

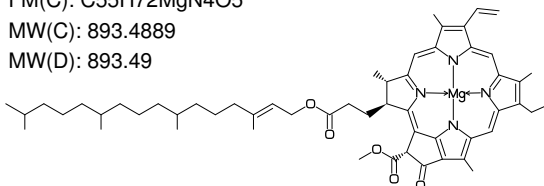
MCF example for luamplib(Lua \LaTeX)

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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)

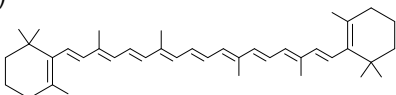
FM(C): C₅₅H₇₂MgN₄O₅
MW(C): 893.4889
MW(D): 893.49



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

(beta-Carotene)

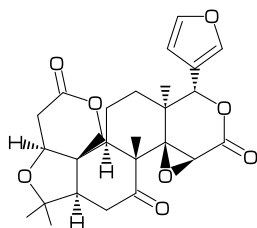
FM(C): C₄₀H₅₆
MW(C): 536.8726
MW(D): 536.888



```
<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)

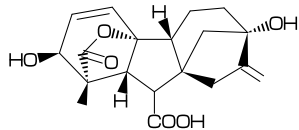
FM(C): C₂₆H₃₀O₈
MW(C): 470.5115
MW(D): 470.51



```
<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)

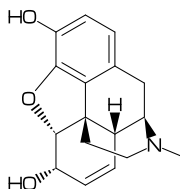
FM(C): C₁₉H₂₂O₆
MW(C): 346.3743
MW(D): 346.37



```
<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)

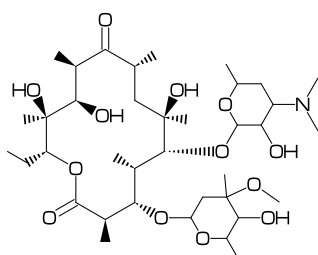
FM(C): C₁₇H₁₉N₃O₃
MW(C): 285.3376
MW(D): 285.343



```
<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): C₃₇H₆₇N₃O₁₃
MW(C): 733.9267
MW(D): 733.93



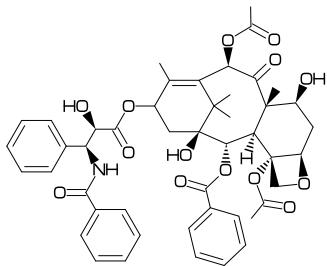
```
<30,|=1,<-120,60,60,60,-60,60,  
60,-60,60,60,60,-60,60,60,=|,1:#,  
14:0,13:/*Et,{1,9}://0,{2,10}:/*_  
{4,6^-35,8,12^35}:/*_  
{6^35,11,12^-35}:/OH,  
$3:\*,0,30,|,{6'}.7,2:0,  
{3,5^35}:/_4:/OH,5^-35:/O!,  
$5:\*^30'1.7,0,!|,{6'}.7,6:0,  
5:/_2:/OH,3:/NMeMe
```

(Paclitaxel)

FM(C): C47H51NO14

MW(C): 853.9061

MW(D): 853.918



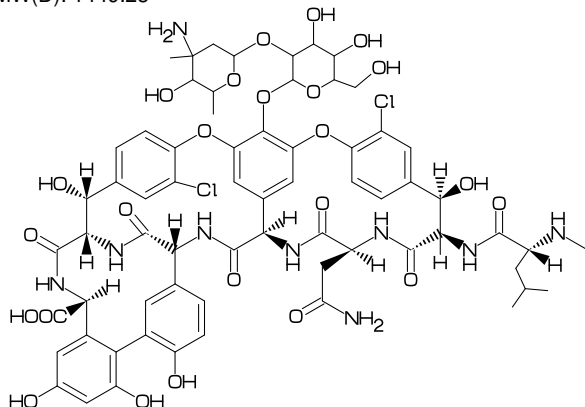
?6,5=d,3:@,|=1,36,45,45,45,45,|=|,\$5:#,
-4=?6,-4=?4,||,-1=wb,-3=wf,-1:0,
{4^35,4^-35,6}:/_,{3^-60,15}:*/OH,
8:/*H^-60,9:*/_^-60,10://0,
\$1:\,0,!,//0,!,*OH,!,/Ph,
60~wf,NH,-60,//0,60,Ph,
\$7:*,0,-45,//0,60,Ph,\$11:*\\,0,-60,//0,60,
.\$12:*^-15,0,60,//0,-60)

(Vancomycin)

