

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

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

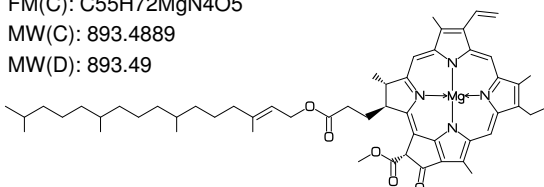
FM(C) : molecular formula calculated by mcf2graph  
MW(C) : molecular weight calculated by mcf2graph  
MW(D) : molecular weight from literature data

## (Chlorophyll a)

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

MW(C): 893.4889

MW(D): 893.49



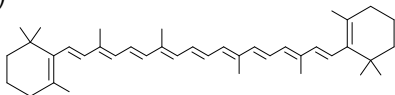
```
|<=1,?5,{2,5}=d1,4:N,3:\,54~d1,  
|,?5,{2,4}=d1,5:N,  
-2:\,54~d1,|,?5,2=d1,5:N,  
-2:\~d1,54,|,?5,5=d1,5:N,-2:\~d1,$5:#,  
-1:@,24,/*C00!^15,72,//0,$1:#,>|,  
4:\^1.45,Mg,17:#,-1:@,11~vb:#,-1:@,23~vb:#,  
{2,9,15,20~zf}:/_8:/!,14:\,!!,  
21:@,-6~wf,!2,//0,!0,!2,!!,  
|,!13,{1,5,9,13}:/_
```

## (beta-Carotene)

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

MW(C): 536.8726

MW(D): 536.888



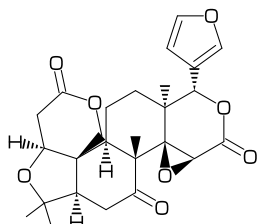
```
<30,?6,3=d1,{3,5^35,5^-35}:/_  
4:\,|,!18,  
{1,3,5,7,9,11,13,15,17}=dr,  
{3,7,12,16}:/_  
|,?6,6=d1,{6,2^35,2^-35}:/_
```

## (Limonin)

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

MW(C): 470.5115

MW(D): 470.51



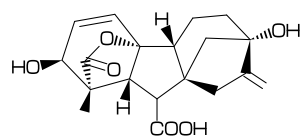
```
<30,?6,{-3,-4}=?6,-5=?3,  
-2=wf,-1=wb,6=?5,-4=?6,-5=wf,  
{13,15,17,20}:0,{3,12,21}://0,  
{4~wf^60,8~zf^60,18^35,18^-35}:/_  
{1^60,5^180,16^60}:/*H,  
14:\*,|,?5,{1,4}=d1,3:0
```

## (Gibberellin A3)

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

MW(C): 346.3743

MW(D): 346.37



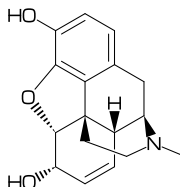
```
<18,?5,3=?7,5=?6[12],8:@,160^1.3,3:#,  
13=d1,6=wf,8=wb,  
5:@,40~zf^1,0,60,//0^180,14~zb:#,  
2:/COOH,7://_,13:*/OH,8:*/OH,  
14:*/_,{1,4}:/H^60)
```

## (Morphine)

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

MW(C): 285.3376

MW(D): 285.343



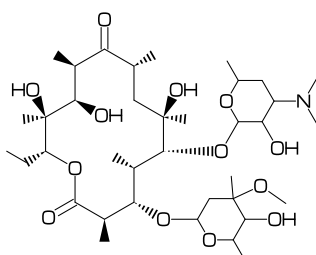
```
<30,Ph,2=?6,-4=?6,(1,12)=?5[2],  
-1:0,-1=zb,  
7:@,60~wf^0.75,70~si^1.3,  
45,N,/_9~wb:#,  
15=d1,  
6:/OH,8^180:*/H,12:*/OH
```

## (Erythromycin)

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

MW(C): 733.9267

MW(D): 733.93



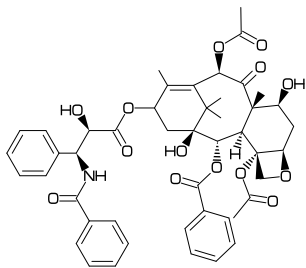
```
<30,|<=1,<-120,60,60,60,-60,60,  
60,-60,60,60,60,-60,60,60,>|,1:#,  
14:0,13:/*Et,{1,9}://0,{2,10}:/_/  
{4,6^-35,8,12^35}:/*_  
{6^35,11,12^-35}:/OH,  
$3:\*,0,30,|,?6^7,2:0,  
{3,5^35}:/_4:/OH,5^-35:/0!,  
$5:\*^30^1.7,0,!|,?6^7,6:0,  
5:/_2:/OH,3:/NMe
```

