

MCF example for luamplib(Lua \LaTeX)

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

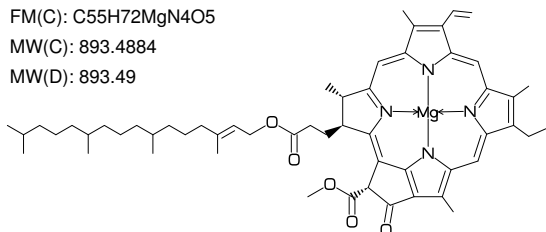
FM(C) : molecular formula calculated by mcf2graph
MW(C) : molecular weight calculated by mcf2graph
MW(D) : molecular weight from literature data

(Chlorophyll a)

FM(C): C₅₅H₇₂MgN₄O₅

MW(C): 893.4884

MW(D): 893.49



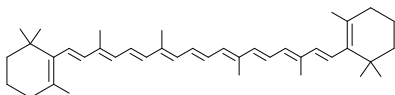
```
|<, '1,?5,{2,5}=d1,4:N,3:\,54~d1,  
|,?5,{2,4}=d1,5:N,  
-2:\,54~d1,|,?5,2=d1,5:N,  
-2:\~d1,54,|,?5,5=d1,5:N,-2:\~d1,&$5,  
-1:@,24,/*C00!^15,72,//0,&$1,>|,  
4:\'1.45,Mg,&17,-1:@,&11~vb,-1:@,&23~vb,  
{2,9,15,20~zf}:/_8:!/!,14:\,!!,  
21:@,-6~wf,!2,//0,!0,!2,!!,  
|,!13,{1,5,9,13}:/_
```

(beta-Carotene)

FM(C): C₄₀H₅₆

MW(C): 536.8722

MW(D): 536.888



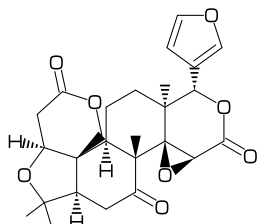
```
<30,?6,3=d1,{3,5^35,5^-35}:/_  
4:\,|,!18,  
{1,3,5,7,9,11,13,15,17}=dr,  
{3,7,12,16}:/_  
|,?6,6=d1,{6,2^35,2^-35}:/_
```

(Limonin)

FM(C): C₂₆H₃₀O₈

MW(C): 470.5113

MW(D): 470.51



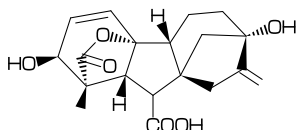
```
<30,?6,{-3,-4}=?6,-5=?3,  
-2=wf,-1=wb,6=?5,-4=?6,-5=wf,  
{13,15,17,20}:0,{3,12,21}://0,  
{4~wf^60,8~zf^60,18^35,18^-35}:/_  
{1^60,5^180,16^60}:/*H,  
14:\*,|,?5,{1,4}=d1,3:0
```

(Gibberellin A3)

FM(C): C₁₉H₂₂O₆

MW(C): 346.3742

MW(D): 346.37



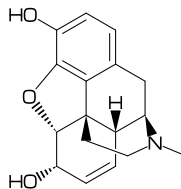
```
<18,?5,3=?7,5=?6[12],8:@,160'1.3,&3,  
13=d1,6=wf,8=wb,  
5:@,40~zf'1,0,60,//0^180,&14~zb,  
2:/COOH,7://_,13:*/OH,8:/*OH,  
14:*/_,{1^60,4^60}:/*H
```

(Morphine)

FM(C): C₁₇H₁₉NO₃

MW(C): 285.3375

MW(D): 285.343



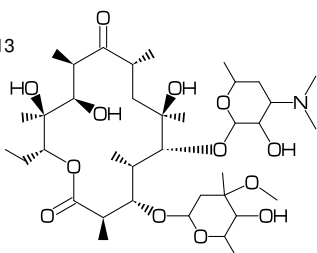
```
<30,Ph,2=?6,-4=?6,(1,12)=?5[2],  
-1:0,-1=zb,  
7:@,60~wf'0.75,70~si_'1.3,  
45,N,/_,&9~wb,  
15=d1,  
6:/OH,8^180:*/H,12:/*OH
```

(Erythromycin)

FM(C): C₃₇H₆₇NO₁₃

MW(C): 733.9263

MW(D): 733.93



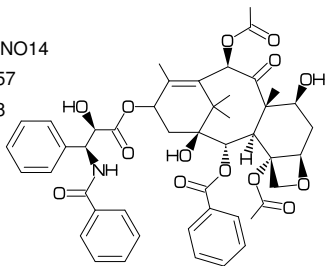
```
<30,|<, '1,<-120,60,60,60,-60,60,  
60,-60,60,60,60,-60,60,60,>|,&1,  
14:0,13:/*Et,{1,9}://0,{2,10}:/*_/  
{4,6^-35,8,12^35}:/*_/  
{6^-35,11,12^-35}:/*OH,  
$3:\*,0,30,|,?6'.7,2:0,  
{3,5^35}:/_4:/OH,5^-35:/0!,  
$5:\*^30'1.7,0,!|,?6'.7,6:0,  
5:/_2:/OH,3:/NMe
```

