

# MCF example for luamplib(Lua $\text{\LaTeX}$ )

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

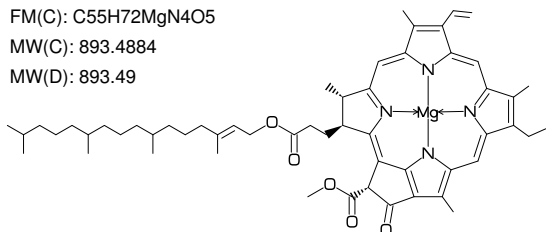
FM(C) : molecular formula calculated by mcf2graph  
MW(C) : molecular weight calculated by mcf2graph  
MW(D) : molecular weight from literature data

(Chlorophyll a)

FM(C): C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>

MW(C): 893.4884

MW(D): 893.49



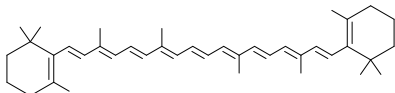
```
|<, '1, ?5, {2,5}=d1,4:N,3:\,54~d1,  
|, ?5, {2,4}=d1,5:N,  
-2:\,54~d1, |, ?5,2=d1,5:N,  
-2:\~d1,54, |, ?5,5=d1,5:N, -2:\~d1, &$5,  
-1:@,24, /*C00!^15,72, //0, &$1, >|,  
4:\ '1.45, Mg, &17, -1:@, &11~vb, -1:@, &23~vb,  
{2,9,15,20~zf}:/_ ,8: /!, 14:\, !!,  
21:@, -6~wf, !2, //0, !, 0, !2, !!,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

(beta-Carotene)

FM(C): C<sub>40</sub>H<sub>56</sub>

MW(C): 536.8722

MW(D): 536.888



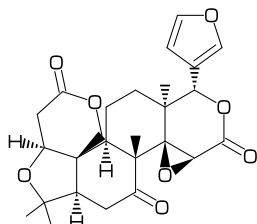
```
<30, ?6, 3=d1, {3,5^35,5^~35}:/_ ,  
4:\, |, !18,  
{1,3,5,7,9,11,13,15,17}=dr,  
{3,7,12,16}:/_ ,  
|, ?6,6=d1, {6,2^35,2^~35}:/_
```

(Limonin)

FM(C): C<sub>26</sub>H<sub>30</sub>O<sub>8</sub>

MW(C): 470.5113

MW(D): 470.51



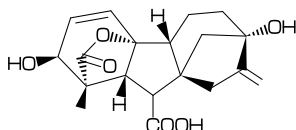
```
<30, ?6, {-3,-4}=?6, -5=?3,  
-2=wf, -1=wb, 6=?5, -4=?6, -5=wf,  
{13,15,17,20}:0, {3,12,21}://0,  
{4~wf^60,8~zf^60,18^35,18^~35}:/_ ,  
{1^60,5^180,16^60}:/*H,  
14:\*, |, ?5, {1,4}=d1, 3:0
```

(Gibberellin A3)

FM(C): C<sub>19</sub>H<sub>22</sub>O<sub>6</sub>

MW(C): 346.3742

MW(D): 346.37



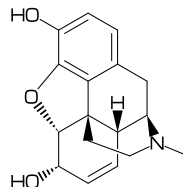
```
<18, ?5, 3=?7, 5=?6 [12], 8:@, 160 '1.3, &3,  
13=d1, 6=wf, 8=wb,  
5:@, 40~zf '1, 0, 60, //0^180, &14~zb,  
2:/COOH, 7://_ , 13:*/OH, 8:/*OH,  
14:*/_ , {1^60,4^60}:/*H
```

(Morphine)

FM(C): C<sub>17</sub>H<sub>19</sub>NO<sub>3</sub>

MW(C): 285.3375

MW(D): 285.343



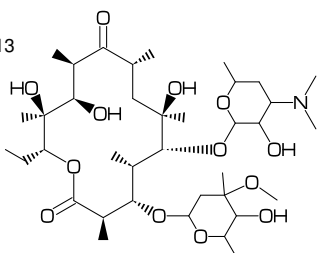
```
<30, Ph, 2=?6, -4=?6, (1,12)=?5 [2],  
-1:0, -1=zb,  
7:@, 60~wf '0.75, 70~si_ '1.3,  
45, N, /_ , &9~wb,  
15=d1,  
6:/OH, 8^180:*/H, 12:/*OH
```

(Erythromycin)

FM(C): C<sub>37</sub>H<sub>67</sub>NO<sub>13</sub>

MW(C): 733.9263

MW(D): 733.93



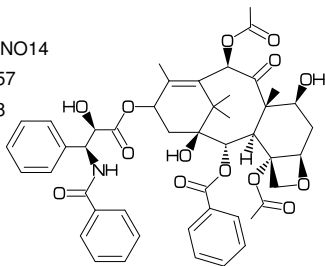
```
<30, |<, '1, <-120, 60, 60, 60, -60, 60,  
60, -60, 60, 60, 60, -60, 60, 60, >|, &1,  
14:0, 13:/*Et, {1,9}://0, {2,10}:/*_ ,  
{4,6^~35,8,12^35}:/*_ ,  
{6^35,11,12^~35}:/*OH,  
$3:\*, 0, 30, |, ?6 ' .7, 2:0,  
{3,5^35}:/_ , 4:/OH, 5^~35:/0!,  
$5:\*^30 '1.7, 0, !, |, ?6 ' .7, 6:0,  
5:/_ , 2:/OH,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

