

MCF example for luamplib(Lua \LaTeX)

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

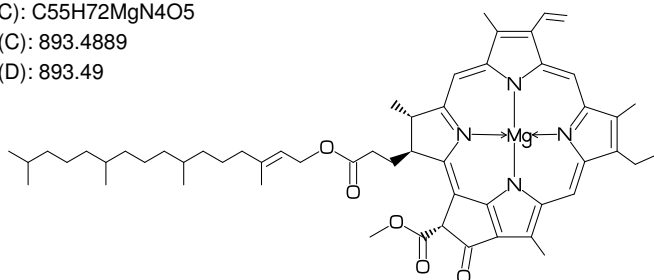
1 MCF example

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

1.1 Chlorophyll a

```
beginfont("NO:1","EN:Chlorophyll a","MW:893.49",
%-----
": <54,#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,##,||,
": {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}:/_
%-----
fsize:=(100mm,50mm);
if check(mc)=0: MC(scantokens(mc)) fi
endfont
```

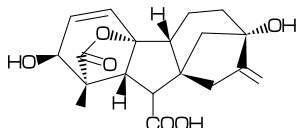
FM(C): C₅₅H₇₂MgN₄O₅
MW(C): 893.4889
MW(D): 893.49



1.2 Gibberellin A3

```
beginfont("NO:4","EN:Gibberellin A3","MW: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
%-----
fsize:=(120mm,30mm);
if check(mc)=0: MC(scantokens(mc)) fi
endfont;
```

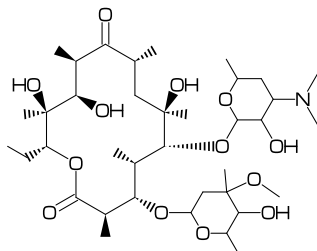
FM(C): C₁₉H₂₂O₆
MW(C): 346.3743
MW(D): 346.37



1.3 Erythromycin

```
beginfont("NO:5","EN:Erythromycin","MW: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:/N?! ")
%-----
fsize:=(120mm,35mm);
if check(mc)=0: MC(scantokens(mc)) fi
endfont;
```

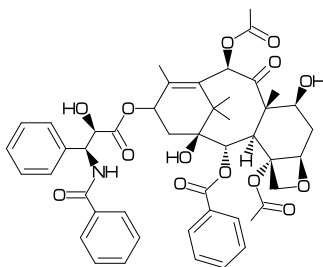
FM(C): C37H67NO13
MW(C): 733.9267
MW(D): 733.93



1.4 Paclitaxel

```
beginfont("EN:Paclitaxel","MW:853.918",
%-----
": ?6,5=d1,@3,#1,36,45,45,45,45,##,&5,-4=?6,-4=?4,-1=wb,-3=wf,-1:0, ",
": 4:??,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:*/OC0!>r1,12:*/OC0!^-15>1r ")
%-----
fsize:=(120mm,35mm);
if check(mc)=0: MC(scantokens(mc)) fi
endfont
```

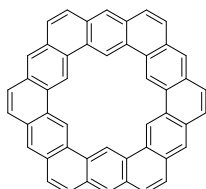
FM(C): C47H51NO14
MW(C): 853.9061
MW(D): 853.918



1.5 Kekulene

```
beginfont("EN:Kekulene","MW:600.7",
%-----
": <30,Ph,{3,-2,-3,-2,-3,-2,-3,-2,-3,-2}=?6,(-3,6)=?6[3],@-4,&6, ",
": {8,12,14,16,18,22,24,26,28,32,34,36,38,42,44,46,48,52,54,56,58}=d1 ")
%-----
fsize:=(120mm,25mm);
if check(mc)=0: MC(scantokens(mc)) fi
endfont
```

