

MCF example for luamplib(Lua \LaTeX)

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Located at : <http://www.ctan.org/pkg/mcf2graph>

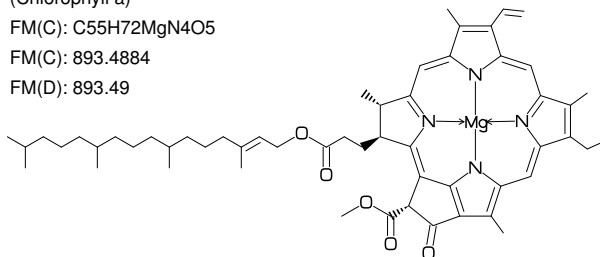
FM(C) : molecular formula calculated by mcf2graph
MW(C) : molecular weight calculated by mcf2graph
MW(D) : molecular weight from literature data

(Chlorophyll a)

FM(C): C₅₅H₇₂MgN₄O₅

FM(C): 893.4884

FM(D): 893.49



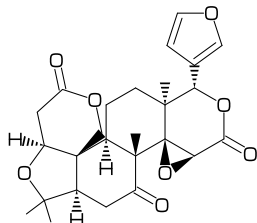
```
|<,' '1,{?5,{2,5}=d1,4:N,3:\,54~d1,
|,{?5,{2,4}=d1,5:N,
-2:\,54~d1,|,{?5,2=d1,5:N,
-2:\~d1,54,|,{?5,5=d1,5:N,-2:\~d1,&#5,
-1:@,24,/C00!\^15,72,/0,&#1,>|,
4:\ '1.45,Mg,&17,-1:@,&11~vb,-1:@,&23~vb,
{2,9,15,20~zf}:/_,8:/!,14:\,!! ,
21:@,-6~wf,!2,/0,! ,0,!2,!! ,
|,!13,{1,5,9,13}:/_,
```

(Limonin)

FM(C): C₂₆H₃₀O₈

FM(C): 470.5113

FM(D): 470.51



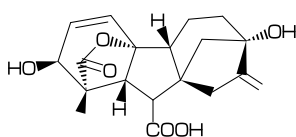
```
<30,{?6,{-3,-4}=?6,-5=?3,
-2=wf,-1=wb,6=?5,-4=?6,-5=wf,
{13,15,17,20}:0,{3,12,21}:/0,
{4~wf^60,8~zf^60,18^35,18^~35}:/_,
{1^60,5^180,16^60}:/*H,
14:\*,|,{?5,{1,4}=d1,3:0
```

(Gibberellin A3)

FM(C): C₁₉H₂₂O₆

FM(C): 346.3742

FM(D): 346.37



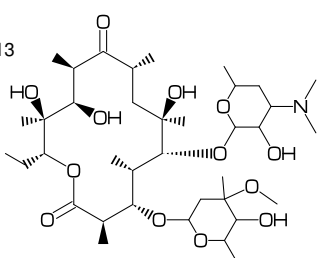
```
<18,{?5,3=?7,5=?6[12],8:@,160 '1.3,&3,
13=d1,6=wf,8=wb,
5:@,40~zf '1,0,60,/0^180,&14~zb,
2:/COOH,7:/_,13:*/OH,8:*/OH,
14:*/_,{1^60,4^60}:/H)
```

(Erythromycin)

FM(C): C₃₇H₆₇NO₁₃

FM(C): 733.9263

FM(D): 733.93



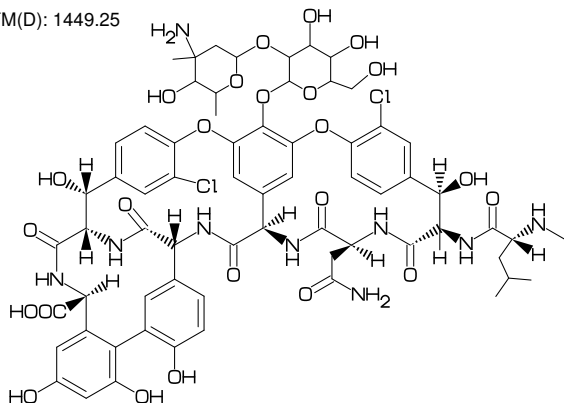
```
<30,|<,' '1,<-120,60,60,60,-60,60,
60,-60,60,60,60,-60,60,60,>|,&1,
14:0,13:/*Et,{1,9}:/0,{2,10}:/_,
{4,6^~35,8,12^35}:/*_ ,
{6^35,11,12^~35}:/OH,
#3:\*,0,30,|,{?6 '.7,2:0,
{3,5^35}:/_,4:/OH,5^~35:/0!,
#5:\*^30 '1.7,0,! ,|,{?6 '.7,6:0,
5:/_,2:/OH,3:/NMeMe
```

(Vancomycin)

