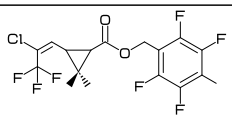
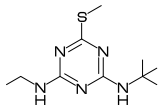
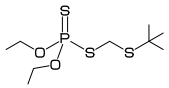
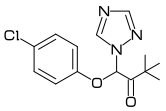
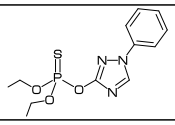
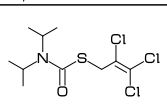
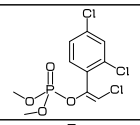
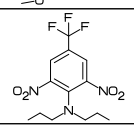
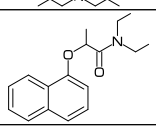
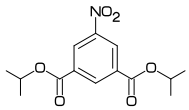
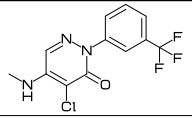
[215] 	Oxacillin	antibiotics	401.4363	401.4362	C19H19N3O5S
	<45,?4,2=?5,2:N,7:S,3^45:/*H,1:?O^15,5:/*COOH,6:??, @4,15~wf,NH!,?O!,<-24,?5,-2'-5=dl,-2:N,-3:O,-4:?,@-1,-24,Ph				
[216] 	Cloxacillin	antibiotics	435.8813	435.8813	C19H18ClN3O5S
	<45,?4,2=?5,2:N,7:S,3^45:/*H,1:?O^15,5:/*COOH,6:??, @4,15~wf,NH!,?O!,<-24,?5,-2'-5=dl,-2:N,-3:O,-4:?,@-1,-24,Ph,-5:/Cl				
[217] 	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,-2'-5=dl,-2:N,-3:O,-4:?,-1^-24:/Ph'(2'6:/Cl)				
[218] 	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				
[219] 	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				
[220] 	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'-2'-3'-5:N, @6,!2,S,!,?5,-3'-5=dl,-1:S,-2:?,-3'-4:N				
[221] 	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,-2'-5=dl,-3:S,-1:N,-2:/NH2, @6,!2,Ph,-2=?6,-10:N,-10:p_^180				
[222] 	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,-2'-5=dl,-3:S,-1:N,-2:/NH2, @6,!2,S,!?O!,?5,-1'-3=dl,-4:O				
[223] 	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,-1'-3=dl,-4:O,@6,!2,O!,?O!,NH2				
[224] 	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				
[225] 	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!				
[226] 	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				
[227] 	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				
[228] 	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!				
[229] 	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				
[230] 	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				
[231] 	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				
[232] 	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				

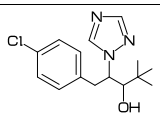
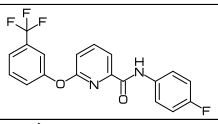
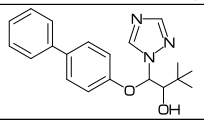
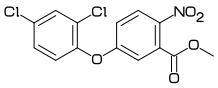
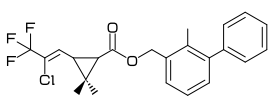
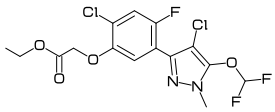
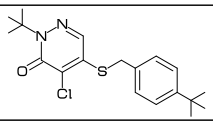
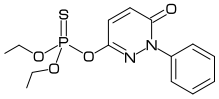
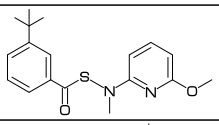
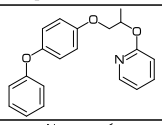
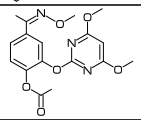
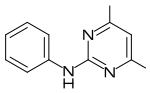
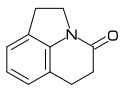
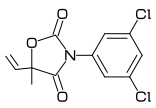
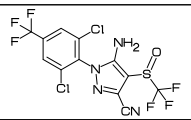
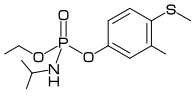
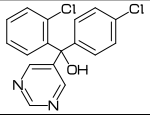
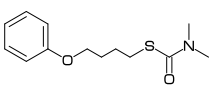
[233] 	Doxycyclin	antibiotics	444.43	444.4345	C22H24N2O8
	<30,Ph,-4’-3’-3=?6,16’19=dl,10’18:?O,7:?w, {5’13~wf^60’11~wf’14’16}:/OH,15:*/N?!,17:/?O!’NH2				
[234] 	Tiamulin	antibiotics	493.74	493.7420	C28H47NO4S
	<-45.5,?8,-3=?5,@8,#.8,-210~zf,?^60,45,56,##,&6~zb, {3^-45’5’8}:?w,@3,30~zf,!d,4:/*OH,11:?O,7:*/H^60, @1,15,O!,?O!2,S,60,60,-60,N?2,!2				
[235] 	BHC	pesticide	290.83	290.8298	C6H6Cl6
	<30,?6,1’*2’3’4’*5’6:*/Cl				
[236] 	pp-DDT	pesticide	354.49	354.4862	C14H9Cl5
	<30,Ph,6:/Cl,@3,!,/?Cl?Cl!Cl,!Ph,-3:/Cl				
[237] 	op-DDT	pesticide	354.49	354.4862	C14H9Cl5
	<30,Ph,4:/Cl,@3,!,/?Cl?Cl!Cl,!Ph,-3:/Cl				
[238] 	pp-DDD	pesticide	320	320.0412	C14H10Cl4
	<30,Ph,6:/Cl,@3,!,/?Cl!Cl,!Ph,-3:/Cl				
[239] 	pp-DDE	pesticide	318	318.0253	C14H8Cl4
	<30,Ph,6:/Cl,@3,!,//?Cl!Cl,!Ph,-3:/Cl				
[240] 	XMC	pesticide	179.2	179.2157	C10H13NO2
	<30,Ph,1’5:?,@3,!O!,?O!,NH!				
[241] 	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				
[242] 	Azaconazole	pesticide	300.139	300.1406	C12H11Cl2N3O2
	<30,Ph,4’6:/Cl,@3,!3,?5,-2’-4=dl,-2’-4’-5:N,@7,?5,-1’-4:O				
[243] 	Acetochlor	pesticide	269.769	269.7671	C14H20ClNO2
	<30,Ph,2:?,4:/!,@3,!N,/?O!2’Cl,!2,O!2				
[244] 	Atrazine	pesticide	215.7	215.6832	C8H14ClN5
	<30,Ph,2’4’6:N,5:/Cl,1:/NH!2,3:/NH’!?!				
[245] 	Alachrol	pesticide	269.8	269.7671	C14H20ClNO2
	<-30,!,O!2,N,/Ph’(-5’-1:/!),!,?O!2,Cl				
[246] 	Isoprcarb	pesticide	193.246	193.2423	C11H15NO2
	<30,Ph,2:/?!,3:/O!’?O!’NH!				
[247] 	Isoprothiolane	pesticide	290.4	290.3989	C12H18O4S2
	<30,!?!,O!,?O!,//?5’(2’5:S),!?O,!O,!?!				
[248] 	Iprobenfos	pesticide	288.34	288.3428	C13H21O3PS
	<30,!?!,O!,P,?O,/O’!?!^170,!,S,!2,Ph				
[249] 	Uninnazole-P	pesticide	291.779	291.7759	C15H18ClN3O
	<30,Ph,6:/Cl,@3,!!d,!,/OH,!,??!,@8,!,|,?5,2’4=dl,1’2’4:N				
[250] 	Esprocarb	pesticide	265.4	265.4142	C15H23NOS
	<30,Ph,@3,!2,S!,?O!,N?2,!,?!,?!				

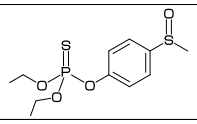
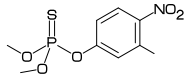
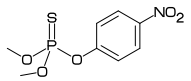
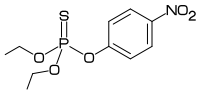
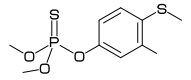
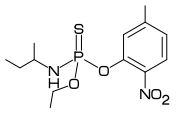
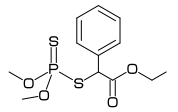
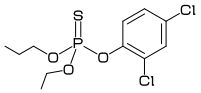
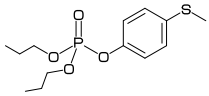
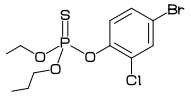
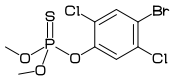
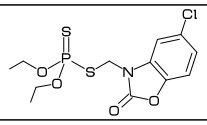
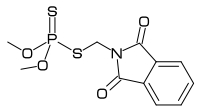
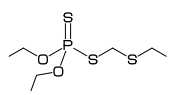
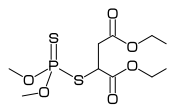
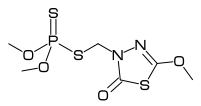
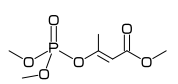
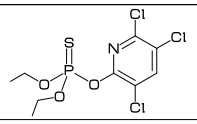
[251] 	Ethalfluralin	pesticide	333.3	333.2631	C13H14F3N3O4
	<30,Ph,1'3:/NO2,5:/?F?F!F,@2,!'1.1,/!,N,!2,?,!d				
[252] 	Ethofenprox	pesticide	376.5	376.4880	C25H28O3
	<30,Ph,@5,!O!,Ph,@10,!,O!3,??,!Ph,-3:/O!2				
[253] 	Endrin	pesticide	380.91	380.9093	C12H8Cl6O
	<30,?6'1.3,3=?6,6=dl,9=?3,-1:O, @2,210~wf'1.5,&5~wb,@7,210~zf'1.5,&10~zb,{1'2'5'6'12^-210'12^-150}:/Cl				
[254] 	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:/??!				
[255] 	Oxadixyl	pesticide	278.3	278.3037	C14H18N2O4
	<30,Ph,2'4:?,@3,!N,!1,?O!2,O!,@7,!,|,?5,1:N,2:O,5:?O				
[256] 	Oxyfluorfen	pesticide	361.701	361.7003	C15H11ClF3NO4
	<30,Ph,6:/?F?F!F,4:/Cl,@3,!O!,Ph,-3:/NO2,-4:/O!2				
[257] 	Cafenstrole	pesticide	350.4	336.4092	C15H20N4O3S
	<30,Ph,2'4'6:?,@3,!,S?O?O,!,|,?5,2'5=dl,2'4'5:N,-2:/?O!'N?'!2				
[258] 	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,-4:?O,-3:/?F!F,-2:?				
[259] 	Carboxin	pesticide	235.301	235.3021	C12H13NO2S
	<30,?6,3=dl,2:S,5:O,4:?,@3,!?O,!NH!,Ph				
[260] 	Quinoxyfen	pesticide	308.13	308.1345	C15H8Cl2FNO
	<30,Ph,4=Ph,10:N,2'6:/Cl,@7,!O!,Ph,-3:/F				
[261] 	Quitozene	pesticide	295.3	295.3347	C6Cl5NO2
	<30,Ph,1'2'3'4'6:/Cl,5:/NO2				
[262] 	Kresoxim-Methyl	pesticide	313.348	313.3477	C18H19NO4
	<30,Ph,@3,!,/?O!'O!,!d,N,!O!,@4,!2,O,!Ph,-1:?				
[263] 	Clomazone	pesticide	239.7	239.6980	C12H14ClNO2
	<30,Ph,2:/Cl,@3,!2,|,?5,1:N,2:O,-2:??,-1:?O				
[264] 	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'(-3:/Cl)				
[265] 	Chlorfenson	pesticide	303.153	303.1611	C12H8Cl2O3S
	<30,Ph,@3,!O!,S?O?O,!Ph,6'12:/Cl				
[266] 	Chlorpropham	pesticide	213.7	213.6607	C10H12ClNO2
	<30,Ph,6:/Cl,@4,!NH!,?O!,O,!?!				
[267] 	Chlorbenside	pesticide	269.183	269.1894	C13H10Cl2S
	<30,Ph,@3,!,S,!2,Ph,6'12:/Cl				
[268] 	Chlorobenzilate	pesticide	325.2	325.1865	C16H14Cl2O3
	<30,Ph,@3,!,/OH^-35,/?O!'O!2^30>lr,!Ph,6'11:/Cl				