FM(C): C66H75Cl2N9O24

MW(C): 1449.253

MW(D): 1449.25



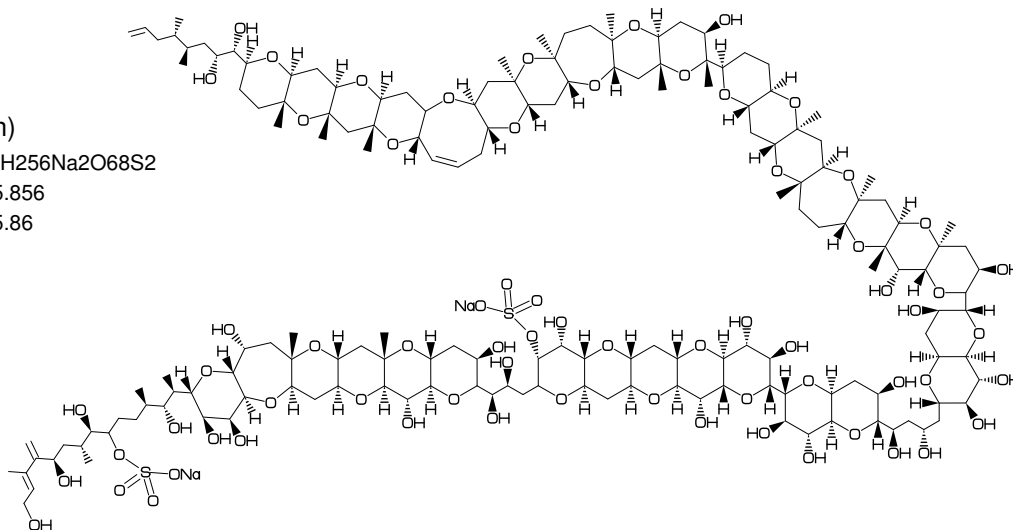
<30,|=1,!12,{1,3,12}=zf,7=wf,
/H^-60,60,*OH,60,Ph,-4:/Cl,
-3:\,0,! ,Ph,-4:\,0,! ,Ph,-1^15:/Cl,
-3:\,/*OH,*H^-60,\$1:#,
\$7:@,\$26:#,\$1:@,120,//0,60,NH,60,
/*H,*COOH^180,-60,
Ph,{-2,-4}:/OH,-1:\,Ph,-5:/OH,-2:@,\$4:#,|=|,
{3^40,6,9,12}://0,{2,5,8,11}:NH,
{1^180,4^180}:*/H,
{7^-60,10^60,14^60}:/*H,
\$10:*\\^-60,60,//0,!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

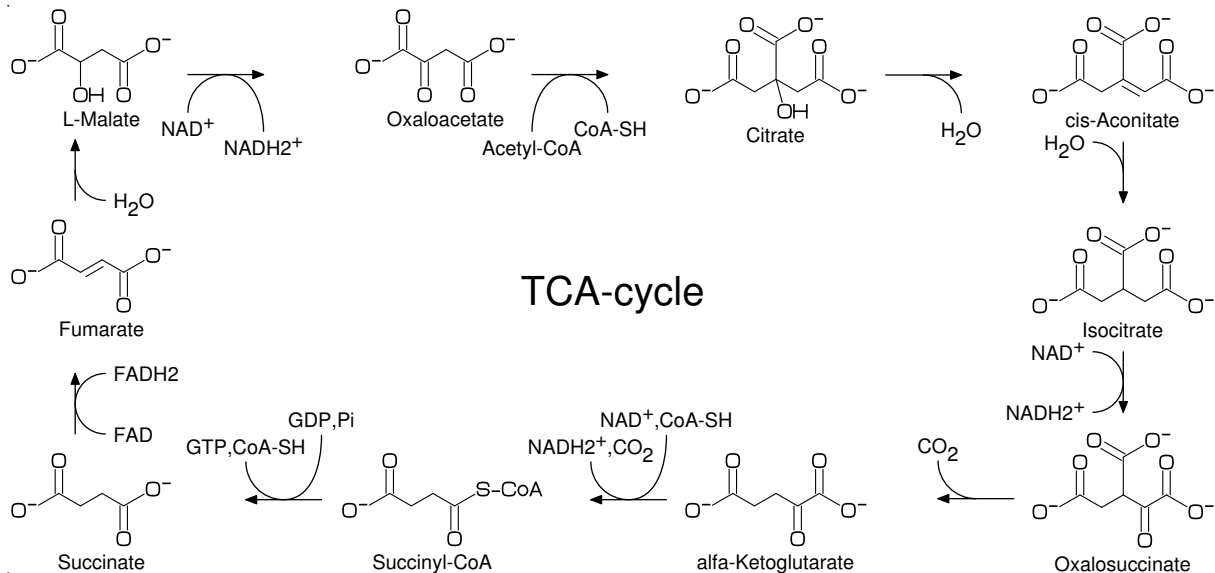
FM(C): C164H256Na2O68S2

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,?6,-3=?6,-3:\,!3,60,<-30,?6,-3=?6,
-3:@,30,<30,?6,{-3,-3}=?6,-3=?7,{-4,-3,-3}=?6,
-2:\,!3,?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")
fsize:=(160mm,75mm);
max_blength:=5mm;
MCat(0.33, 1)(<30,0[-1],!0,//0,! ,//0,!2,//0,! ,0[-1])
MCat(0.66, 1)(<30,0[-1],!0,//0,!4,//0,! ,0[-1],-4'1:\,//0,! ,0[-1],4:/OH^-165)
MCat(1, 1)(<30,0[-1],!0,//0,!2,!~dr,! ,//0,! ,0[-1],-4'1:\,//0,! ,0[-1])
MCat(1, 0.55)(<30,0[-1],!0,//0,!4,//0,! ,0[-1],-4:\'1,//0,! ,0[-1])
MCat(1, 0.05)(<30,0[-1],!0,//0,!3,//0,! ,//0,! ,0[-1],-4:\'1,//0,! ,0[-1])
MCat(0.66,0.05)(<30,0[-1],!0,//0,!3,//0,! ,//0,! ,0[-1])
MCat(0.33,0.05)(<30,0[-1],!0,//0,!3,//0,! ,"{S-CoA}")
MCat(0, 0.05)(<30,0[-1],!0,//0,!3,//0,! ,0[-1])
MCat(0, 0.55)(<30,0[-1],!0,//0,! ,!~dr,! ,//0,! ,0[-1])
MCat(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)(" ",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^+^",1.7)("NADH2^+^",1.7)("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

```