(Paclitaxel)

FM(C): C47H51NO14

MW(C): 853.9057

MW(D): 853.918



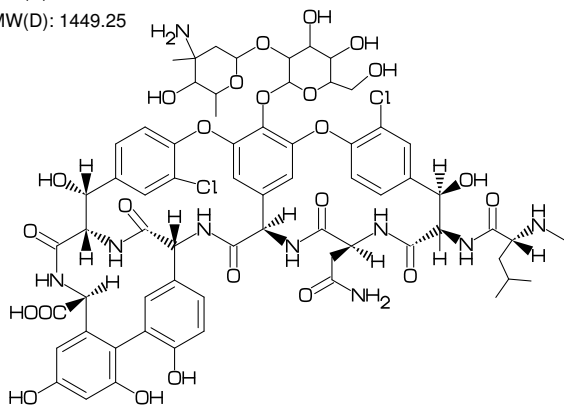
?6,5=d,3:@,|<,' '1,36,45,45,45,45,>|,&\$5,
 -4=?6,-4=?4,||,-1=wb,-3=wf,-1:0,
 {4^35,4^~35,6}:/_,{3^~60,15}:/OH,
 8:/*H^~60,9:*/_~60,10://0,
 \$1:\,0,!//0,!*/OH,!/Ph,60~wf,NH,-
 60,//0,60,Ph,
 \$7:*,0,-45,//0,60,Ph,\$11:* \,0,-60,//0,60,
 \$12:*^~15,0,60,//0,-60)

(Vancomycin)

FM(C): C66H75Cl2N9O24

MW(C): 1449.253

MW(D): 1449.25



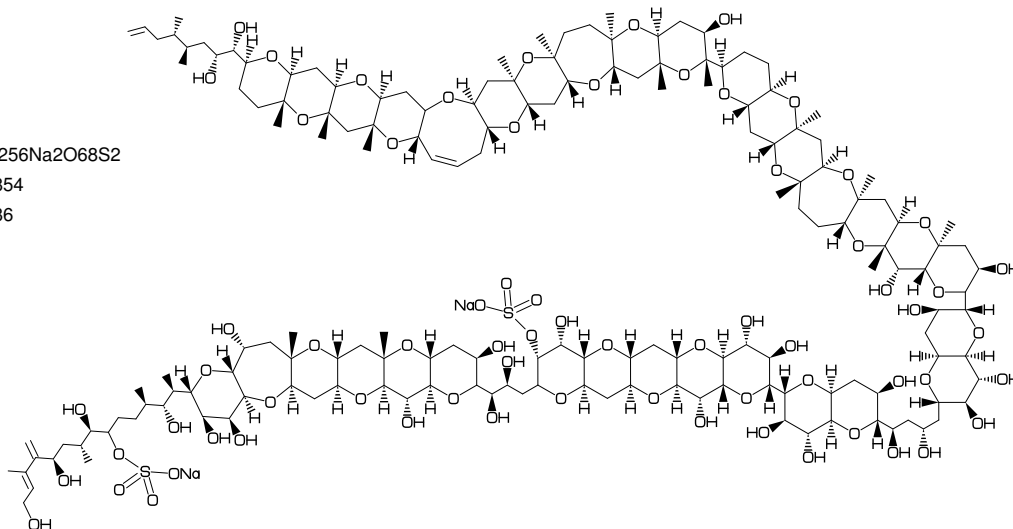
<30,|<,' '1,!12,{1,3,12}=zf,7=wf,
 /H^~60,60,*/OH,60,Ph,-4:/Cl,
 -3:\,0,!Ph,-4:\,0,!Ph,-1^15:/Cl,
 -3:\,/*OH,*H^~60,&\$1,
 \$7:@,&\$26,\$1:@,120,//0,60,NH,60,
 /*H,*COOH^180,-60,
 Ph,{-2,-4}:/OH,-1:\,Ph,-5:/OH,-2:@,&\$4,>|,
 {3^40,6,9,12}://0,{2,5,8,11}:NH,
 {1^180,4^180}:/H,
 {7^~60,10^60,14^60}:/H,
 \$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)

