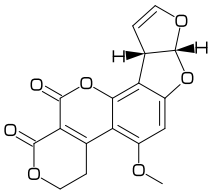
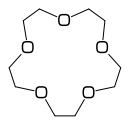
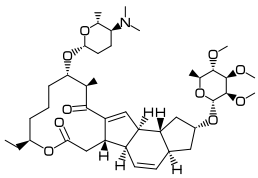
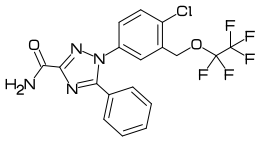
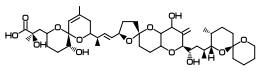
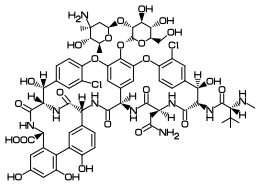
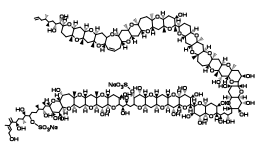
[(No)] (EXA)	(Name)	(Category)	(MW)*1	(mw)*2	(fm)*3
(Structure)	(Molecular_Coding_Format)		*1_(MW):Molecular_weight(data) *2_(mw):Molecular_weight(calculated) *3_(fm):Molecular_formula(calculated)		
[1] 2 	Aflatoxin␣G1	biological	328.27	328.2729	C17H12O7
	<30,Ph,6=?6,-2=?6,4=?5,-2=?5,{-2,10}=dl,{7,12,15,18}:O, 2:/O!,{8,11}://O,{16^-54,17^54}:*/H				
[2] 2 	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				
[3] 2 	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,*,O,66~zb,?6‘.7,-1:O,#.5,-2:*/_,{-3',-4,-5}:*/O!,8:*/_,5^-65:*/H,##, @9,*,O,!~zb,|,?6‘.7,6:O,#.5,5:/*_,4:*/N?!				
[4] 2 	Flupoxam	pesticide	460.8	446.7584	C18H12ClF5N4O2
	<30,Ph,4:/Cl,@1,\,?5,{-2,-4}=db,{-2,-4,-5}:N,-1:/Ph,@-3,\,//O,!,NH2, @3,\,!,O,!,/F^35,/F^-35,!,CF3				
[5] 2 	Okadaic␣acid	biological	805.00	805.0029	C44H68O13
	<30,?6,@4,?6,@-4,\,!3,<-12,?5,@-3,<-12,?6,-3=?6,@-3,*\,!3, ?6,@-4,?6,@6,\,!,/*_^-40,*/OH^20,!,//O,!1,OH, 3=wb,11=dl,15=dr,17=wf,19=wf,38=wb,{5,7,16,24,25,33,42}:O, 32:*/H^60,10:/_,{12,31,37'}:*/_,27://_,28:/OH,{3,29}:/*OH				
[6] 2 	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,*\^-60,60,//O,!,NH2,@13,*\,NH,!,//O,!,/??!,*/H^60,!~zf,NH,!, @23,\,O,!~zf,|,?6‘.7,2:O,3^10:*/!OH,{4',5}:*/OH, @-1,*,O,!~wb,|,?6‘.7,6:O,{3'^35,5}:*/_,3^-35:/NH2,4:/*OH,				
[7] 2 	Maitotoxin	biological	3425.86	3425.856	C164H256Na2O68S2
	<55.8,?6,-4=?7␣,{-4,-3,-3,-3}=?6,@-3,\,!3,?6,{-4,-3,-3,-3}=?6,@-3,\,?6,-3=?6, @-3,\,!3,60,<-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}:*/_^60‘1,{80,88,97,108',115,120,124}:/*_^-60‘1, @$6,\,|,!11,60~dr,-60,60,OH,{2',7,10}:*/OH,{1,3,8'}:*/_,11://_,12:/_, @6,\,O,3O,SO3Na, @$36,-45~zf,O,3O,SO3Na, @$150,\,|,!7,{1,2}:/*OH,4:*/_,5:/*_,7=dl				