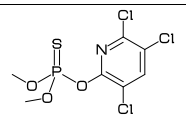
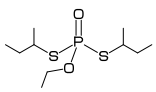
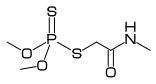
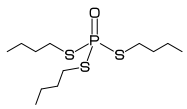
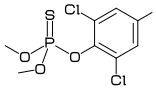
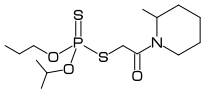
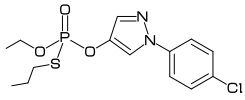
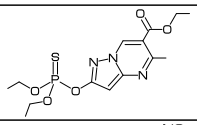
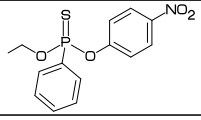
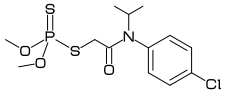
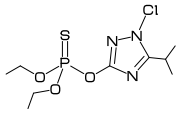
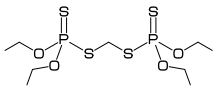
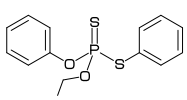
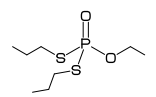
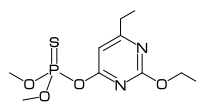
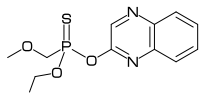
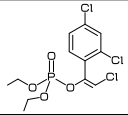
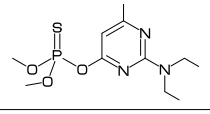
[269] 	Chlorantraniliprole	pesticide	483.15	483.1460	C18H14BrCl2N5O2
	<30,Ph,1:/Cl,3:?,@5,!?O,60,NH!,@4,!NH!,?O!,<24,?5,-1’-3=db,-3’-4:N,-2:/Br, @-4,24,Ph,-5:N,-1:/Cl				
[270] 	Chlorothalonil	pesticide	265.9	265.911	C8Cl4N2
	<30,Ph,4’6:/CN,1’2’3’5:/Cl				
[271] 	Chlornitrofen	pesticide	318.5	318.5399	C12H6Cl3NO3
	<30,Ph,6:/NO2,@3,!O!,Ph,-1’-3’-5:/Cl				
[272] 	Fthalide	pesticide	271.9	271.9122	C8H2Cl4O2
	<30,Ph,3=?5,8:O,9:?O,1’2’5’6:/Cl				
[273] 	Azoxystrobin	pesticide	403.4	403.3874	C22H17N3O5
	<30,Ph,2:/CN,@3,!O!,Ph,-1’-3:N,@-4,!O!,Ph,@-5,!,/?O!’O!,!d,!O!				
[274] 	Thiuram	pesticide	240.43	240.4328	C6H12N2S4
	<30,!,N?!,?S,!,S,!,S,!,?S,!,N?!				
[275] 	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				
[276] 	Penflufen	pesticide	317.41	317.4010	C18H24FN3O
	<30,Ph,@3,!NH!,?O!,?5,-1’-4=db,-2’-3:N,-2’-4:?,-1:/F,@4,!?,60,!?!				
[277] 	MCPA	pesticide	200.62	200.6189	C9H9ClO3
	<30,Ph,1:/Cl,5:?,4:/O!2’COOH				
[278] 	Asulam	pesticide	230.2	230.2409	C8H10N2O4S
	<30,Ph,1:/NH2,@3,!,S?O?O,!NH!,?O!,O!				
[279] 	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,-1’-5:N,-2’-4:/O!				
[280] 	Triaziflam	pesticide	333.4	333.4037	C17H24FN5O
	<30,Ph,2’6:?,@4,!,O!2,?!,NH!,Ph,-1’-3’-5:N,-2:/NH2,-4:/??’!F				
[281] 	Trichlopyr	pesticide	256.47	256.4705	C7H4Cl3NO3
	<30,Ph,2:N,1’4’6:/Cl,3:/O!2’COOH				
[282] 	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!				
[283] 	Flupoxam	pesticide	460.8	460.7850	C19H14ClF5N4O2
	<30,Ph,4:/Cl,@1,!,?5,-2’-4=db,-2’-4’-5:N,-1:/Ph,-3:/?O!’NH2, @3,!2,O!2,/F^35,/F^-35,!,?F?F!F				
[284] 	Cyanazine	pesticide	240.7	240.6927	C9H13ClN6
	<30,Ph,2’4’6:N,5:/Cl,1:/NH!2,3:/NH!’??’!CN				
[285] 	Diethofencarb	pesticide	267.3	267.3208	C14H21NO4
	<30,Ph,@4,!NH!,?O!,O,!?!,1’6:/O!2				
[286] 	Diclofop-methyl	pesticide	341.2	341.1859	C16H14Cl2O4
	<30,Ph,4’6:/Cl,@3,!O!,Ph,@-4,!O,!?!,?O,!O!				

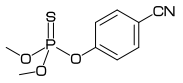
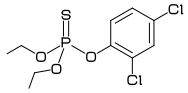
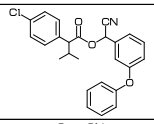
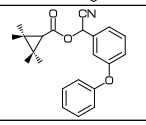
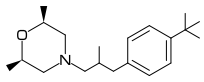
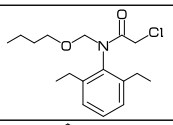
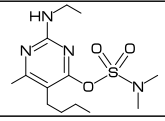
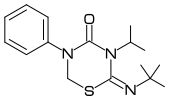
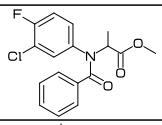
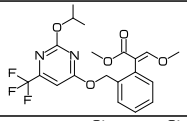
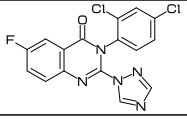
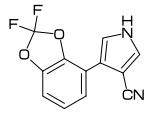
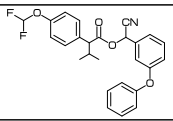
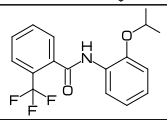
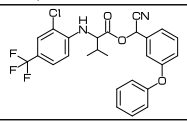
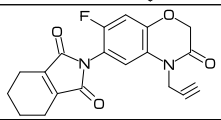
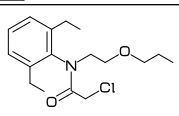
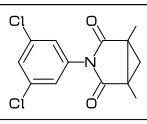
[287] 	Cyhalothrin	pesticide	449.86	449.8500	C23H19ClF3NO3
	<-30,?3,{2^-35'*2^35}:?w,@1,!!d,/?F?F!F,!Cl,@3,!?O,!O!,/CN,!Ph,-4:/O!'Ph>rl				
[288] 	Cyhalofop-Buthyl	pesticide	357.381	357.3754	C20H20FNO4
	<30,Ph,1:/CN,4:/F,@3,!O!,Ph,@-3,!O,!?!,?O!,O,!4				
[289] 	Diphenamid	pesticide	239.3	239.3122	C16H17NO
	<30,Ph,@3,!2,Ph,-5:/?O!'N?!				
[290] 	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				
[291] 	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)				
[292] 	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				
[293] 	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				
[294] 	Simazine	pesticide	201.7	201.6566	C7H12ClN5
	<30,Ph,2'4'6:N,5:/Cl,1:/NH!2,3:/NH!2				
[295] 	Dimethametryn	pesticide	255.4	255.3829	C11H21N5S
	<30,Ph,2'4'6:N,5:/S!,1:/NH!2,3:/NH'!?!'?!				
[296] 	Dimethenamid	pesticide	275.8	275.7948	C12H18ClNO2S
	<-6,?5,3'5=dl,2:S,3'5:?,@4,!,N!,?O!2,Cl,6:/?!2'O!				
[297] 	Simetryn	pesticide	213.3	213.3032	C8H15N5S
	<30,Ph,2'4'6:N,5:/S!,1'3:/NH!2				
[298] 	Dimepiperate	pesticide	263.4	263.3983	C15H21NOS
	<30,Ph,@3,!??,!S!,?O!,?6,-6:N				
[299] 	Diazinon	pesticide	304.35	304.3455	C12H21N2O3PS
	<30,!2,O!,P,?S,/O!2^160>rl,!O!,|,Ph,4'6:N,5:?,3:/?!				
[300] 	Thiobencarb	pesticide	257.776	257.7795	C12H16ClNOS
	<30,Ph,1:/Cl,@4,!2,S!,?O!,N?2,!2				
[301] 	Thiometon	pesticide	246.34	246.3508	C6H15O2PS3
	<-30,!O!,P,?S,/O!^160,!,S!3,S!2				
[302] 	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,-5'-1:/Br,-3:/O!'?F?F!F				
[303] 	Dieldrin	pesticide	380.895	380.9093	C12H8Cl6O
	<30,?6'1.2,3=?6,6=dl,9=?3,-1:O,@2,148~wf'1.4,&5~wb, @7,145~wf'1.3,&10~zb,{1'2'5'6'12^-210'12^-150}:/Cl				
[304] 	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				