(Paclitaxel)

FM(C): C47H51NO14

MW(C): 853.9057

MW(D): 853.918



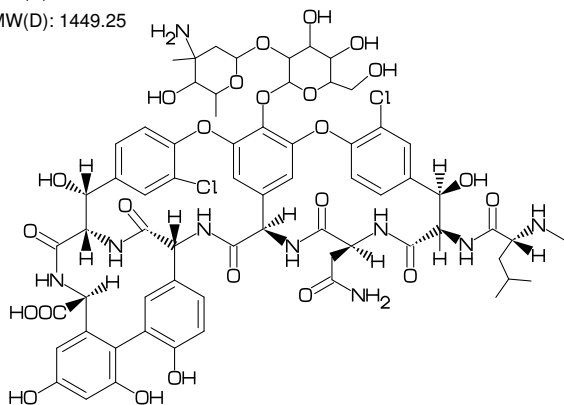
?6,5=d,3:@,|<,' '1,36,45,45,45,45,>|,&\$5,  
-4=?6,-4=?4,||,-1=wb,-3=wf,-1:0,  
{4^35,4^~35,6}:/\_,{3^~60,15}:/OH,  
8:/\*H^~60,9:\*/\_~60,10://0,  
\$1:\,0,!//0,!\*/OH,!/Ph,60~wf,NH,-  
60,//0,60,Ph,  
\$7:\\*,0,-45,//0,60,Ph,\$11:\* \,0,-60,//0,60,  
\$12:\\*^~15,0,60,//0,-60)

(Vancomycin)

