

MCF example for luamplib(Lua \LaTeX)

Author : Akira Yamaji Date : April 16, 2018
Located at : <http://www.ctan.org/pkg/mcf2graph>

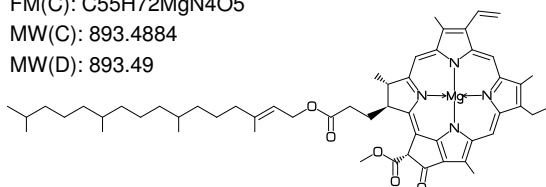
FM(C) : molecular formula calculated by mcf2graph
MW(C) : molecular weight calculated by mcf2graph
MW(D) : molecular weight from literature data

(Chlorophyll a)

FM(C): C₅₅H₇₂MgN₄O₅

MW(C): 893.4884

MW(D): 893.49



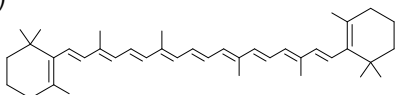
```
|<=1,?5,{2,5}=d1,4:N,3:\,54~d1,  
|,?5,{2,4}=d1,5:N,  
-2:\,54~d1,|,?5,2=d1,5:N,  
-2:\~d1,54,|,?5,5=d1,5:N,-2:\~d1,$5:&,  
-1:@,24,/*C00!~15,72,//0,$1:&,>|,  
4:\'1.45,Mg,17:&,-1:@,11~vb:&,-1:@,23~vb:&,  
{2,9,15,20~zf}:/_,8:!/!,14:\,!!,  
21:@,-6~wf,!2,//0,!0,!2,!!,  
|,!13,{1,5,9,13}:/_,
```

(beta-Carotene)

FM(C): C₄₀H₅₆

MW(C): 536.8722

MW(D): 536.888



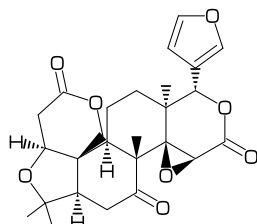
```
<30,?6,3=d1,{3,5^35,5^-35}:/_,  
4:\,|,!18,  
{1,3,5,7,9,11,13,15,17}=dr,  
{3,7,12,16}:/_,  
|,?6,6=d1,{6,2^35,2^-35}:/_
```

(Limonin)

FM(C): C₂₆H₃₀O₈

MW(C): 470.5113

MW(D): 470.51



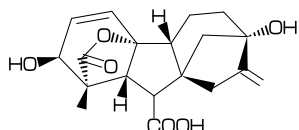
```
<30,?6,{-3,-4}=?6,-5=?3,  
-2=wf,-1=wb,6=?5,-4=?6,-5=wf,  
{13,15,17,20}:0,{3,12,21}:/0,  
{4~wf^60,8~zf^60,18^35,18^-35}:/_,  
{1^60,5^180,16^60}:/*H,  
14:\*,|,?5,{1,4}=d1,3:0
```

(Gibberellin A3)

FM(C): C₁₉H₂₂O₆

MW(C): 346.3742

MW(D): 346.37



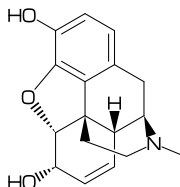
```
<18,?5,3=?7,5=?6[12],8:@,160'1.3,3:&,  
13=d1,6=wf,8=wb,  
5:@,40~zf'1,0,60,//0^180,14~zb:&,  
2:/COOH,7:/_ ,13:*/OH,8:/*OH,  
14:*/_,{1^60,4^60}:/H
```

(Morphine)

FM(C): C₁₇H₁₉NO₃

MW(C): 285.3375

MW(D): 285.343



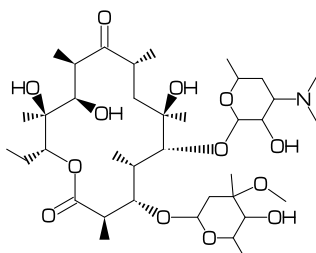
```
<30,Ph,2=?6,-4=?6,(1,12)=?5[2],  
-1:0,-1=zb,  
7:@,60~wf'0.75,70~si_'1.3,  
45,N,/_ ,9~wb:&,  
15=d1,  
6:/OH,8^180:*/H,12:/*OH
```

