

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

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

## 1 Change color

(use with metapost only)

MC(

<30,Ph,{2,5}:N,3:/NH2,4:/COOH,

%-----

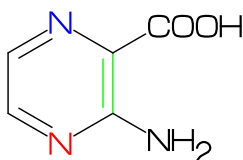
2:red,        % red    A2

5:blue,      % blue   A5

3=green      % green B3

%-----

)



## 2 Change font

(use with metapost only)

%-----

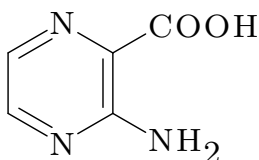
atomfont:="cmr8";

%-----

MC(

<30,Ph,{2,5}:N,3:/NH2,4:/COOH

)



## 3 MCF example

FM(C) : molecular formula calculated by mcf2graph

MW(C) : molecular weight calculated by mcf2graph

MW(D) : molecular weight from literature data

### 3.1 Chlorophyll a

beginfont("N0:1","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);

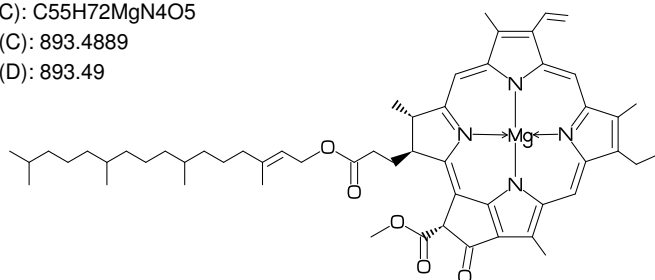
if check\_mc(mc)=0: MC(scantokens(mc)) fi

endfont

FM(C): C55H72MgN4O5

MW(C): 893.4889

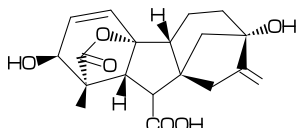
MW(D): 893.49



### 3.2 Gibberellin A3

```
beginfont("NO:4","EN:Gibberellin A3","MW:346.37",
%-----
": <18,?5,3=?7,5=?6[12],@8,160'1.3,&3,13=dl,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,20mm);
if check_mc(mc)=0: MC(scantokens(mc)) fi
endfont;
```

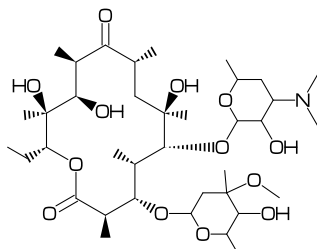
FM(C): C19H22O6  
MW(C): 346.3743  
MW(D): 346.37



### 3.3 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:/O!, ",
": @.$5,\*^30'1.7,0,!,|,?6'.7,6:0,5:/_2:/OH,3:/N?! ")
%-----
fsize:=(120mm,35mm);
if check_mc(mc)=0: MC(scantokens(mc)) fi
endfont;
```

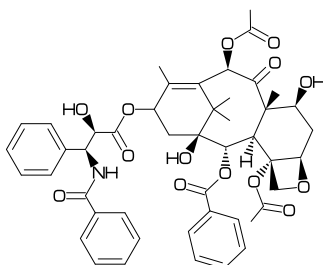
FM(C): C37H67NO13  
MW(C): 733.9267  
MW(D): 733.93



### 3.4 Paclitaxel

```
beginfont("EN:Paclitaxel","MW:853.918",
%-----
": ?6,5=dl,@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>lr ")
%-----
fsize:=(120mm,35mm);
if check_mc(mc)=0: MC(scantokens(mc)) fi
endfont
```

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



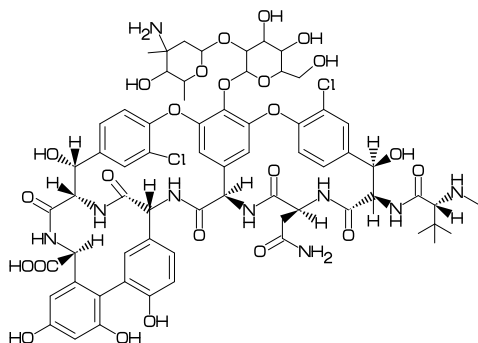
### 3.5 Vancomycin

```

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): C<sub>66</sub>H<sub>75</sub>Cl<sub>2</sub>N<sub>9</sub>O<sub>24</sub>  
 MW(C): 1449.253  
 MW(D): 1449.25