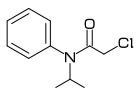
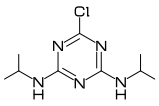
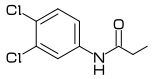
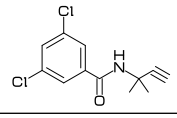
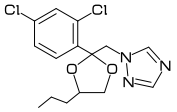
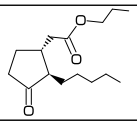
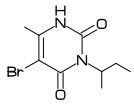
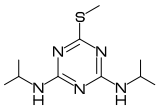
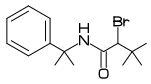
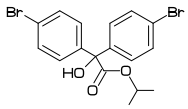
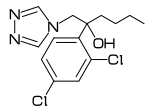
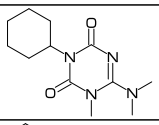
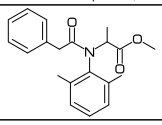
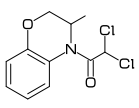
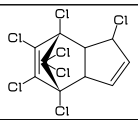
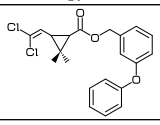
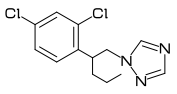
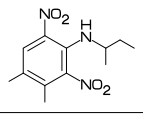
[305] 	Tecnazene	pesticide	260.879	260.8896	C6HCl4NO2
	<30,Ph,{1,3,4,6}:/Cl,5:/NO2				
[306] 	Tetrachlorvinfos	pesticide	365.97	365.9618	C10H9Cl4O4P
	<-30,!O!,P,?O,/O!^160,!O!,/Ph'(2'4'5:/Cl),!d,!Cl				
[307] 	Tetraconazole	pesticide	372.14	372.1455	C13H11Cl2F4N3O
	<-6,?5,2'5=dl,1'2'4:N,@4,!4,O!,/F^35,/F^-35,!,?F!F,7:/Ph'(4'6:/Cl)				
[308] 	Tetradifon	pesticide	356.038	356.0518	C12H6Cl4O2S
	<30,Ph,@3,!,S?O?O,!Ph,6'10'11'13:/Cl				
[309] 	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,				
[310] 	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				
[311] 	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:/??!				
[312] 	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:?				
[313] 	Terbutryn	pesticide	241.4	241.3563	C10H19N5S
	<30,Ph,2'4'6:N,5:/S!,1:/NH!2,3:/NH!'??!				
[314] 	Terbufos	pesticide	288.42	288.4306	C9H21O2PS3
	<30,!2,O!,P,?S,/O!2^160>rl,!,S!2,S!,??!				
[315] 	Triadimefon	pesticide	293.8	293.7487	C14H16ClN3O2
	<30,Ph,6:/Cl,@3,!,O!2,?O!,??!,@8,!,|,?5,2'4=dl,1'2'4:N				
[316] 	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				
[317] 	Triallate	pesticide	304.7	304.6641	C10H16Cl3NOS
	<-30,!?!,N,/?!,!?O!,S!2,/Cl,!d,/Cl,!Cl				
[318] 	Dimethylvinphos	pesticide	331.52	331.5167	C10H10Cl3O4P
	<-30,!O!,P,?O,/O!^160,!O!,/Ph'(2'4:/Cl)'1,!d,!Cl				
[319] 	Trifluralin	pesticide	335.3	335.2790	C13H16F3N3O4
	<30,Ph,1'3:/NO2,5:/?F?F!F,@2,!N,/!2,!3				
[320] 	Napropamide	pesticide	271.4	271.3541	C17H21NO2
	<-30,Ph,4=Ph,@10,!O!,?!,?O!,N?2,!2				
[321] 	Nitrothal-isopropyl	pesticide	295.3	295.2878	C14H17NO6
	<30,Ph,5:/NO2,1'3:/?O!'O!'?!				
[322] 	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)				

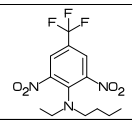
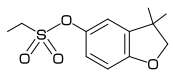
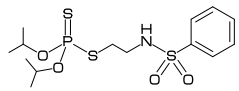
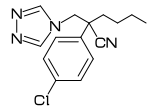
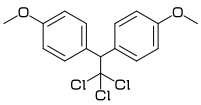
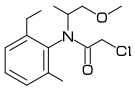
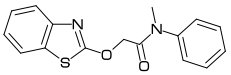
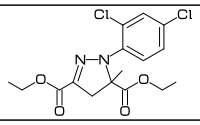
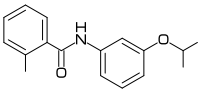
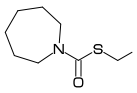
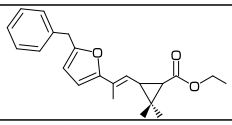
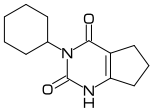
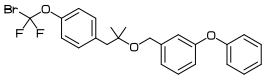
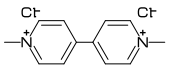
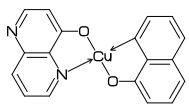
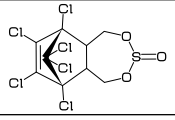
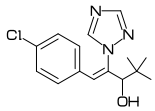
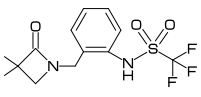
[323] 	Paclobutrazole	pesticide	293.795	293.7917	C15H20ClN3O
	<30,Ph,6:/Cl,@3,!3,/OH,!,??!,@8,!,|,?5,2'4=dl,1'2'4:N				
[324] 	Picolinafen	pesticide	376.331	376.3043	C19H12F4N2O2
	<30,Ph,5:/?F?F!F,@3,!O!,Ph,-5:N,@-4,!?O,!NH!,Ph,-3:/F				
[325] 	Bitertanol	pesticide	337.4	337.4155	C20H23N3O2
	<30,Ph,@3,!Ph,@-3,!,O!2,/OH,!,??!,@14,!,|,?5,2'4=dl,1'2'4:N				
[326] 	Bifenox	pesticide	342.14	342.1309	C14H9Cl2NO5
	<30,Ph,4'6:/Cl,@3,!O!,Ph,-4:/?O!'O!,-3:/NO2				
[327] 	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				
[328] 	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				
[329] 	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:/??!				
[330] 	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				
[331] 	Pyributicarb	pesticide	330.4	330.4444	C18H22N2O2S
	<30,Ph,5:/??!,@3,!?O!,S!,N?!,Ph,-5:N,-4:/O!				
[332] 	Pyriproxyfen	pesticide	321.5	321.3697	C20H19NO3
	<30,Ph,@5,!O!,Ph,@-3,!,O!2,?!,O,-60,Ph,-5:N				
[333] 	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!				
[334] 	Pyrimethanil	pesticide	199.257	199.2517	C12H13N3
	<30,Ph,@3,!NH!,|,Ph,2'6:N,3'5:?				
[335] 	Pyroquilon	pesticide	173.2	173.2111	C11H11NO
	<30,Ph,3=?6,10:N,9:?O,11--4=?5				
[336] 	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)				
[337] 	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				
[338] 	Fenomiphos	pesticide	303.36	303.3574	C13H22NO3PS
	<30,!2,O!,P,?O,/NH'!?!^160,!O!,Ph,-4:?,-3:/S!				
[339] 	Fenarimol	pesticide	331.2	331.1959	C17H12Cl2N2O
	<30,Ph,@3,!2,Ph,4'11:/Cl,7:/OH^30,7^-30:/Ph'(3'5:N)				
[340] 	Fenothiocarb	pesticide	253.4	253.3604	C13H19NO2S
	<30,Ph,@3,!O,!5,S,!?O!,N?!				

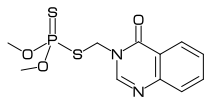
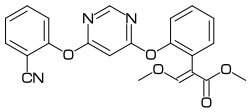
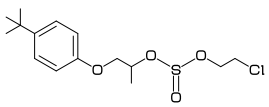
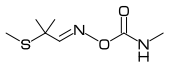
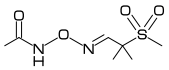
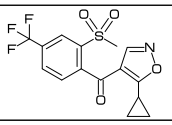
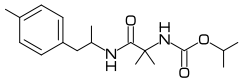
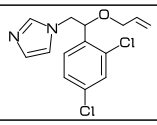
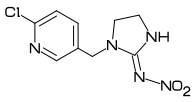
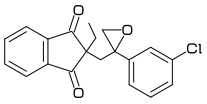
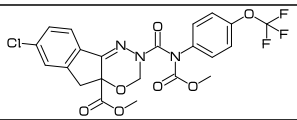
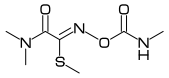
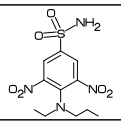
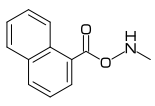
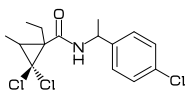
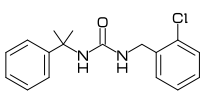
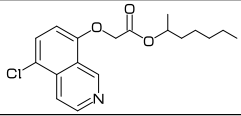
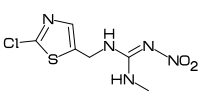
[341] 	Fensulfothion	pesticide	308.35	308.3540	C11H17O4PS2
	<30,!2,O!,P,?S,/O!2^160>rl,!O!,Ph,-3:/S'?O!				
[342] 	Fenitrothion	pesticide	277.23	277.2340	C9H12NO5PS
	<-30,!O!,P,?S,/O!^160,!O!,Ph,-4:?,-3:/NO2				
[343] 	Parathion-methyl	pesticide	263.2	263.2074	C8H10NO5PS
	<-30,!O!,P,?S,/O!^160,!O!,Ph,-3:/NO2				
[344] 	Parathion	pesticide	291.3	291.2606	C10H14NO5PS
	<30,!2,O!,P,?S,/O!2^160>rl,!O!,Ph,-3:/NO2				
[345] 	Fenthion	pesticide	278.33	278.3280	C10H15O3PS2
	<-30,!O!,P,?S,/O!^160,!O!,|,Ph,3:?,4:/S!				
[346] 	Butamifos	pesticide	332.36	332.3556	C13H21N2O4PS
	<-30,!2,?!,NH!,P,?S,/O!2^170>rl,!O!,|,Ph,2:/NO2,5:?				
[347] 	Phenthoate	pesticide	320.358	320.3647	C12H17O4PS2
	<-30,!O!,P,?S,/O!^160,!,S,!,/Ph,!?O!,O!2				
[348] 	Prothyophos	pesticide	329.18	329.1797	C11H15Cl2O3PS
	<-30,!3,O!,P,?S,/O!2^160>rl,!O!,Ph,-5'-3:/Cl				
[349] 	Propaphos	pesticide	304.343	304.3422	C13H21O4PS
	<-30,!3,O!,P,?O,/O!3^160>rl,!O!,Ph,-3:/S!				
[350] 	Profenofos	pesticide	373.6	373.6307	C11H15BrClO3PS
	<30,!2,O!,P,?S,/O!3^160>rl,!O!,Ph,-5:/Cl,-3:/Br				
[351] 	Bromophos	pesticide	365.99	365.9960	C8H8BrCl2O3PS
	<-30,!O!,␣P,?S,/O!^160,!O!,|,Ph,3'6:/Cl,4:/Br				
[352] 	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				
[353] 	Phosmet	pesticide	317.32	317.3210	C11H12NO4PS2
	<-30,!O!,P,?S,/O!^160,!,S,!2,|,?5,3=Ph2,1:N,2'5:?O				
[354] 	Phorate	pesticide	260.4	260.3774	C7H17O2PS3
	<30,!2,O!,P,?S,!,S!2,S!2,4:/O!2^160>rl				
[355] 	Malathion	pesticide	330.35	330.3580	C10H19O6PS2
	<-30,!O!,P,?S,/O!^160,!S!,/!?O!'O!2'1,!?O!,O!2				
[356] 	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!				
[357] 	Mevinphos	pesticide	224.15	224.1482	C7H13O6P
	<-30,!O!,P,?O,/O!^160,!O,!?,!d,!?O!,O!				
[358] 	Chlorpyrifos	pesticide	350.59	350.5863	C9H11Cl3NO3PS
	<30,!2,O!,P,?S,/O!2^160>rl,!O!,|,Ph,6:N,2'4'5:/Cl				