(Paclitaxel)

FM(C): C47H51NO14

MW(C): 853.9061

MW(D): 853.918



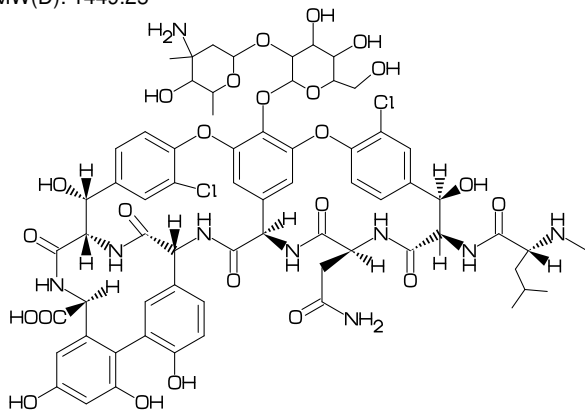
?6,5=d,3:@,|<=1,36,45,45,45,45,>|,\$5:#,  
-4=?6,-4=?4,||,-1=wb,-3=wf,-1:0,  
{4^35,4^-35,6}:/\_,{3^-60,15}:/OH,  
8:/\*H^-60,9:\*/\_60,10://0,  
\$1:\,0,!//0,!\*/OH,!/Ph,  
60~wf,NH,-60,//0,60,Ph,  
\$7:\\*,0,-45,//0,60,Ph,\$11:\*\\,0,-60,//0,60,  
\$12:\*^-15,0,60,//0,-60)

(Vancomycin)

FM(C): C66H75Cl2N9O24

MW(C): 1449.253

MW(D): 1449.25



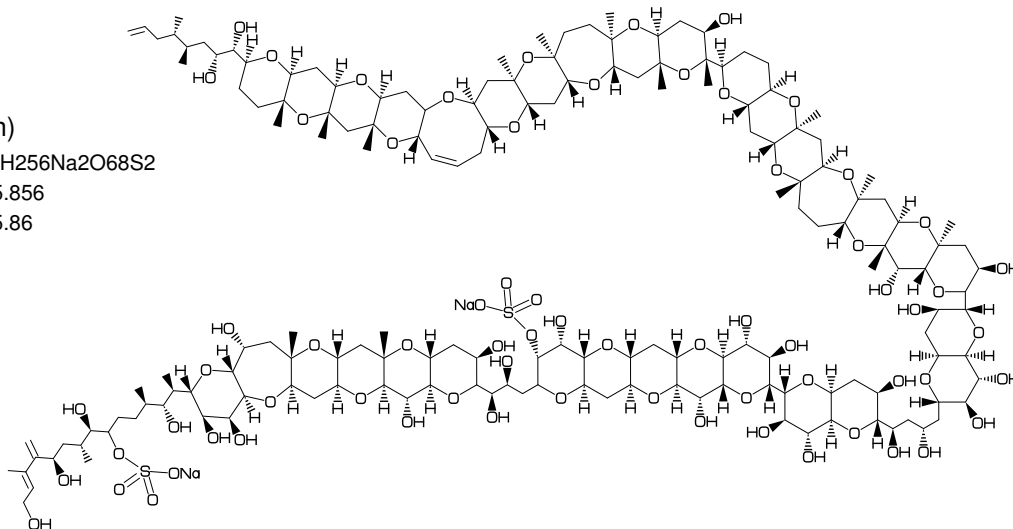
<30,|<=1,!12,{1,3,12}=zf,7=wf,  
/H^-60,60,\*/OH,60,Ph,-4:/Cl,  
-3:\,0,!Ph,-4:\,0,!Ph,-1^15:/Cl,  
-3:\,/\*OH,\*H^-60,\$1:#,  
\$7:@,\$26:#,\$1:@,120,//0,60,NH,60,  
/\*H,\*COOH^180,-60,  
Ph,{-2,-4}:/OH,-1:\,Ph,-5:/OH,-2:@,\$4:#,>|,  
{3^40,6,9,12}://0,{2,5,8,11}:NH,  
{1^180,4^180}:/H,  
{7^-60,10^60,14^60}:/H,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

