MCF example for luamplib(LuaLaTeX)

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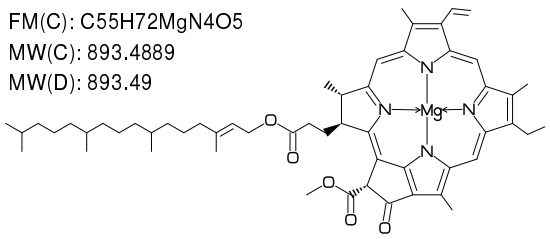
Located at : http://www.ctan.org/pkg/mcf2graph

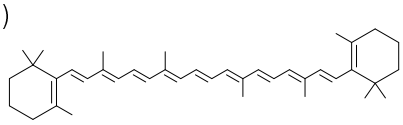
FM(C) : molecular formula calculated by mcf2graph
MW(C) : molecular weight calculated by mcf2graph
MW(D) : molecular weight from literature data

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



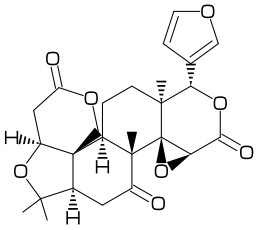
```
|=1,?5,{2,5}=dl,4:N,3:\,54~dl,
|,?5,{2,4}=dl,5:N,
-2:\,54~dl,|,?5,2=d,5:N,-2:\~dl,54,
|,?5,5=d,5:N,-2:\~dl,$5:#,
-1:@,24,/*COO!^15,72,//O,$1:#,=|,||,
 {2,9,15,20~zf}:/_,8:/!,14:\,!!,
 4:\‘1.45,Mg,17:#,-1:@,11~vb:#,
 -1:@,23~vb:#,
 21:@,-6~wf,!2,//O,!,O,!2,!!,
|,!13,{1,5,9,13}:/_
```

(beta-Carotene)
FM(C): C40H56
MW(C): 536.8726
MW(D): 536.888



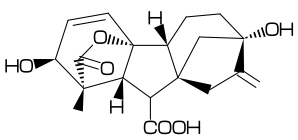
```
<30,?6,3=dl,{3,5^35,5^-35}:/_,
4:\,|,!18,
{1,3,5,7,9,11,13,15,17}=dr,
{3,7,12,16}:/_,
|,?6,6=dl,{6,2^35,2^-35}:/_
```

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



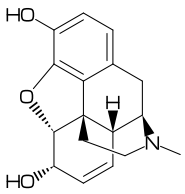
```
<30,?6,{-3,-4}=?6,-5=?3,
-2=wf,-1=wb,6=?5,-4=?6,-5=wf,
{13,15,17,20}:O,{3,12,21}://O,
{4~wf^60,8~zf^60,18^35,18^-35}:/_,
{1^60,5^180,16^60}:/*H,
14:\*,|,?5,{1,4}=dl,3:O
```

(Gibberellin A3)
FM(C): C19H22O6
MW(C): 346.3743
MW(D): 346.37



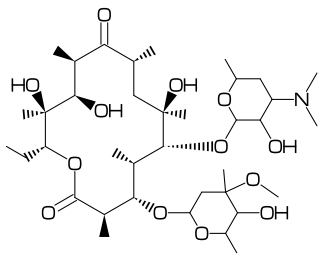
```
<18,?5,3=?7,5=?6[12],8:@,160‘1.3,3:#,
13=dl,6=wf,8=wb,
5:@,40~zf‘1,O,60,//O^180,14~zb:#,
2:/COOH,7://_,13:*/OH,8:/*OH,
14:*/_,{1,4}:*/H^60)
```

(Morphine)
FM(C): C17H19NO3
MW(C): 285.3376
MW(D): 285.343



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

(Erythromycin)
FM(C): C37H67NO13
MW(C): 733.9267
MW(D): 733.93



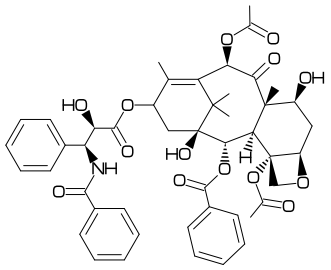
```
<30,|=1,<-120,60,60,60,-60,60,
60,-60,60,60,60,-60,60,60,=|,1:#,
14:O,13:/*Et,{1,9}://O,{2,10}:*/_,
{4,6^-35,8,12^35}:/*_,
{6^35,11,12^-35}:*/OH,
$3:\*,O,30,|,?6‘.7,2:O,
{3,5^35}:/_,4:/OH,5^-35:/O!,
$5:\*^30‘1.7,O,!,|,?6‘.7,6:O,
5:/_,2:/OH,3:/NMeMe
```

