

# 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, .

%-----

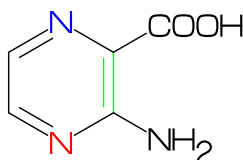
2:red,        % red    A2

5:blue,      % blue   A5

3=green      % green B3

%-----

)



## 2 Change font

(use with metapost only)

%-----

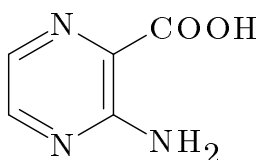
atomfont:="cmr8";

%-----

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")

  fsize:=(100mm,50mm);

  MC(

    <54,|=1,?5,{2,5}=d1,4:N,3:\,54~d1,|,?5,{2,4}=d1,5:N,

    -2:\,54~d1,|,?5,2=d,5:N,-2:\~d1,54,|,?5,5=d,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}:/\_

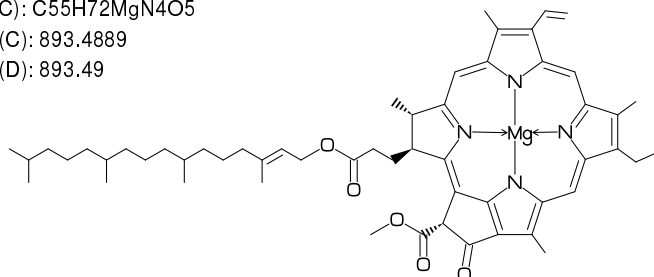
  )

endfont

FM(C): C55H72MgN4O5

MW(C): 893.4889

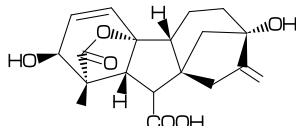
MW(D): 893.49



### 3.2 Gibberellin A3

```
beginfont("N0:4","EN:Gibberellin A3","MW:346.37");
  fsize:=(120mm,20mm);
  MC(
    <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
  )
endfont;
```

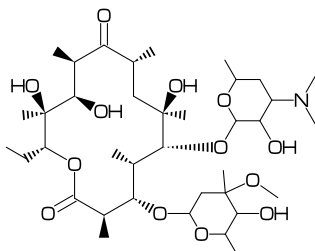
FM(C): C<sub>19</sub>H<sub>22</sub>O<sub>6</sub>  
MW(C): 346.3743  
MW(D): 346.37



### 3.3 Erythromycin

```
beginfont("N0:5","EN:Erythromycin","MW:733.93");
  fsize:=(120mm,35mm);
  MC(
    <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:/NMeMe
  )
endfont;
```

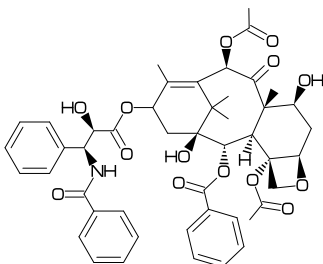
FM(C): C<sub>37</sub>H<sub>67</sub>NO<sub>13</sub>  
MW(C): 733.9267  
MW(D): 733.93



### 3.4 Paclitaxel

```
beginfont("EN:Paclitaxel","MW:853.918")
  fsize:=(120mm,35mm);
  MC(
    ?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
  )
endfont
```

FM(C): C<sub>47</sub>H<sub>51</sub>NO<sub>14</sub>  
MW(C): 853.9061  
MW(D): 853.918



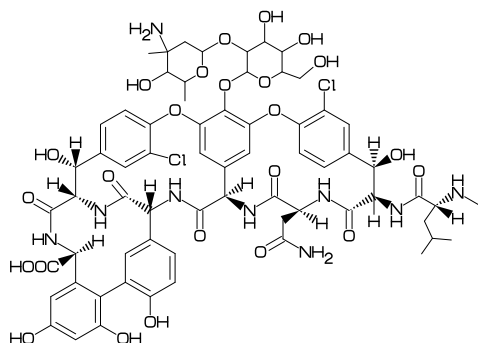
### 3.5 Vancomycin

```

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,!,/!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)
endfont;