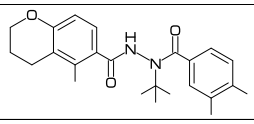
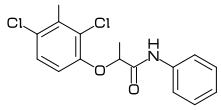
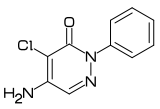
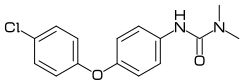
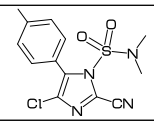
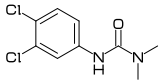
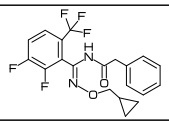
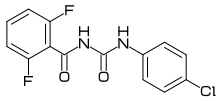
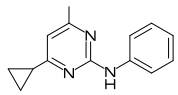
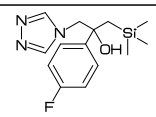
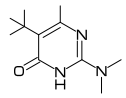
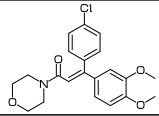
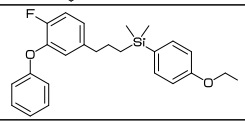
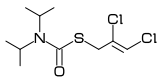
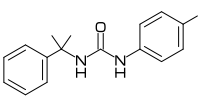
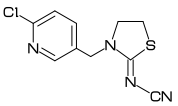
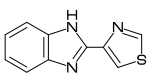
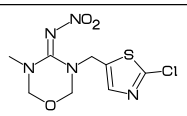
[359] 	Chlorpyrifos-methyl	pesticide	322.53	322.5331	C7H7Cl3NO3PS
	<-30,!O!,P,?S,/O!^160>rl,!O!,|,Ph,6:N,2'4'5:/Cl				
[360] 	Cadusafos	pesticide	270.386	270.3921	C10H23O2PS2
	<-30,!2,?!,S!,P,?O,/O!2^160>rl,!,S,!?,!2				
[361] 	Dimethoate	pesticide	229.25	229.2574	C5H12NO3PS2
	<-30,!O!,P,?S,/O!^160,!,S!2,?O,!NH!				
[362] 	Tribufos	pesticide	314.50	314.5109	C12H27OPS3
	<30,!4,S,!,P,?O,/S'!4^160>rl,!,S,!4				
[363] 	Tolclofos-methyl	pesticide	301.13	301.1266	C9H11Cl2O3PS
	<-30,!O!,P,?S,/O!^160,!O!,|,Ph,2'6:/Cl,4:?				
[364] 	Piperophos	pesticide	353.48	353.4807	C14H28NO3PS2
	<-30,!3,O!,P,?S,/O'!?!^160>rl,!,S!2,?O!,|,?6,1:N,6:?				
[365] 	Pyraclofos	pesticide	360.80	360.7960	C14H18ClN2O3PS
	<30,!2,O!,P,?O,/S!3^160>rl,!O!,<-12,|,?5,1'4=dl,3'4:N,@-3,-12,Ph,-3:/Cl				
[366] 	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				
[367] 	EPN	pesticide	323.303	323.3040	C14H14NO4PS
	<30,!2,O!,P,?S,/Ph^170,!O!,Ph,-3:/NO2				
[368] 	Anilofos	pesticide	367.9	367.8516	C13H19ClNO3PS2
	<-30,!O!,P,?S,/O!^160,!,S,!2,?O!,N,/?!,!Ph,-3:/Cl				
[369] 	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:/?!				
[370] 	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				
[371] 	Edifenphos	pesticide	310.37	310.3714	C14H15O2PS2
	<30,Ph,@3,!O!,P,?S,/O!2>rl^160,!,S,!Ph				
[372] 	Ethoprophos	pesticide	242.33	242.3390	C8H19O2PS2
	<-30,!3,S,!,P,?O,/S!3^160>rl,!,O!2				
[373] 	Ethrimfos	pesticide	292.29	292.2917	C10H17N2O4PS
	<-30,!O!,P,?S,/O!^160,!O!,|,Ph,2'4:N,5:/!,3:/O!2				
[374] 	Quinalphos	pesticide	298.30	298.2978	C12H15N2O3PS
	<30,!,O!2,P,?S,/O!2^160>rl,!O!,|,Ph,3=Ph,2'5:N				
[375] 	Chlorfenvinphos	pesticide	359.58	359.5699	C12H14Cl3O4P
	<30,!2,O!,P,?O,/O!2^160>rl,!O!,/Ph'(2'4:/Cl)'1,!d,!Cl				
[376] 	Pirimiphos-methyl	pesticide	305.333	305.3335	C11H20N3O3PS
	<-30,!O!,P,?S,/O!^160,!O!,Ph,-5'-3:N,-2:?,-4:/N?2'!2				

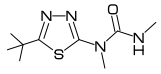
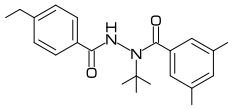
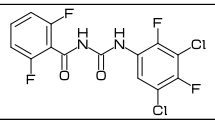
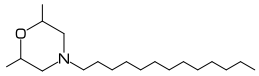
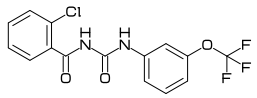
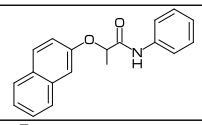
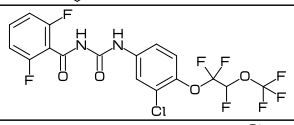
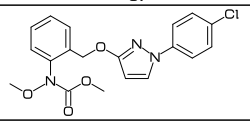
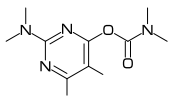
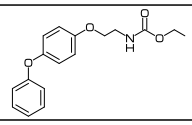
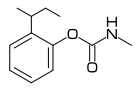
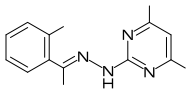
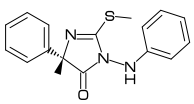
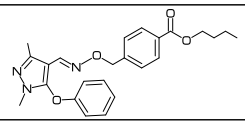
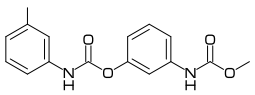
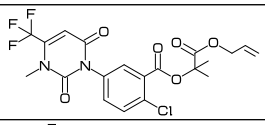
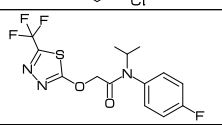
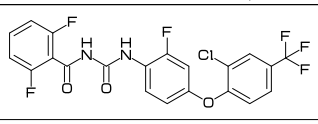
[377] 	Cyanophos	pesticide	243.22	243.2193	C9H10NO3PS
	<-30,!O!,P,?S,/O!^160,!O!,Ph,-3:/CN				
[378] 	Dichlofenthion	pesticide	315.2	315.1531	C10H13Cl2O3PS
	<30,!2,O!,P,?S,/O!2^160>rl,!O!,Ph,-5'-3:/Cl				
[379] 	Fenvalerate	pesticide	419.91	419.9000	C25H22ClNO3
	<30,Ph,6:/Cl,@3,!,/?!,!?O,!O!,/CN,!Ph,-4:/O'!Ph>rl				
[380] 	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				
[381] 	Fenpropimorph	pesticide	303.49	303.4821	C20H33NO
	<30,?6,3:N,6:O,1'5:?w,@3,!,!?,!2,Ph,-3:/??!				
[382] 	Butachlor	pesticide	311.85	311.8468	C17H26ClNO2
	<30,!4,O!2,N,/Ph'(-1'-5:/!)'1,!,?O!2,Cl				
[383] 	Bupirimate	pesticide	316.42	316.4196	C13H24N4O3S
	<30,Ph,4'6:N,1:?,@3,!O!,S?O?O,!,N?!,2:/!3,5:/NH!2				
[384] 	Buprofezin	pesticide	305.4	305.4383	C16H23N3OS
	<-30,?6,1'5:N,1:/Ph,3:S,6:?O,5:/?!,4://N'!??!				
[385] 	Flamprop-methyl	pesticide	335.8	335.7572	C17H15ClFNO3
	<30,Ph,1:/Cl,6:/F,@3,!N,/?O!'Ph>rl,!?!,?O,!O!				
[386] 	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!				
[387] 	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)				
[388] 	Fludioxonil	pesticide	248.2	248.1850	C12H6F2N2O2
	<30,Ph,5=?5,7'9:O,{8^-40'8^40}:/F,@4,!,|,?5,2'5=dl,-2:NH,-4:/CN				
[389] 	Flucythrinate	pesticide	451.5	451.4619	C26H23F2NO4
	<30,Ph,@6,!O!,/F,!,F,@3,!,/?!,!?O,!O!,/CN,!Ph,-4:/O!'Ph>rl				
[390] 	Flutolanil	pesticide	323.3	323.3096	C17H16F3NO2
	<30,Ph,2:/?F?F!F,@3,!?O,!NH!,Ph,-1:/O'!?!				
[391] 	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				
[392] 	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				
[393] 	Pretilachlor	pesticide	311.85	311.8468	C17H26ClNO2
	<30,Ph,2'4:/!,@3,!N,/?O!2'Cl'1,!3,O!3				
[394] 	Procymidone	pesticide	284.136	284.1379	C13H11Cl2NO2
	?6,1:N,@3,&5,2'6:?O,3'5:?,1:/Ph'(3'5:/Cl)				