(Paclitaxel)

FM(C): C47H51NO14

MW(C): 853.9061

MW(D): 853.918



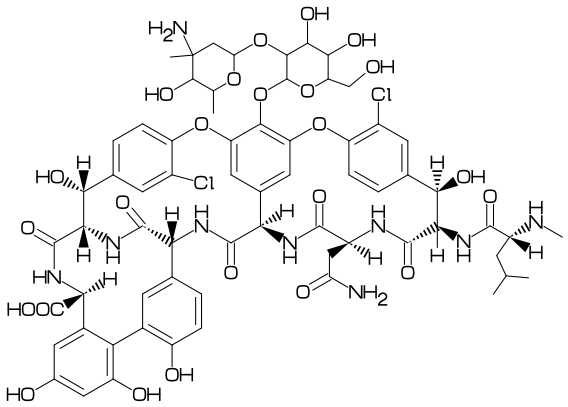
```
?6,5=d,3:@,|=1,36,45,45,45,45,=|,$5:#,
-4=?6,-4=?4,||,-1=wb,-3=wf,-1:O,
{4^35,4^-35,6}:/_,{3^-60,15}:*/OH,
8:/*H^-60,9:*/_^60,10://O,
$1:\,O,!,//O,!,*/OH,!,/Ph,
60~wf,NH,-60,//O,60,Ph,
$7:\*,O,-45,//O,60,Ph,$11:*\,O,-60,//O,60,
$12:\*^-15,O,60,//O,-60)
```

(Vancomycin)

FM(C): C66H75Cl2N9O24

MW(C): 1449.253

MW(D): 1449.25



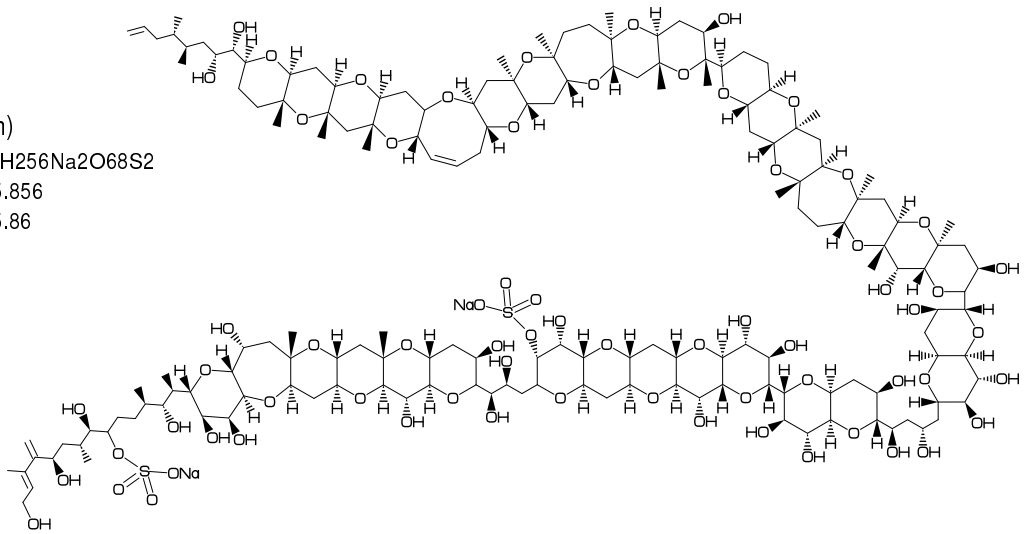
```
<30,|=1,!12,{1,3,12}=zf,7=wf,
/H^-60,60,*/OH,60,Ph,-4:/Cl,
-3:\,O,!,Ph,-4:\,O,!,Ph,-1^15:/Cl,
-3:\,/*OH,*/H^-60,$1:#,
$7:@,$26:#,$1:@,120,//O,60,NH,60,
 /*H,*/COOH^180,-60,
Ph,{-2,-4}:/OH,-1:\,Ph,-5:/OH,-2:@,$4:#,=|,
{3^40,6,9,12}://O,{2,5,8,11}:NH,
{1^180,4^180}:*/H,
{7^-60,10^60,14^60}:/*H,
$10:*\^-60,60,//O,!,NH2,$13:*\,NH,!,//O,!,
 /!iPr^-35>60,*/H^60 ,!~zf,NH,!,
$23:\,O,!,|,?6‘.7,2:O,3^10:/!OH,{4,5}:/OH,
-1:\,O,!,|,?6‘.7,6:O,
{3^35,5}:/_,3^-35:/NH2,4:/OH
```