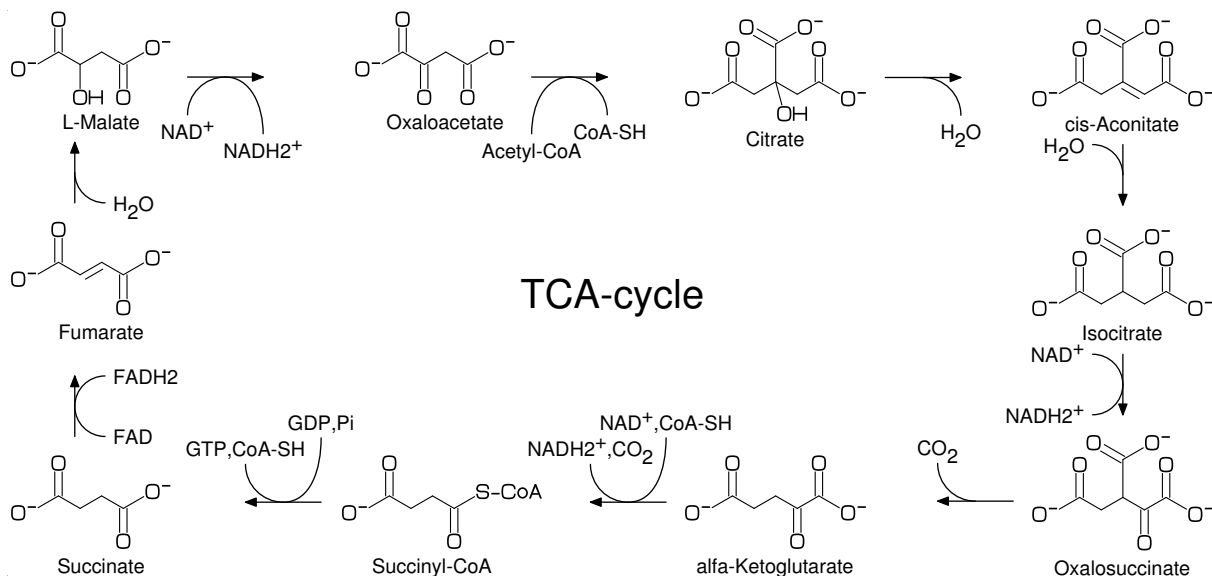
FM(C): C164H256Na2O68S2

MW(C): 3425.856

MW(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:\,!?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;
MCa(0.33, 1)(<30,0[-1],!0,//0,!//0,!2,//0,!0[-1])
MCa(0.66, 1)(<30,0[-1],!0,//0,!4,//0,!0[-1],-4'1:\,//0,!0[-1],4:/OH^-165)
MCa(1, 1)(<30,0[-1],!0,//0,!2,!~dr,!//0,!0[-1],-4'1:\,//0,!0[-1])
MCa(1, 0.55)(<30,0[-1],!0,//0,!4,//0,!0[-1],-4:\'1,//0,!0[-1])
MCa(1, 0.05)(<30,0[-1],!0,//0,!3,//0,!//0,!0[-1],-4:\'1,//0,!0[-1])
MCa(0.66,0.05)(<30,0[-1],!0,//0,!3,//0,!//0,!0[-1])
MCa(0.33,0.05)(<30,0[-1],!0,//0,!3,//0,!,"{S-CoA}")
MCa(0, 0.05)(<30,0[-1],!0,//0,!3,//0,!0[-1])
MCa(0, 0.55)(<30,0[-1],!0,//0,!,!~dr,!//0,!0[-1])
MCa(0, 1)(<30,0[-1],!0,//0,!3,//0,!0[-1],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)("Acetyl-CoA",1.5)("CoA-SH",1);
r_arrow(10mm)( 0)(p2+(1.1w2,.4h2))("","0)("","0)("H_2_O",1);
r_arrow( 8mm)(270)(p3+(.5w3,-.4h3))("","0)("H_2_O",1)("","0");
r_arrow( 8mm)(270)(p4+(.5w4,-.4h4))("","0)("NAD^+",1)("NADH2^+",1);
r_arrow(10mm)(180)(p5+(-.1w5,.4h5))("","0)("","0)("CO_2",1);
r_arrow(10mm)(180)(p6+(-.1w6,.5h6))("","0)("NAD^+",CoA-SH,1.7)("NADH2^+",CO_2,1);
r_arrow(10mm)(180)(p7+(-.1w7,.5h7))("","0)("GDP,Pi",1.7)("GTP,CoA-SH",1);
r_arrow( 8mm)( 90)(p8+(.4w8,1.2h8))("","0)("FAD",1)("FADH2",1);
r_arrow( 8mm)( 90)(p9+(.4w9,1.2h9))("","0)("H_2_O",1)("","0");
r_arrow(10mm)( 0)(p10+(1.1w10,.3h10))("","0)("NAD^+",1)("NADH2^+",1.5);
defaultscale:=1.5;
label("TCA-cycle",(0.5w,0.5h));
)
endfont

```