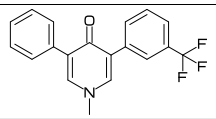
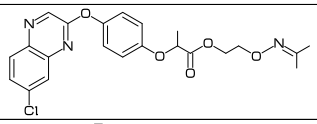
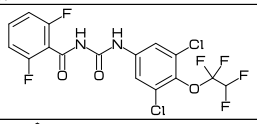
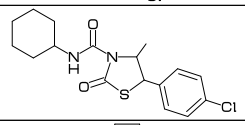
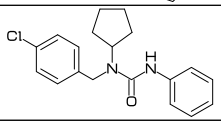
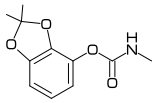
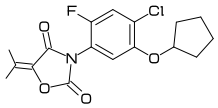
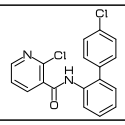
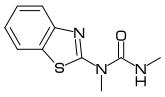
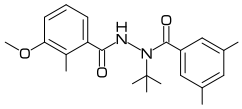
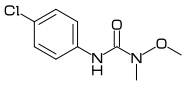
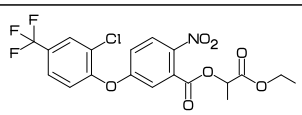
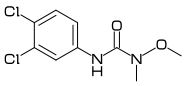
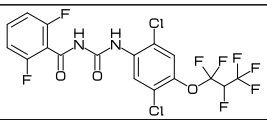
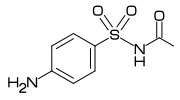
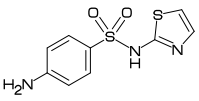
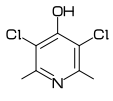
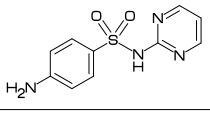
[395] 	Propachlor	pesticide	211.689	211.6879	C11H14ClNO
	<30,Ph,@3,!N,/?!,!,?O!2,Cl				
[396] 	Propazine	pesticide	229.7	229.7098	C9H16ClN5
	<30,Ph,2'4'6:N,5:/Cl,1'3:/NH'!?!				
[397] 	Propanil	pesticide	218.077	218.0798	C9H9Cl2NO
	<30,Ph,1'6:/Cl,3:/NH!'?O!2				
[398] 	Propyzamide	pesticide	256.1	256.1278	C12H11Cl2NO
	<30,Ph,1'5:/Cl,@3,!?O,!NH,!??!,!t				
[399] 	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,-3:/!2^-15				
[400] 	Prohydrojasmon	pesticide	254.37	254.3651	C15H26O3
	<18,?5,2:?O,3:*/!4^-12,4:/*!?O!'O!3				
[401] 	Bromacil	pesticide	261.119	261.1157	C9H13BrN2O2
	<30,?6,6=dl,3:N,1:/Br,2'4:?O,5:NH,6:?,3:/?!2				
[402] 	Prometryn	pesticide	241.4	241.3563	C10H19N5S
	<30,Ph,2'4'6:N,5:/S!,1'3:/NH'!?!				
[403] 	Bromobutide	pesticide	312.2	312.2452	C15H22BrNO
	<30,Ph,@3,!??,!NH!,?O!,/Br,!??!				
[404] 	Bromopropylate	pesticide	428.12	428.1151	C17H16Br2O3
	<30,Ph,@3,!2,Ph,6'11:/Br,7:/OH^-45,@7,30,?O!,O,-60,?!				
[405] 	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				
[406] 	Hexazinone	pesticide	252.31	252.3127	C12H20N4O2
	<30,?6,3=dl,2'4'6:N,2:?,1'5:?O,6:/?6,3:/N?!				
[407] 	Benalaxyl	pesticide	325.4	325.4015	C20H23NO3
	<30,Ph,@3,!2,?O!,N,/Ph'(-5'-1:?),!?!,?O,!O!				
[408] 	Benoxacor	pesticide	260.1	260.1165	C11H11Cl2NO2
	<90,Ph,3=?6,7:N,10:O,8:?,@7,!?O!,/Cl,!Cl				
[409] 	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				
[410] 	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				
[411] 	Penconazole	pesticide	284.184	284.1843	C13H15Cl2N3
	<30,Ph,4'6:/Cl,@3,!,/!2,!2,|,<30,?5,2'4=dl,1'2'4:N				
[412] 	Pendimethalin	pesticide	281.3	267.2810	C12H17N3O4
	<30,Ph,3'5:/NO2,1'2:?,@4,!,NH,!?,!2				

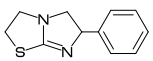
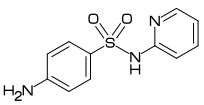
[413] 	Benfluralin	pesticide	335.3	335.2790	C13H16F3N3O4
	<30,Ph,1'3:/NO2,5:/?F?F!F,2:/N?2'!4				
[414] 	Benfuresate	pesticide	256.3	256.3180	C12H16O4S
	<30,Ph,3=?5,7:O,9:??,@6,!O!,S?O?O,!2				
[415] 	Bensulide	pesticide	397.5	397.5134	C14H24NO4PS3
	<30,!?!,O!,P,?S,/O'!?!^160>rl,!,S!3,NH!,S?O?O,!Ph				
[416] 	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				
[417] 	Methoxychlor	pesticide	345.644	345.6481	C16H15Cl3O2
	<30,Ph,@3,!2,Ph,6'11:/O!,7:/?Cl?Cl!Cl				
[418] 	Metolachlor	pesticide	283.8	283.7936	C15H22ClNO2
	<30,Ph,5:/!,3:?,@4,!N,/?!2'O!,!,?O!2,Cl				
[419] 	Mefenacet	pesticide	298.4	298.3595	C16H14N2O2S
	<12,Ph,3=?5,9=dl,9:N,7:S,@8,!,O!2,?O!,N?!,Ph				
[420] 	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				
[421] 	Mepronil	pesticide	269.3	269.3382	C17H19NO2
	<30,Ph,2:?,@3,!?O,!NH!,Ph,-2:/O'!?!				
[422] 	Molinate	pesticide	187.3	187.3023	C9H17NOS
	<47,?7,3:N,@3,!?O!,S!2				
[423] 	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				
[424] 	Lenacil	pesticide	234.3	234.2942	C13H18N2O2
	<30,?6,3=?5,3=dl,6:N,2:NH,1'5:?O,6:/?6				
[425] 	Halfenprox	pesticide	477.4	477.3384	C24H23BrF2O3
	<30,Ph,@6,!O!,/F^35,/F^-35,!,Br,@3,!,!??!,O!2,Ph,-2:/O!'Ph>rl				
[426] 	Paraquat	pesticide	257.16	257.1589	C12H14Cl2N2
	Ph,@4,!Ph,1'10:N?,1:p_^-90,10:p_^90,@1,@(O'1.2),Cl,n_^15,@10,@(O'1.2),Cl,n_^15				
[427] 	Oxine-Copper	pesticide	351.852	351.8460	C18H12CuN2O2
	Ph,4:N,5=Ph,@-4,!O,-60,<90,Cu,-90,O,60,Ph,-2=Ph,10:N,@4,&12~vf,@23,&12~vf				
[428] 	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				
[429] 	Uniconazole-P	pesticide	291.779	291.7759	C15H18ClN3O
	<30,Ph,6:/Cl,@3,!!d,!,/OH,!??!,@8,!,|,?5,2'4=dl,1'2'4:N				
[430] 	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				

[431] 	Azinphos-methyl	pesticide	317.318	316.3362	C11H13N2O3PS2
	<-30,!O!,P,?S,/O!^160,!,S!2,|,?6,-3=?6,2'4'8'10=dl,1'3:N,6:?O				
[432] 	Azoxystorbin	pesticide	403.394	403.3874	C22H17N3O5
	<30,Ph,2:/CN,@3,!O!,Ph,-1'-3:N,@-4,!O!,Ph,@-5,!,//!O!,!?O!,O!				
[433] 	Aramite	pesticide	334.859	334.8587	C15H23ClO4S
	<30,Ph,6:/??!,@3,!,O!2,?!,O!,S,?O,!,O!3,Cl				
[434] 	Aldicarb	pesticide	190.3	190.2632	C7H14N2O2S
	<-30,!,S,!??,!!d,N,!O!,?O,!NH!				
[435] 	Aldoxycarb	pesticide	222.3	222.2620	C7H14N2O4S
	<30,!?O,!NH!,O!,N,!d,!??,!,S?O?O,!				
[436] 	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				
[437] 	Iprovalicarb	pesticide	320.4	320.4265	C18H28N2O3
	<30,Ph,6:?,@3,!,!?!,NH!,?O!,??,!NH!,?O!,O,!?!				
[438] 	Imazalil	pesticide	297.2	297.1797	C14H14Cl2N2O
	<-30,!,/Ph'(4'6:/Cl),!,O!2,!d,@1,60,|,?5,2'4=dl,1'3:N				
[439] 	Imidacloprid	pesticide	255.662	255.661	C9H10ClN5O2
	<30,Ph,1:N,6:/Cl,@3,!2,|,?5,1:N,3:NH,2://N'!NO2				
[440] 	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				
[441] 	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!				
[442] 	Oxamyl	pesticide	219.3	219.2614	C7H13N3O3S
	<-30,!,N?!,?O!,/S!,!d,N,!O!,?O!,NH!				
[443] 	Oryzalin	pesticide	346.4	332.3329	C11H16N4O6S
	<30,Ph,1'3:/NO2,5:/S?O?O'!NH2,2:/N?2'!3				
[444] 	Carbaryl	pesticide	201.22	201.2212	C12H11NO2
	<30,Ph,5=Ph,@4,!?O,!O!,NH!				
[445] 	Carpropamid	pesticide	334.665	334.6685	C15H18Cl3NO
	<-30,?3,1:?,{2^-35'*2^35}:*/Cl,3^70:/!,@3,!?O!,NH,!?!,Ph,-3:/Cl				
[446] 	Cumyluron	pesticide	302.802	302.7985	C17H19ClN2O
	<30,Ph,@4,!??,!NH!,?O!,NH,!2,Ph,-1:/Cl				
[447] 	Cloquintocet-methyl	pesticide	335.83	335.8251	C18H22ClNO3
	<90,Ph,4=Ph,2:N,10:/Cl,@7,!,O!2,?O!,O,!?,!5				
[448] 	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				