```

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



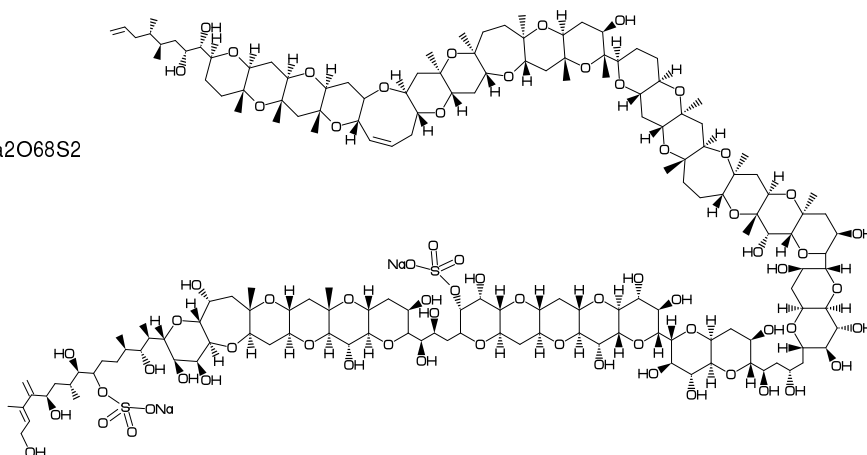
### 3.6 Maitotoxin

```

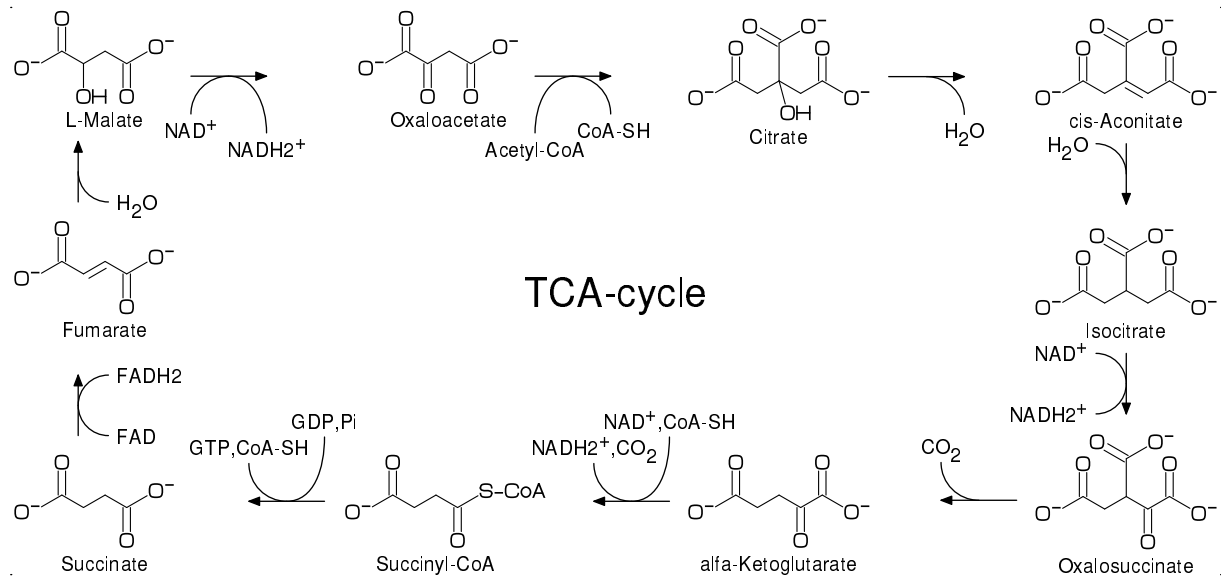
beginfont("N0:7","EN:Maitotoxin","MW:3425.86")
fsize:=(170mm,70mm);
MC(<55.8,?6,-4=?7,{4,-3,-3,-3}=?6,-3:\,!3,?6,{4,-3,-3,-3}=?6,-3:\,?6,-3=?6,
  -3:\,!3,60,<-30,?6,-3=?6,-3:@,30,<30,?6,{3,-3}=?6,-3=?7,{4,-3,-3}=?6,
  -2:\,?6,-3=?6,-3=?7,{3,-3}=?6,-3=?8,-3=d1,{5,-3,-3,-3}=?6,
  {5,7,15,16,23,24,32,40,41,48,49,58,59,72,73,82,83,90,91,99,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

```

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



### 3.7 TCA cycle



```

beginfont("EN:TCA cycle")
fsize:=(160mm,75mm);
max_blength:=5mm;
C00m:='(/0,!,0[-1]);
OmCO:='(0[-1],!,/0);
MCat(0.33, 1)(<30,OmCO,!,/0,!,2,C00m)
MCat(0.66, 1)(<30,OmCO,!,4,C00m,-4'1:\,C00m,4:/OH~-165)
MCat(1, 1)(<30,OmCO,!,2,!~dr,!,C00m,-4'1:\,C00m)
MCat(1, 0.55)(<30,OmCO,!,4,C00m,-4:\'1,C00m)
MCat(1, 0.05)(<30,OmCO,!,3,/0,!,C00m,-4:\'1,C00m)
MCat(0.66,0.05)(<30,OmCO,!,3,/0,!,C00m)
MCat(0.33,0.05)(<30,OmCO,!,3,/0,!, "{S-CoA}")
MCat(0, 0.05)(<30,OmCO,!,3,C00m)
MCat(0, 0.55)(<30,OmCO,!,!~dr,!,C00m)
MCat(0, 1)(<30,OmCO,!,3,C00m,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)("H_2_0",1);
r_arrow( 8mm)(270)(p3+ ( 0.5w3,-0.4h3))("H_2_0",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^+^,CO_2",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))("H_2_0",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

```