(Maitotoxin)

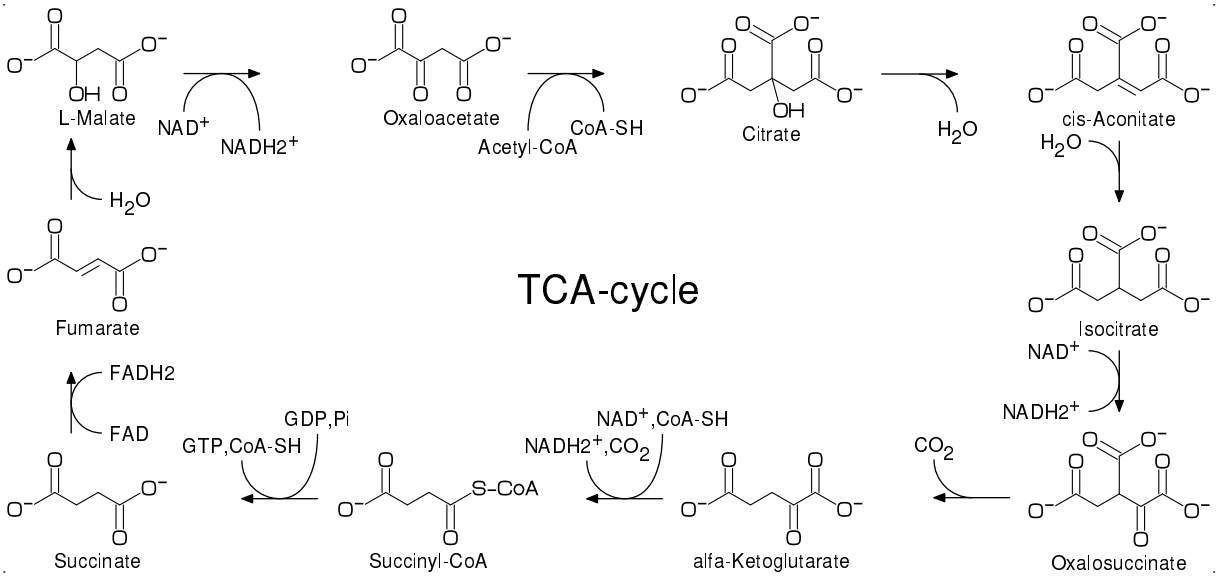
FM(C): C164H256Na2O68S2

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:\,?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=dl,{-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}:O,
{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:\,O,30,SOO,30,"O{Na}",
$36:@,-45~zf,O,30,SOO,30,"O{Na}",$150:\,|,!7,{1,2}:/*OH,4:*/_,5:/*_,7=dl
```




```
beginfont("EN:TCA cycle")
fsize:=(160mm,75mm);
max_blength:=5mm;
MCat(0.33,   1)(<30,O[-1],!O,//O,!,//O,!2,//O,!,O[-1])
MCat(0.66,   1)(<30,O[-1],!O,//O,!4,//O,!,O[-1],-4‘1:\,//O,!,O[-1],4:/OH^-165)
MCat(1,      1)(<30,O[-1],!O,//O,!2,!~dr,!,//O,!,O[-1],-4‘1:\,//O,!,O[-1])
MCat(1,   0.55)(<30,O[-1],!O,//O,!4,//O,!,O[-1],-4:\‘1,//O,!,O[-1])
MCat(1,   0.05)(<30,O[-1],!O,//O,!3,//O,!,//O,!,O[-1],-4:\‘1,//O,!,O[-1])
MCat(0.66,0.05)(<30,O[-1],!O,//O,!3,//O,!,//O,!,O[-1])
MCat(0.33,0.05)(<30,O[-1],!O,//O,!3,//O,!,"{S-CoA}")
MCat(0,   0.05)(<30,O[-1],!O,//O,!3,//O,!,O[-1])
MCat(0,   0.55)(<30,O[-1],!O,//O,!,!~dr,!,//O,!,O[-1])
MCat(0,      1)(<30,O[-1],!O,//O,!3,//O,!,O[-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_O",1);
r_arrow( 8mm)(270)(p3+(.5w3,-.4h3))("",0)("",0)("H_2_O",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_O",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
```