[449] 	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:?				
[450] 	Clomeprop	pesticide	324.2	324.2018	C16H15Cl2NO2
	<30,Ph,4’6:/Cl,5:?,@3,!O,!?!,?O,!NH!,Ph				
[451] 	Chloridazon	pesticide	221.6	221.6430	C10H8ClN3O
	<30,?6,3’4:N,2’6=dl,5:?O,1:/NH2,6:/Cl,4:/Ph				
[452] 	Chloroxuron	pesticide	290.745	290.7448	C15H15ClN2O2
	<30,Ph,6:/Cl,@3,!O!,Ph,@-3,!NH!,?O!,N?!				
[453] 	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:?				
[454] 	Diuron	pesticide	233.1	233.0945	C9H10Cl2N2O
	<30,Ph,1’6:/Cl,@3,!NH!,?O!,N?!				
[455] 	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				
[456] 	Diflubenzuron	pesticide	310.7	310.6832	C14H9ClF2N2O2
	<30,Ph,2’4:/F,@3,!?O,!NH!,?O,!NH!,Ph,-3:/Cl				
[457] 	Cyprodinil	pesticide	225.295	225.2889	C14H15N3
	<30,Ph,2’4:N,5:?,1:/?3,3:/NH!’Ph				
[458] 	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),				
[459] 	Dimethirimol	pesticide	209.29	209.2880	C11H19N3O
	<30,?6,3’5=dl,1:?O,2:NH,3:/N?!,4:N,5:?,6:/??!				
[460] 	Dimethomorph	pesticide	387.86	387.8566	C21H22ClNO4
	<30,?6,1:O,4:N,@4,!?O!,!d‘1,/Ph’(4:/Cl),!,|,Ph,4’5:/O!				
[461] 	Silafluofen	pesticide	408.588	408.5804	C25H29FO2Si
	<30,Ph,@5,!O!,Ph,-1:/F,@10,!4,Si,??,!Ph,-3:/O!2				
[462] 	Di-allate	pesticide	270.212	270.2190	C10H17Cl2NOS
	<-30,!?!,N!,?O!,S,!2,!d,!Cl,3:/?!,7:/Cl				
[463] 	Daimuron	pesticide	268.4	268.3534	C17H20N2O
	<30,Ph,@4,!??,!NH!,?O,!NH!,Ph,-3:?				
[464] 	Thiacloprid	pesticide	252.72	252.7232	C10H9ClN4S
	<30,Ph,1:N,6:/Cl,@3,!2,<-12,|,?5,1:N,3:S,-4://N’!CN				
[465] 	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				
[466] 	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				

[467] 	Tebuthiuron	pesticide	228.3	228.3145	C9H16N4OS
	<18,?5,3'5=dl,4'5:N,2:S,1:/??!,@3,!,N?!,?O,!NH!				
[468] 	Tebufenozide	pesticide	352.5	352.4699	C22H28N2O2
	<30,Ph,6:/!,@3,!?O,!NH!,N,/??!,!?O,!Ph,-4'-2:?				
[469] 	Teflubenzuron	pesticide	381.1	381.1092	C14H6Cl2F4N2O2
	<30,Ph,2'4:/F,@3,!?O,!NH!,?O,!NH!,|,Ph,3'5:/Cl,4'6:/F				
[470] 	Tridemorph	pesticide	297.5	297.5190	C19H39NO
	<30,?6,3:N,6:O,1'5:?,3:/!12				
[471] 	Triflumuron	pesticide	358.701	358.6997	C15H10ClF3N2O3
	<30,Ph,4:/Cl,@3,!?O,!NH!,?O,!NH!,Ph,-2:/O!'?F?F!F				
[472] 	Naproanilide	pesticide	291.35	291.3437	C19H17NO2
	<30,Ph,4=Ph,@8,!O,!?!,?O,!NH!,Ph				
[473] 	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				
[474] 	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!				
[475] 	Pirimicarb	pesticide	238.291	238.2862	C11H18N4O2
	<30,Ph,1'5:N,2'3:?,6:/N?!,@4,!O!,?O!,N?!				
[476] 	Fenoxycarb	pesticide	301.35	301.3370	C17H19NO4
	<30,Ph,@5,!O!,Ph,@-3,!,O!3,NH!,?O!,O!2				
[477] 	Fenobucarb	pesticide	207.3	207.2688	C12H17NO2
	<30,Ph,5:/?!2,@4,!O!,?O,!NH!				
[478] 	Ferimzone	pesticide	254.337	254.3302	C15H18N4
	<30,Ph,4:?,@3,!?,!d,N,!NH!,|,Ph,2'6:N,3'5:?				
[479] 	Fenamidone	pesticide	311.403	311.4013	C17H17N3OS
	<18,?5,4=dl,3'5:N,2:?O,@3,!NH!,Ph,4:/S!,1^52:?w,1^-48:/*Ph				
[480] 	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				
[481] 	Phenmedipham	pesticide	300.32	300.3092	C16H16N2O4
	<30,Ph,5:?,@3,!NH!,?O!,O,!Ph,-4:/NH!'?O!'O!				
[482] 	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				
[483] 	Flufenacet	pesticide	363.331	363.3305	C14H13F4N3O2S
	<6,?5,2'5=dl,1'2:N,4:S,5:/?F?F!F,@3,!O!,!?O!,N,/?!,!Ph,-3:/F				
[484] 	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				

[485] 	Fluridone	pesticide	329.3	329.3157	C19H14F3NO
	<30,?6,3'6=dl,2:N,2:?,5:?O,@4,!Ph,-4:/?F?F!F,6:/Ph				
[486] 	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,?!				
[487] 	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				
[488] 	Hexathiazox	pesticide	352.877	352.8788	C17H21ClN2O2S
	<30,?6,@3,!NH!,?O!,<-24,|,?5,1:N,3:S,2:?O,5:?,@4,!Ph,-3:/Cl				
[489] 	Pencycuron	pesticide	328.84	328.8358	C19H21ClN2O
	<30,Ph,6:/Cl,@3,!2,N,/?5,!?O,!NH!,Ph				
[490] 	Bendiocarb	pesticide	223.228	223.2252	C11H13NO4
	<30,Ph,5=?5,7'9:O,8:??,@4,!O!,?O,!NH!				
[491] 	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				
[492] 	Boscalid	pesticide	343.21	343.2066	C18H12Cl2N2O
	<30,Ph,5:N,4:/Cl,@3,!?O,!NH!,Ph,@-1,!Ph,-3:/Cl				
[493] 	Methabenzthiazuron	pesticide	221.3	221.2788	C10H11N3OS
	Ph,3=?5,9=dl,7:S,9:N,@8,!,N?!,?O,!NH!				
[494] 	Methoxyfenozide	pesticide	368.48	368.4693	C22H28N2O3
	<30,Ph,2:?,1:/O!,@3,!?O,!NH!,N,/??!,!?O,!Ph,-4'-2:?				
[495] 	Monolinuron	pesticide	214.6	214.6488	C9H11ClN2O2
	<30,Ph,6:/Cl,@3,!NH!,?O!,N?!,O!				
[496] 	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				
[497] 	Linuron	pesticide	249.1	249.0938	C9H10Cl2N2O2
	<30,Ph,1'6:/Cl,@3,!NH!,?O!,N?!,O!				
[498] 	Lufenuron	pesticide	511.15	511.1502	C17H8Cl2F8N2O3
	<30,Ph,2'4:/F, @3,!?O,!NH!,?O,!NH!,Ph,-1'-4:/Cl,@-3,!O!,/F^35,/F^-35,!,/F,!,?F?F!F				
[499] 	Sulfacetamide	antibacterial	214.239	214.2415	C8H10N2O3S
	<30,Ph,1:/NH2,@4,!,S?O?O,!NH!,?O!				
[500] 	Sulfatiazole	antibacterial	255.31	255.3166	C9H9N3O2S2
	<30,Ph,1:/NH2,@4,!,S?O?O,!NH!,|,?5,1'3=dl,2:N,5:S				
[501] 	Chlopidol	antibacterial	192.039	192.0425	C7H7Cl2NO
	<30,Ph,1'3:?,2:N,4'6:/Cl,5:/OH				
[502] 	Sulfadiadine	antibacterial	250.276	250.2769	C10H10N4O2S
	<30,Ph,1:/NH2,@4,!,S?O?O,!NH!,Ph,-5'-1:N				