(Erythromycin)

FM(C): C₃₇H₆₇NO₁₃

MW(C): 733.9263

MW(D): 733.93



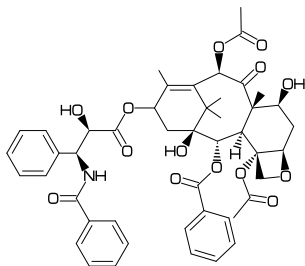
```
<30,|<=1,<-120,60,60,60,-60,60,  
60,-60,60,60,60,-60,60,60,>|,1:&,  
14:0,13:/*Et,{1,9}:/0,{2,10}:/_,  
{4,6^-35,8,12^35}:/*_ ,  
{6^35,11,12^-35}:/OH,  
$3:\*,0,30,|,?6'.7,2:0,  
{3,5^35}:/_,4:/OH,5^-35:/0!,  
$5:\*^30'1.7,0,! ,?6'.7,6:0,  
5:/_,2:/OH,3:/NMeMe
```

(Paclitaxel)

FM(C): C47H51NO14

MW(C): 853.9057

MW(D): 853.918



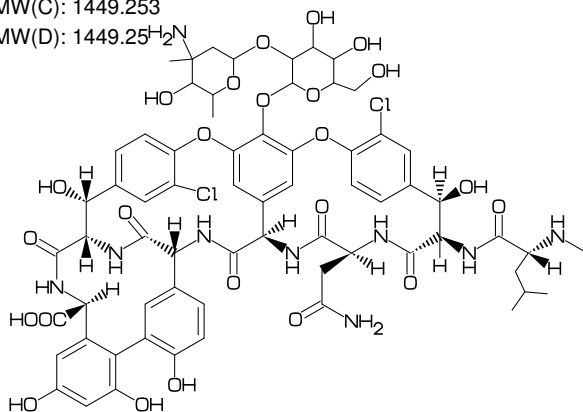
?6,5=d,3:@,|<=1,36,45,45,45,45,>|,\$5:&,
-4=?6,-4=?4,||,-1=wb,-3=wf,-1:0,
{4~35,4~35,6}:/_,{3~60,15}:*/OH,
8:/*H~60,9:*/_60,10://0,
\$1:\,0,!//0,!*/OH,!/Ph,
60~wf,NH,-60,//0,60,Ph,
\$7:*,0,-45,//0,60,Ph,\$11:*\\,0,-60,//0,60,
\$12:*~15,0,60,//0,-60)

(Vancomycin)