FM(C): C48H24
MW(C): 600.7041
MW(D): 600.7



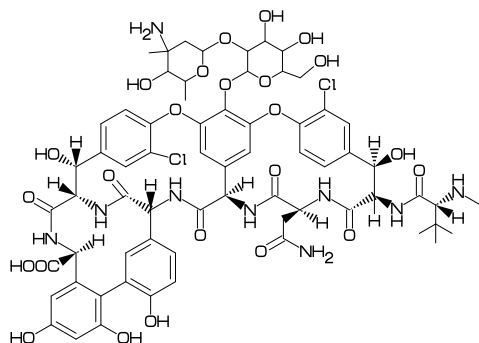
1.6 Vancomycin

```

beginfont("N0:6","EN:Vancomycin","MW:1449.25");
fsize:=(150mm,50mm);
MC(<-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,@$1,60,/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,{1,4^180}:*/H,{7^-60,10^60,14^60}:*/H,
  @10,*^-60,60,/0,! ,NH2,@13,*\,NH,! ,/0,! ,/??!,*/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)
endfont;

```

FM(C): C₆₆H₇₅Cl₂N₉O₂₄
 MW(C): 1449.253
 MW(D): 1449.25



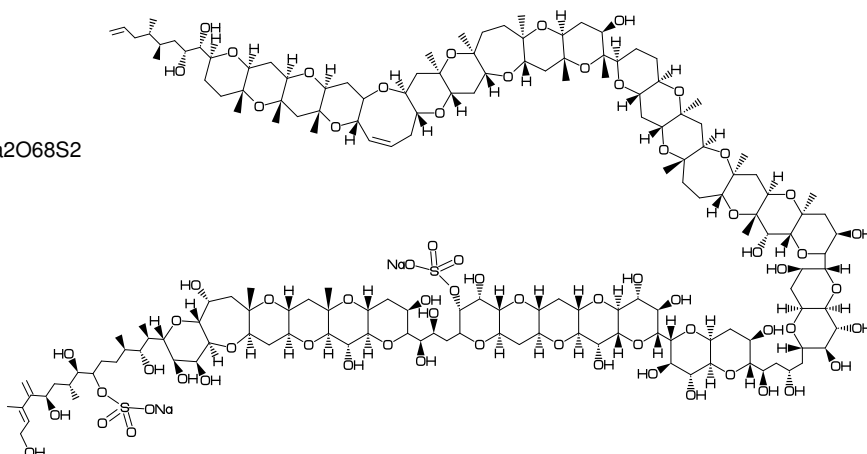
1.7 Maitotoxin

```

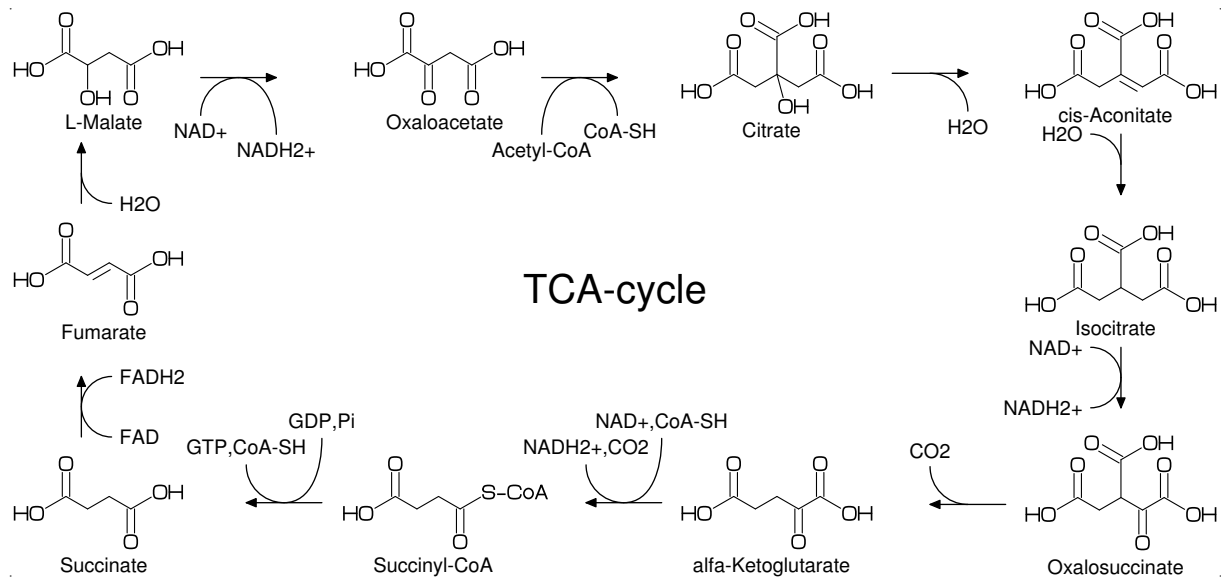
beginfont("N0:7","EN:Maitotoxin","MW:3425.86")
fsize:=(170mm,70mm);
MC(<55.8,?6,-4=?7 ,{-4,-3,-3,-3}=?6,@-3,\,!3,?6,{-4,-3,-3,-3}=?6,@-3,\,!3,?6,-3=?6,
  @-3,\,!3,60,<-30,?6,-3=?6,@-3,30,<30,?6,{-3,-3}=?6,-3=?7,{-4,-3,-3}=?6,
  @-2,\,!3,?6,-3=?6,-3=?7,{-3,-3}=?6,-3=?8,-3=d1,{-5,-3,-3,-3}=?6,
  {5,7,15,16,23,24,32,40,41,48,49,58,59,72,73,82,83,90,91,99,
    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,\,!17,{1,2}:/*OH,4:/*/_ ,5:/*/_ ,7=d1)
endfont