FM(C): C66H75Cl2N9O24

MW(C): 1449.253

MW(D): 1449.25



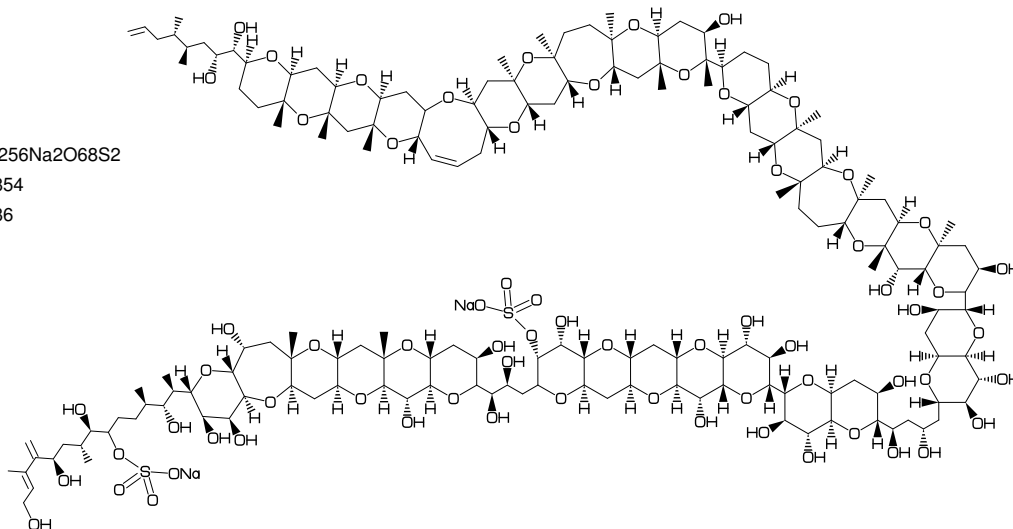
<30,|<,' '1,!12,{1,3,12}=zf,7=wf,  
/H^~60,60,\*/OH,60,Ph,-4:/Cl,  
-3:\,0,!Ph,-4:\,0,!Ph,-1^15:/Cl,  
-3:\,/\*OH,\*H^~60,&\$1,  
\$7:@,&\$26,\$1:@,120,//0,60,NH,60,  
/\*H,\*COOH^180,-60,  
Ph,{-2,-4}:/OH,-1:\,Ph,-5:/OH,-2:@,&\$4,>|,  
{3^40,6,9,12}://0,{2,5,8,11}:NH,  
{1^180,4^180}:/H,  
{7^~60,10^60,14^60}:/H,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

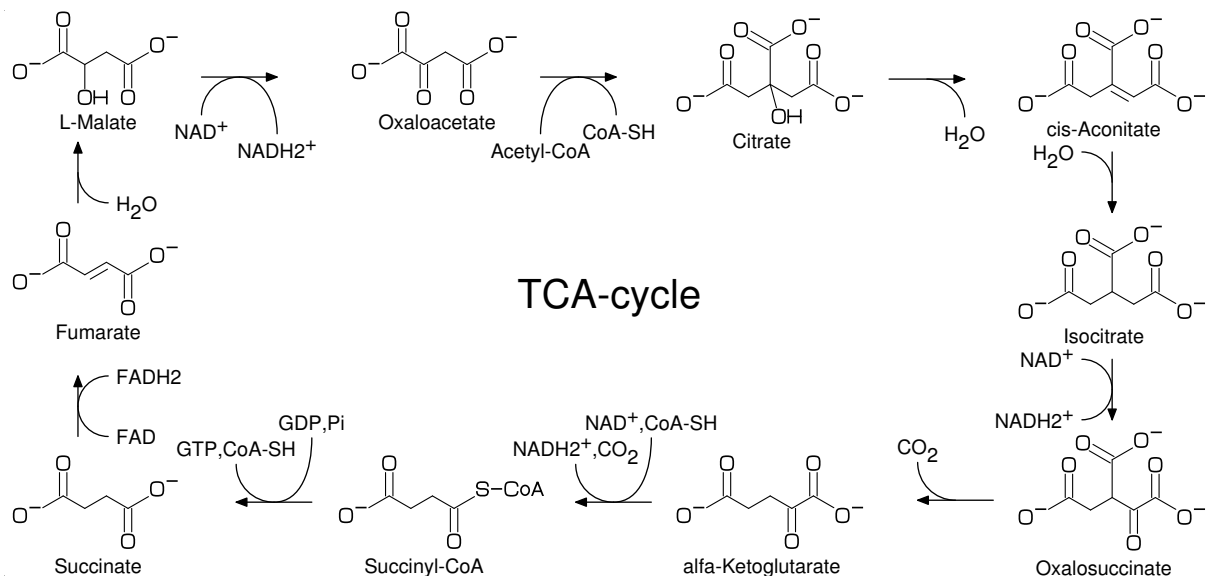
FM(C): C164H256Na2O68S2

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_2_0",1);
r_arrow( 8mm)(270)(p3+(.5w3,-.4h3))("","0)("","0)("H_2_0",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_2_0",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

```