FM(C): C66H75Cl2N9O24

MW(C): 1449.253

MW(D): 1449.25H2N



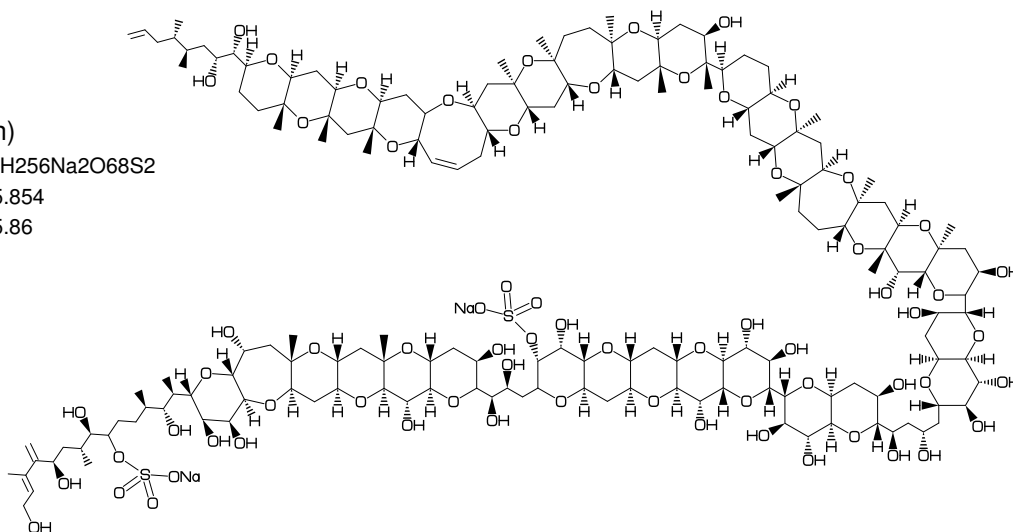
<30,|<=1,!12,{1,3,12}=zf,7=wf,
/H~60,60,*/OH,60,Ph,-4:/Cl,
-3:\\,0,!Ph,-4:\\,0,!Ph,-1^15:/Cl,
-3:\\,/*OH,*/H~60,\$1:&,
\$7:@,\$26:&,\$1:@,120,//0,60,NH,60,
/*H,*/COOH^180,-60,
Ph,{2,-4}:/OH,-1:\\,Ph,-5:/OH,-2:@,\$4:&,>|,
{3^40,6,9,12}://0,{2,5,8,11}:NH,
{1^180,4^180}:*/H,
{7~60,10^60,14^60}:/*H,
\$10:*\\~60,60,//0,!NH2,\$13:*\\,NH,!//0,!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

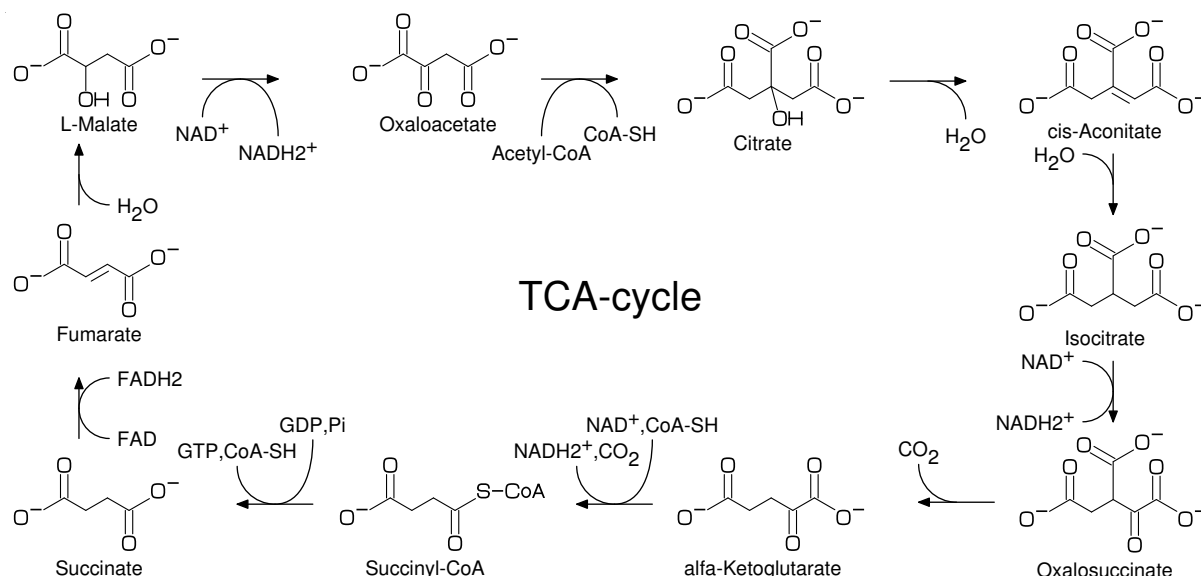
FM(C): C164H256Na2O68S2

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:='{"O^-~"}';
Mca(0.33, 1)(<30,Om,!0,/,0,!,/,0,!,/,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

```