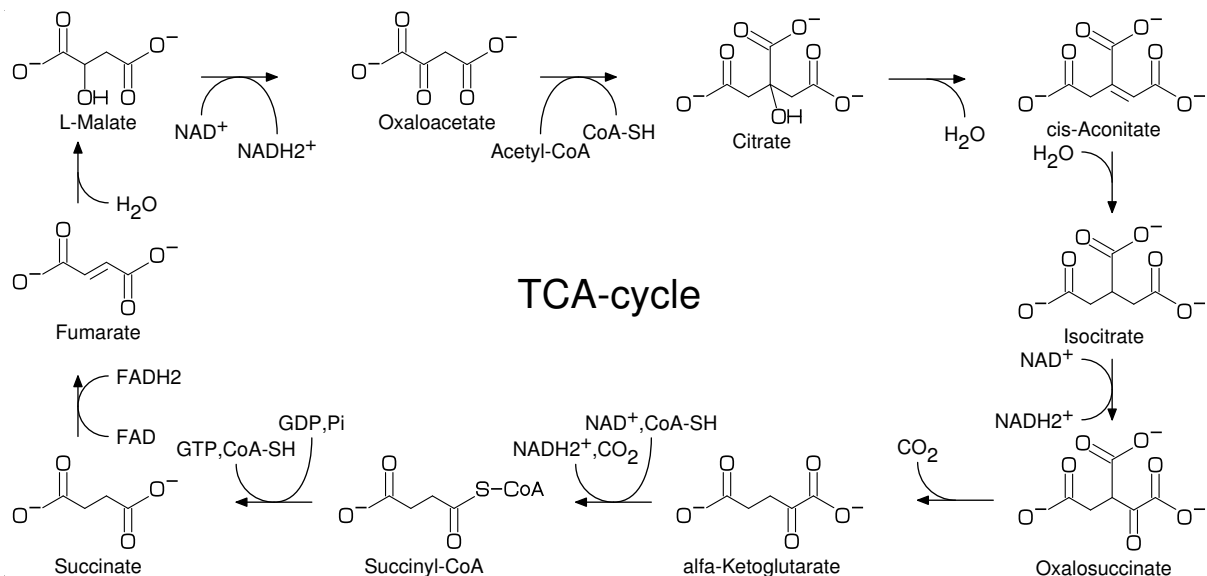
FM(C): C164H256Na2O68S2

MW(C): 3425.854

MW(D): 3425.86



<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=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



```

beginfont("EN:TCA cycle")
font_wd:=160mm;
font_ht:=75mm;
max_bond_length:=5mm;
Om:='{"0^-~}";
Mca(0.33, 1)(<30,Om,!0,//0,! ,//0,!2,//0,! ,Om)
Mca(0.66, 1)(<30,Om,!0,//0,!4,//0,! ,Om,-4'1:\,//0,! ,Om,4:/OH^-165)
Mca(1, 1)(<30,Om,!0,//0,!2,!~dr,! ,//0,! ,Om,-4'1:\,//0,! ,Om)
Mca(1, 0.55)(<30,Om,!0,//0,!4,//0,! ,Om,-4:\'1,//0,! ,Om)
Mca(1, 0.05)(<30,Om,!0,//0,!3,//0,! ,//0,! ,Om,-4:\'1,//0,! ,Om)
Mca(0.66,0.05)(<30,Om,!0,//0,!3,//0,! ,//0,! ,Om)
Mca(0.33,0.05)(<30,Om,!0,//0,!3,//0,! ,{"S-CoA"})
Mca(0, 0.05)(<30,Om,!0,//0,!3,//0,! ,Om)
Mca(0, 0.55)(<30,Om,!0,//0,! ,!~dr,! ,//0,! ,Om)
Mca(0, 1)(<30,Om,!0,//0,!3,//0,! ,Om,3:/OH)
EXT(
defaultfont:="uhvr8r";
defaultscale:=0.75;
ext_setup;
save dx; pair dx; dx:=(12mm,0);
label.bot("Oxaloacetate",p1+dx); label.bot("Citrate",p2+dx);
label.bot("cis-Aconitate",p3+dx); label.bot("Isocitrate",p4+dx);
label.bot("Oxalosuccinate",p5+dx); label.bot("alfa-Ketoglutarate",p6+dx);
label.bot("Succinyl-CoA",p7+dx); label.bot("Succinate",p8+dx);
label.bot("Fumarate",p9+dx); label.bot("L-Malate",p10+dx);
sw_label_emu:=1;
ext_setup;
r_arrow(10mm)( 0)(p1+(1.1w1,.3h1))("","0)("","0)("Acetyl-CoA",1.5)("CoA-SH",1);
r_arrow(10mm)( 0)(p2+(1.1w2,.4h2))("","0)("","0)("","0)("H_2O",1);
r_arrow( 8mm)(270)(p3+(.5w3,-.4h3))("","0)("","0)("H_2O",1)("","0");
r_arrow( 8mm)(270)(p4+(.5w4,-.4h4))("","0)("","0)("NAD^+",1)("NADH2^+",1);
r_arrow(10mm)(180)(p5+(-.1w5,.4h5))("","0)("","0)("","0)("CO_2",1);
r_arrow(10mm)(180)(p6+(-.1w6,.5h6))("","0)("","0)("NAD^+^",CoA-SH",1.7)("NADH2^+^",CO_2",1);
r_arrow(10mm)(180)(p7+(-.1w7,.5h7))("","0)("","0)("GDP,Pi",1.7)("GTP,CoA-SH",1);
r_arrow( 8mm)( 90)(p8+(.4w8,1.2h8))("","0)("","0)("FAD",1)("FADH2",1);
r_arrow( 8mm)( 90)(p9+(.4w9,1.2h9))("","0)("","0)("H_2O",1)("","0");
r_arrow(10mm)( 0)(p10+(1.1w10,.3h10))("","0)("","0)("NAD^+",1)("NADH2^+",1.5);
defaultscale:=1.5;
label("TCA-cycle",(0.5w,0.5h));
)
endfont

```