[503] 	Levamisole	antibacterial	204.29	204.2913	C11H12N2S
	?5,3=?5,6=dl,2:S,4'6:N,7:/Ph				
[504] 	Sulfapyrizine	antibacterial	249.288	249.2889	C11H11N3O2S
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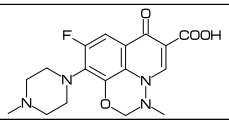
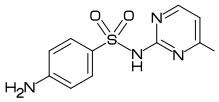
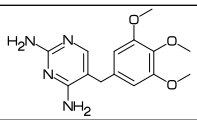
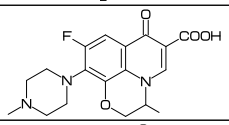
[505] 	Marbofloxacin	antibacterial	362.361	362.3555	C17H19FN4O4
	<30,Ph,3'(2--7)=?6,9=dl,6:/F,7'13:N,11:O,9:/COOH,10:?O,13:?,@1,!,?6,-6:N,-3:N?				
[506] 	Sulfamerazine	antibacterial	264.303	264.3035	C11H12N4O2S
	<30,Ph,1:/NH2,@4,!,S?O?O,!NH!,Ph,-5'-1:N,-4:?				
[507] 	Trimethoprim	antibacterial	290.323	290.3177	C14H18N4O3
	<30,Ph,1'5:N,2'6:/NH2,3:/!Ph'(4'5'6:/O!)				
[508] 	Ofloxacin	antibacterial	361.373	361.3675	C18H20FN3O4
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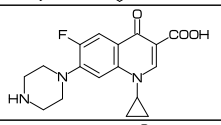
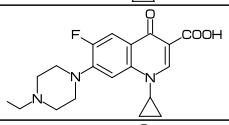
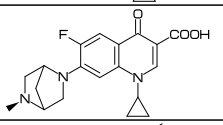
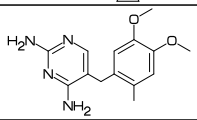
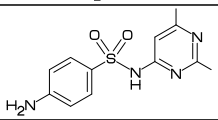
[509] 	Ciprofloxacin	antibacterial	331.347	331.3415	C17H18FN3O3
	<30,Ph,3=?6,9=dl,7:N,6:/F,7:/?3,9:/COOH,10:?O,1:/?6'(1:N)'(4:NH)				
[510] 	Enrofloxacin	antibacterial	359.401	359.3946	C19H22FN3O3
	<30,Ph,3=?6,9=dl,7:N,6:/F,7:/?3,9:/COOH,10:?O,@1,!,?6,-6:N,-3:N?2				
[511] 	Danofloxacin	antibacterial	357.385	357.3788	C19H20FN3O3
	<30,Ph,3=?6,9=dl,7:N,6:/F,7:/?3,9:/COOH,10:?O, @1,!,|,?6,@2,-200'1.1,&5,1'4:N,4:?w				
[512] 	Ormetoprim	antibacterial	274.324	274.3183	C14H18N4O2
	<30,Ph,1'5:N,2'6:/NH2,@3,!2,|,Ph,2:?,4'5:/O!				
[513] 	Sulfadimidine	antibacterial	278.33	278.3301	C12H14N4O2S
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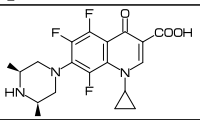
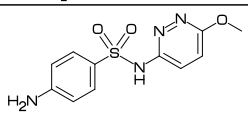
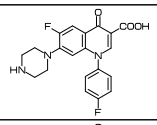
[514] 	Orbifloxacin	antibacterial	395.382	395.3756	C19H20F3N3O3
	<30,Ph,3=?6,9=dl,7:N,2'5'6:/F,7:/?3,9:/COOH,10:?O,@1,!,|,?6,1:N,3'5:?w,4:NH				
[515] 	Sulfamethoxypyridazine	antibacterial	280.302	280.3029	C11H12N4O3S
	<30,Ph,1:/NH2,@4,!,S?O?O,!NH!,|,Ph,5'6:N,4:/O!				
[516] 	Sarafloxacin	antibacterial	385.371	385.3640	C20H17F2N3O3
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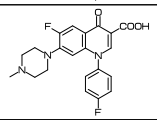
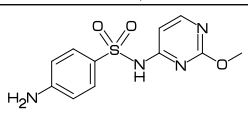
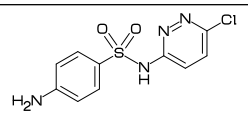
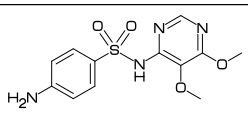
[517] 	Difloxacin	antibacterial	399.398	399.3906	C21H19F2N3O3
	<30,Ph,3=?6,9=dl,7:N,6:/F,9:/COOH,10:?O,7:/Ph'(4:/F),1:/?6'(1:N)'(4:N?)				
[518] 	Sulfamonomethoxine	antibacterial	280.302	280.3029	C11H12N4O3S
	<30,Ph,1:/NH2,@4,!,S?O?O,!NH!,|,Ph,2'4:N,3:/O!				
[519] 	Sulfachlorpyridazine	antibacterial	284.723	284.7220	C10H9ClN4O2S
	<30,Ph,1:/NH2,@4,!,S?O?O,!NH!,|,Ph,5'6:N,4:/Cl				
[520] 	Sulfadoxine	antibacterial	310.328	310.3289	C12H14N4O4S
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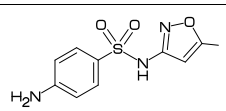
[521] 	Sulfamethoxazole	antibacterial	253.276	253.2776	C10H11N3O3S
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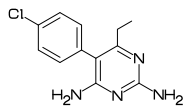
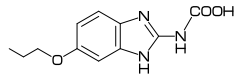
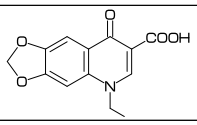
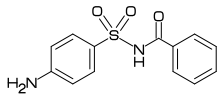
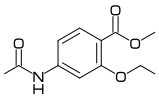
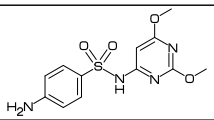
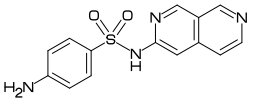
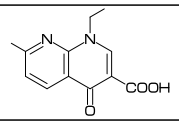
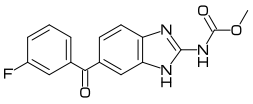
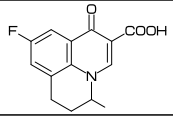
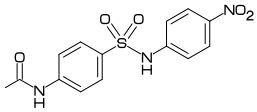
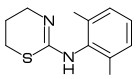
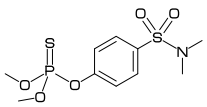
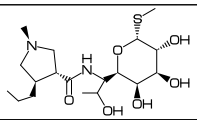
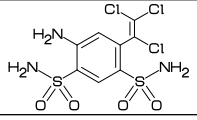
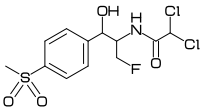
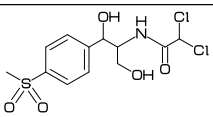
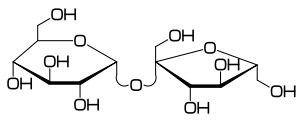
[522] 	Pirimethamin	antibacterial	248.714	248.7114	C12H13ClN4
	<30,Ph,6:/Cl,@3,!Ph,-2'-4:N,-1:/!,-3'-5:/NH2				
[523] 	Oxibendazole	antibacterial	249.27	235.2392	C11H13N3O3
	<30,Ph,3=?5,9=dl,7:NH,9:N,1:/O!3,8:/NH!'COOH				
[524] 	Oxolinic acid	antibacterial	261.233	261.2301	C13H11NO5
	<30,Ph,3=?6,6=?5,9=dl,7:N,11'13:O,10:?O,7:/!,9:/COOH				
[525] 	Sulfabenzamide	antibacterial	276.31	276.3109	C13H12N2O3S
	<30,Ph,1:/NH2,@4,!,S?O?O,!NH!,?O,!Ph				
[526] 	Ethopabate	antibacterial	237.255	237.2518	C12H15NO4
	<30,Ph,1:/NH!'?O!,3:/O!2,4:/?O!'O!				
[527] 	Sulfadimethoxine	antibacterial	310.33	310.3289	C12H14N4O4S
	<30,Ph,1:/NH2,@4,!,S?O?O,!NH!,|,Ph,2'4:N,3'5:/O!				
[528] 	Sulfaquinoxaline	antibacterial	300.337	300.3356	C14H12N4O2S
	<30,Ph,1:/NH2,@4,!,S?O?O,!NH!,Ph,-4=Ph,-5'-2:N				
[529] 	Nalidixic acid	antibacterial	232.239	232.2352	C12H12N2O3
	<30,Ph,3=?6,9=dl,5'10:N,6:?,7:?O,8:/COOH,10:/!				
[530] 	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!				
[531] 	Flumequine	antibacterial	261.225	261.2483	C14H12FNO3
	<30,Ph,3'(2--7)=?6,9=dl,7:N,6:/F,9:/COOH,10:?O,13:?				
[532] 	Sulfanitran	antibacterial	335.334	335.3351	C14H13N3O5S
	<30,Ph,@1,!NH!,?O!,@4,!,S?O?O,!NH!,Ph,-3:/NO2				
[533] 	Xylazine	antibacterial	220.334	220.3338	C12H16N2S
	<30,?6,3=dl,2:S,4:N,@3,!NH!,Ph,-5'-1:?				
[534] 	Famphur	antibacterial	325.3	325.3415	C10H16NO5PS2
	<-30,!O!,P,?S,/O!^160,!O!,Ph,-3:/S?O?O!'N?!				
[535] 	Lincomycin	antibacterial	406.54	406.5373	C18H34N2O6S
	<6,?5,5:N,5:?w,2:*/!2, @3,!z,?O,!NH!,!wb,?6,-1:O,*-3'-4'-5:*/OH,-2:/*S!,8:/?!'OH^-30>lr				
[536] 	Chlorsulon	antibacterial	380.66	380.6558	C8H8Cl3N3O4S2
	<30,Ph,6:/NH2,1'3:/S?O?O'!NH2,@4,!,/Cl,60^dl,/Cl,!Cl				
[537] 	Florfenicol	antibacterial	358.21	358.2132	C12H14Cl2FNO4S
	<30,Ph,1:/S?O?O!,@4,!,/OH,!,/!F,!NH!,?O!,/Cl,!Cl				
[538] 	Thiamphenicol	antibacterial	356.22	356.2221	C12H15Cl2NO5S
	<30,Ph,1:/S?O?O!,@4,!,/OH,!,/!OH,!'1.1,NH,!'1.1,?O!,/Cl,!Cl				

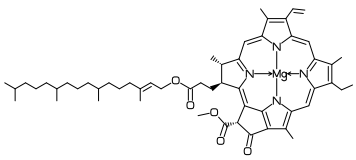
[1]



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,
 |,#1.4,-35~wf_r,35~bd_r‘1,30~wb_r,130‘1.66,O,&1,##,
 #.5,{2^$270'3^$90}:/OH,{1^$90'4^$270}:/!OH
```

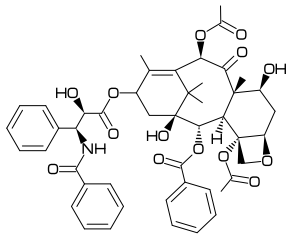
[2]



Chlorophyll a	biological	893.509	893.4889	C55H72MgN4O5

```
<-36,#1,?5,@3,!,54,?5,@-2,!,54,?5,@-2,!,54,?5,@-2,!,&5,@6,22,70,&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:?
```

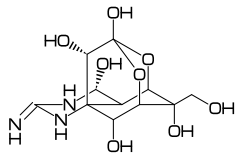
[3]



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!
```

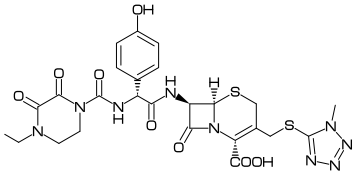
[4]



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
```

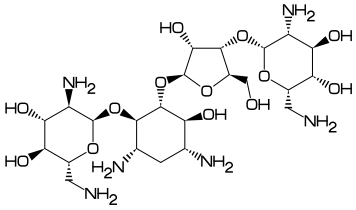
[5]



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,-3'-6:N,-4'-5:?O,-3:/!,
 @6,!2,S,!,?5,-3'-5=dl,-1:?,-1'-2'-3'-4:N,
```