```

FM(C): C₁₆₄H₂₅₆Na₂O₆₈S₂
 MW(C): 3425.856
 MW(D): 3425.86



1.8 TCA cycle



```

beginfont("EN:TCA cycle")
fsize:=(160mm,75mm);
max_blength:=5mm;
COOH:='(/O,! ,OH);
HOCO:='(OH,! ,/O,);
MCat(0.33, 1)(<30,HOCO,! ,/O,! 2,COOH)
MCat(0.66, 1)(<30,HOCO,! 4,COOH,@-4'1,\,COOH,4:/OH~-165)
MCat(1, 1)(<30,HOCO,! 2,! ~dr,! ,COOH,@-4'1,\,COOH)
MCat(1, 0.55)(<30,HOCO,! 4,COOH,@-4,\ '1,COOH)
MCat(1, 0.05)(<30,HOCO,! 3,/O,! ,COOH,@-4,\ '1,COOH)
MCat(0.66,0.05)(<30,HOCO,! 3,/O,! ,COOH)
MCat(0.33,0.05)(<30,HOCO,! 3,/O,! ,"{S-CoA}")
MCat(0, 0.05)(<30,HOCO,! 3,COOH)
MCat(0, 0.55)(<30,HOCO,! ,! ~dr,! ,COOH)
MCat(0, 1)(<30,HOCO,! 3,COOH,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, 0.3h1))("Acetyl-CoA",1.5)(" CoA-SH",1);
r_arrow(10mm)( 0)(p2+ ( 1.1w2, 0.4h2))("",0)("H2O",1);
r_arrow( 8mm)(270)(p3+ ( 0.5w3,-0.4h3))("H2O",1)("",0);
r_arrow( 8mm)(270)(p4+ ( 0.5w4,-0.4h4))("NAD+",1)("NADH2+",1);
r_arrow(10mm)(180)(p5+ (-0.1w5, 0.4h5))("",0)("CO_2_",1);
r_arrow(10mm)(180)(p6+ (-0.1w6, 0.5h6))("NAD+,CoA-SH",1.7)("NADH2+,CO2",1);
r_arrow(10mm)(180)(p7+ (-0.1w7, 0.5h7))("GDP,Pi",1.7)("GTP,CoA-SH",1);
r_arrow( 8mm)( 90)(p8+ ( 0.4w8, 1.2h8))("FAD",1)("FADH2",1);
r_arrow( 8mm)( 90)(p9+ ( 0.4w9, 1.2h9))("H2O",1)("",0);
r_arrow(10mm)( 0)(p10+( 1.1w10,0.3h10))("NAD+",1)("NADH2+",1.5);
defaultscale:=1.5;
label("TCA-cycle",(0.5w,0.5h));
)
endfont

```