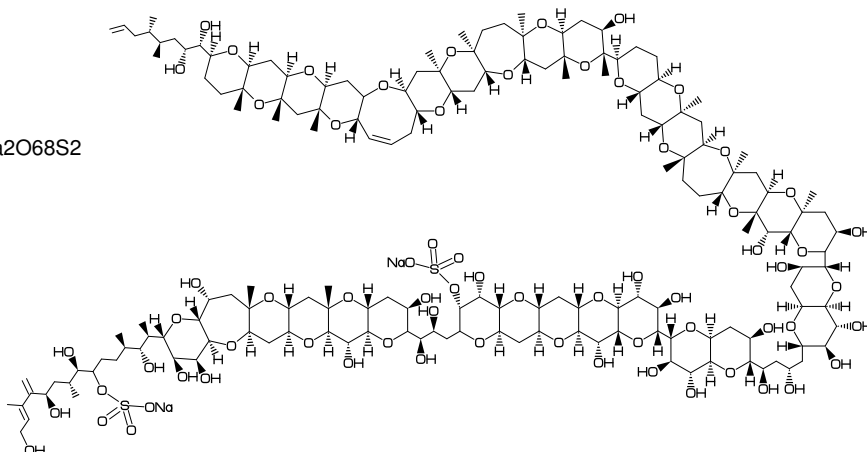
### 3.6 Maitotoxin

```

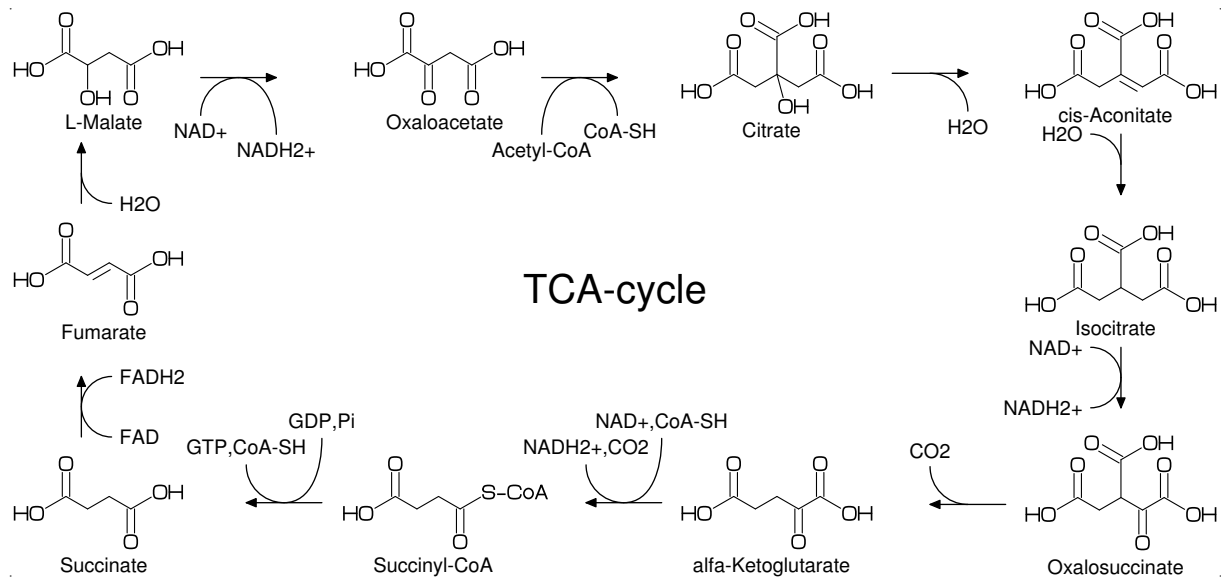
beginfont("N0:7","EN:Maitotoxin","MW:3425.86")
fsize:=(170mm,70mm);
MC(<55.8,?6,-4=?7 ,{-4,-3,-3,-3}=?6,@-3,\,!3,?6,{-4,-3,-3,-3}=?6,@-3,\,!3,?6,-3=?6,
  @-3,\,!3,60,<-30,?6,-3=?6,@-3,30,<30,?6,{-3,-3}=?6,-3=?7,{-4,-3,-3}=?6,
  @-2,\,!3,?6,-3=?6,-3=?7,{-3,-3}=?6,-3=?8,-3=d1,{-5,-3,-3,-3}=?6,
  {5,7,15,16,23,24,32,40,41,48,49,58,59,72,73,82,83,90,91,99,
    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): C<sub>164</sub>H<sub>256</sub>Na<sub>2</sub>O<sub>68</sub>S<sub>2</sub>  
 MW(C): 3425.856  
 MW(D): 3425.86



### 3.7 TCA cycle



```

beginfont("EN:TCA cycle")
fsize:=(160mm,75mm);
max_blength:=5mm;
COOH:=' (/0,!,OH);
HOCO:=' (OH,!,/0,);
MCat(0.33, 1)(<30,HOCO,!,/0,!,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,/0,!,COOH,@-4,\ '1,COOH)
MCat(0.66,0.05)(<30,HOCO,!,3,/0,!,COOH)
MCat(0.33,0.05)(<30,HOCO,!,3,/0,!, "{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

```