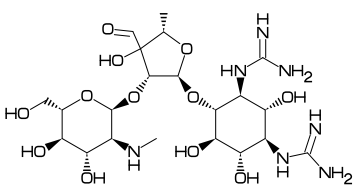
[6]



Neomycin	antibiotics	614.644	614.6437	C23H46N6O13

```
<30,?6,3:O,2:/*!NH2,1'*6:*/OH,5:*/NH2,
 @4,!w,O,!wb,?6,{-3,-5^15}:/*NH2,-2:*/OH^-15,
 @-1,!z,O,-72~wb,?5,-4:O,-1:/*OH>vt,-3:*/!OH>vt,
 @-2,-24~zf,O,-60~zb,?6,-5:O,-1:/*NH2,-2'*-3:*/OH,-4:/*!NH2>60
```

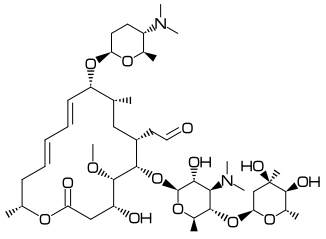
[7]



Streptmycin	antibiotics	581.574	581.5740	C21H39N7O12

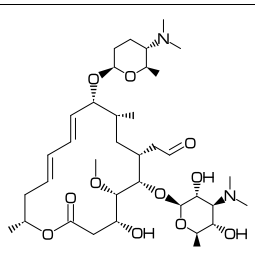
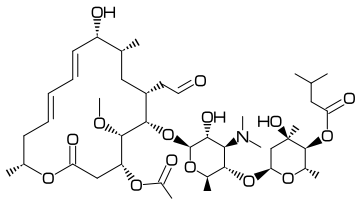
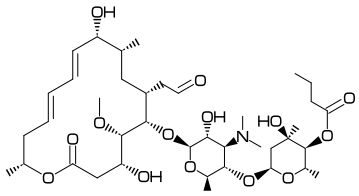
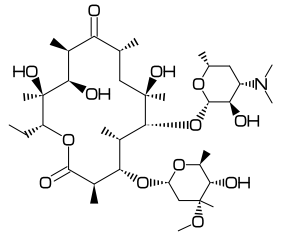
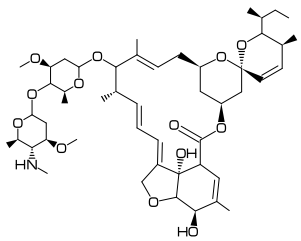
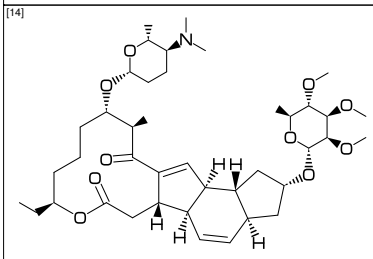
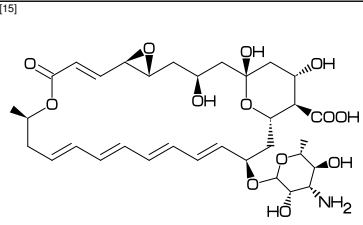
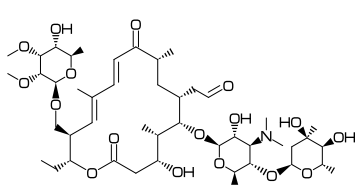
```
<54,?5,3:O,4:?z,5:/OH^45,@1,!z,O,-24~wb,?6,-5:O,@2,!w,O,24~zb,?6,
  5:/!dO^-48,10'*11'15'*16'*18:*/OH,9:/*!OH,12:*/NH!,{17^-18'19}:*/NH!'?NH'!NH2
```

[8]

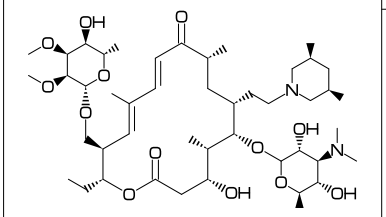


Spiramycin	antibiotics	843.1	843.0526	C43H74N2O14

```
<-90,#1,60,60,-60,60,60,-60,60,60,-60,60,60,60,-60,60,-60,&1,##,
 12'14=dl,2:O,{1'10^-30}:?z,5:/*OH,3:?O,6:/*O!>vt,8:/*!'!dO,
 @-6,!z^-30,O,!wb,?6‘.7,-5:O,#.5,-3:/*N?!,-4:?w,##,
 @7,!z,O,O~wb,?6‘.7,-5:O,#.5,-2:*/N?!,-1:/*OH,-4:?w,##,
   @-3,!z‘1,O,60~wb,?6‘.7,-5:O,#.5,{-2^35'-3}:*/OH,{-2^-35'-4}:?z,##,
```

[9] 	Neospiramycin	antibiotics	698.9	698.8842	C36H62N2O11
	<-90,#1,60,60,-60,60,60,-60,60,60,-60,60,60,60,-60,60,-60,&1,##, 12'14=dl,2:O,{1'10^-30}:?z,5:/*OH,3:?O,6:/*O!>vt,8:/*!'!dO, @-6,!z^-30,O,!wb,?6'.7,-5:O,#.5,-3:/*N?!,-4:?w,##, @7,!z,O,O~wb,?6'.7,-5:O,#.5,-2:*/N?!,-4:?w,-1'-3:/*OH,##,				
[10] 	Josamycin	antibiotics	827.995	827.9949	C42H69NO15
	<-90,#1,60,60,-60,60,60,-60,60,60,-60,60,60,60,-60,60,-60,&1,##, 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,O~wb,?6'.7,-5:O,#.5,-2:*/N?!,-1:/*OH,-4:?w,##, @-3,!z'1,O,60~wb,?6'.7,-5:O,#.5,-2^35:*/OH,{-2^-35'-4}:?z,##, @-3,!w,O,60,?O,60,-60,?,!				
[11] 	Leucomycin A5	antibiotics	771.942	771.9317	C39H65NO14
	<-90,#1,60,60,-60,60,60,-60,60,60,-60,60,60,60,-60,60,-60,&1,##, 12'14=dl,2:O,1:?z,3:?O,10:?z,6:/*O!>vt,-6:/*OH,5:/*OH,8:/*!'!dO, @7,!z,O,O~wb,?6'.7,-5:O,#.5,-2:*/N?!,-1:/*OH,-4:?w,##, @-3,!z'1,O,60~wb,?6'.7,-5:O,#.5,-2^35:*/OH,{-2^-35'-4}:?z,##, @-3,!w,O,60,?O,60,-60,60				
[12] 	Erythromycin	antibiotics	733.93	733.9267	C37H67NO13
	<30,#1,<-120,60,60,60,-60,60,60,-60,60,60,60,-60,60,60,60,##,&1, 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,?O,-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, 17:?,19:?z,@18,!O!,?6'.7,-1:O,#.5,-2:?w,-4:*/O!,##, @-3,!O,60,?6'.7,-5:O,#.5,-4:?w,-3:/*NH!,-2:*/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,-1:O,#.5,-2:?w,*-3'-4'-5:*/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,O,-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,-1:O,#.5,-3'*-5:*/OH,-4:/*NH2,-2:?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,O~wb,?6'.7,-5:O,#.5,-3:/*OH,-4:?w,-1'-2:/*O!,##, @7,!z,O,O~wb,?6'.7,-5:O,#.5,-2:*/N?!,-1:/*OH,-4:?w,##, @-3,!z'1,O,60~wb,?6'.7,-5:O,#.5,{-2^35'-3}:*/OH,{-2^-35'-4}:?z,##				

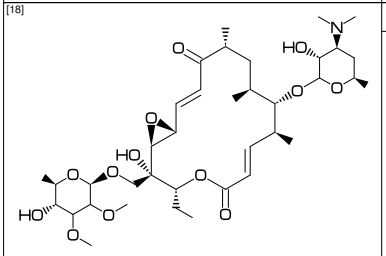
[17]



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,-5:O,#.5,-1’-2:*/O!,-3:*/OH,-4:?z,##,
 @7,!z,O,O,?6‘.7,-5:O,#.5,-2:*/N?!,-1’-3:/*OH,-4:?w,##,
 @8,!z,!2,?6‘.7,-6:N,#.5,-2’-4:?w
```

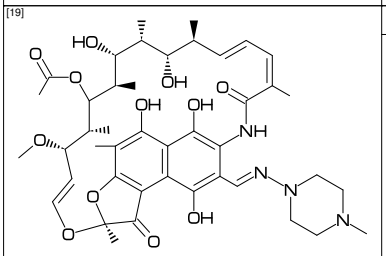
[18]



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,##,
 @8,!z,O,O,?6‘.7,-5:O,#.5,-2:*/N?!,-1:/*OH,-4:?w,##,
 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,-5:O,#.5,-3:/*OH,-4:?w,-1’-2:/O!
```

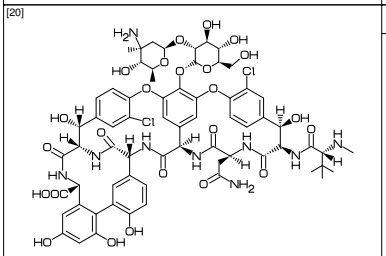
[19]



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?
```

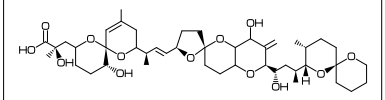
[20]



Vancomycin	antibiotics	1449.25	1449.253	C66H75Cl2N9O24

```
<-30,#1,!12,1’3’12=zf,7=wf,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,|,?6‘.7,2:O,3^10:*/!OH,*4’5:*/OH,
 @-1,!z,O,!wb,|,?6‘.7,6:O,{*3^35’5}:?w,3^-35:/NH2,4:/*OH
```

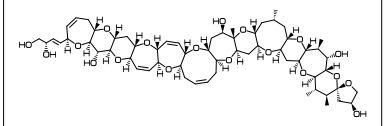
[21]



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
```

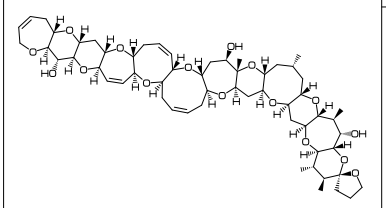
[22]



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
```

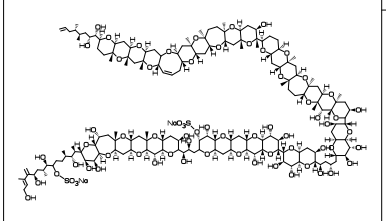
[23]



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
```