FM(C): C₆₆H₇₅Cl₂N₉O₂₄

FM(C): 1449.253

FM(D): 1449.25



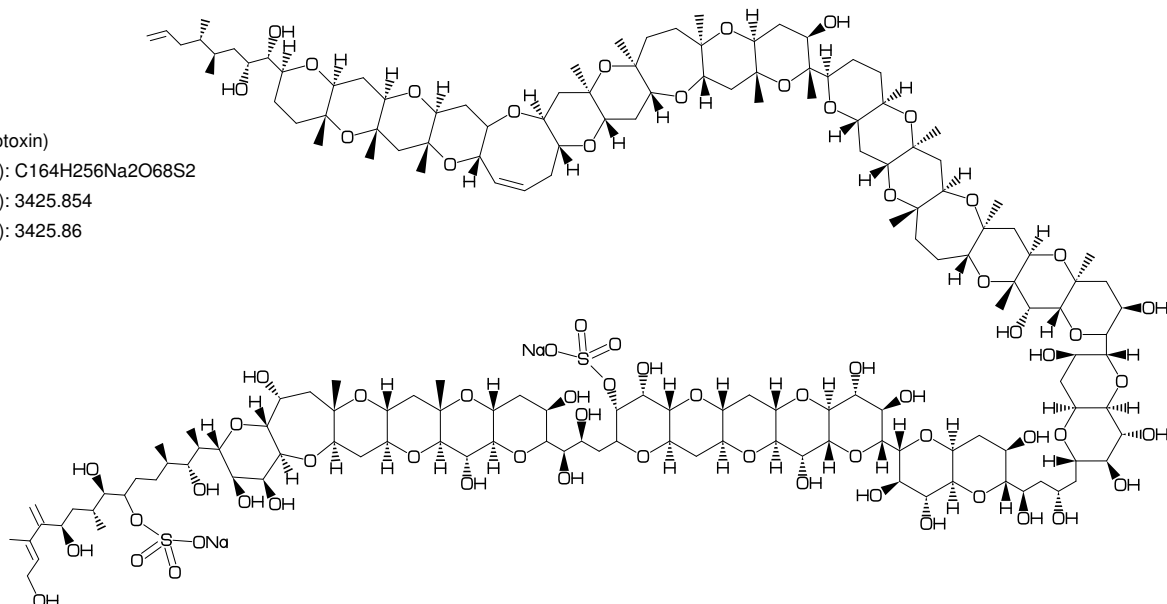
```
<30,|<,' '1,!12,{1,3,12}=zf,7=wf,
/H^~60,60,*/OH,60,Ph,-4:/Cl,
-3:\,0,! ,Ph,-4:\,0,! ,Ph,-1^15:/Cl,
-3:\,/OH,*/H^~60,&#1,
#7:@,&#26,#1:@,120,/0,60,NH,60,
/*H,*/COOH^180,-60,
Ph,{-2,-4}:/OH,-1:\,Ph,-5:/OH,-2:@,&#4,>|,
{3^40,6,9,12}:/0,{2,5,8,11}:NH,
{1^180,4^180}:/H,
{7^~60,10^60,14^60}:/*H,
#10:\^~60,60,/0,! ,NH2,#13:* \,NH,! ,/0,! ,
/!iPr^~35>60,*/H^60 ,!~zf,NH,! ,
#23:\,0,! ,|,{?6 '.7,2:0,3^10:/!OH,{4,5}:/OH,
-1:\,0,! ,|,{?6 '.7,6:0,
{3^35,5}:/_,3^~35:/NH2,4:/OH
```

(Maitotoxin)

FM(C): C164H256Na2O68S2

FM(C): 3425.854

FM(D): 3425.86



<55.8,?6,-4=?7 ,{-4,-3,-3,-3}=?6,-3:\,!3,?6,{-4,-3,-3,-3}=?6,
-3:\,!3,60,<-30,?6,-3=?6,
-3:@,30,<30,?6,{-3,-3}=?6,-3=?7,{-4,-3,-3}=?6,
-2:\,!3,60,<-30,?6,-3=?6,-3=?7,{-3,-3}=?6,-3=?8,-3=d1,{-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}:0,
{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,{47,57,71}:/*H^60,
{3,8,13,17,21,33,38,42,56,70,84,92,101,106,111,128,138,142,146,150}:/*H^-60,
{4,14,22,34,39,43,81,89,98,102,116,121,125,129,133}:*/H^60,
{6,46,50,53,60,67,74}:*/H^-60,{9,18,85,93,112,139,143,147}:*/_ '1^60,
{80,88,97,115,120,124}:/*_ '1^-60,108:/*_ '1^-60,
#6:\,!11,60~dr,-60,60,OH,2:/*OH,{7,10}:/*OH,{1,3}:*/_,{8~zf,11~dm,12}:/_,
6:\,0,30,S00,30,"O{Na}",
#36:@,-45~zf,0,30,S00,30,"O{Na}",#150:\,!7,{1,2}:/*OH,4:*/_ ,5:/*_ ,7=d1

TCA-cycle

