

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

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

## 1 MCF example

use molecular data base file 'mcf\_exa\_data.mcf'

FM(fm) : molecular formula (calculated)

MW(mw) : molecular weight (calculated)

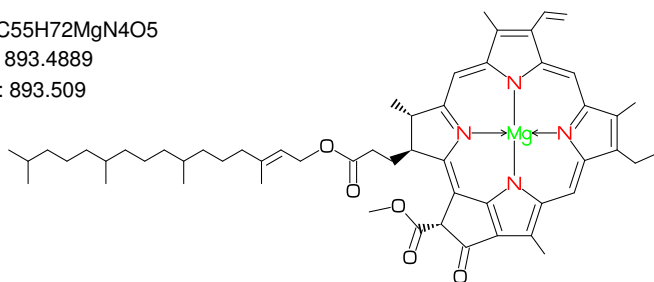
### 1.1 Chlorophyll a

```
beginfont("f:mcf_data_base.mcf","t:EN","v:Chlorophyll a","NO:-",
          ":",||,{4,11,17,23}:red,27:green)  %%% change color of atoms %%%
fsize:=(100mm,45mm);
if check(mc)=0: MC(scantokens(mc)) fi
ext(defaultscale:=0.8;
    label.lrt("fm: "&cal_FM,(0,h-5mm));
    label.lrt("mw: "&cal_MW,(0,h-9mm));
    label.lrt("MW: "&inf_MW,(0,h-13mm));)
endfont
```

fm: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>

mw: 893.4889

MW: 893.509



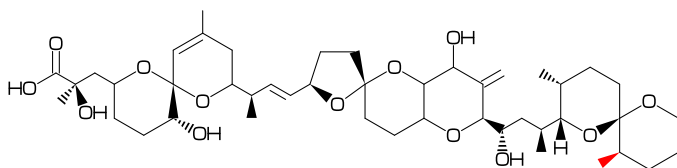
### 1.2 Dinophysistoxin-1

```
beginfont("t:EN","v:Okadaic acid","EN:Dinophysistoxin-1",
          "MW:819",":,38:*/_,65=red)  %%% add methyl group (color red) %%%
fsize:=(150mm,35mm);
if check(mc)=0: MC(scantokens(mc)) fi
ext(defaultscale:=0.8;
    label.lrt("fm: "&cal_FM,(0,h-5mm));
    label.lrt("mw: "&cal_MW,(0,h-9mm));
    label.lrt("MW: "&inf_MW,(0,h-13mm));)
endfont;
```

fm: C<sub>45</sub>H<sub>70</sub>O<sub>13</sub>

mw: 819.0294

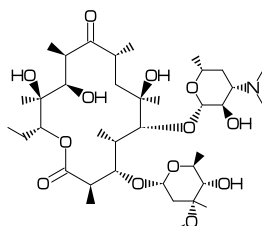
MW: 819



## 1.3 Erythromycin

```
beginfont("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',4,6^-35,8,10',12^35}:/*_ ,      ",
": {6^35,11,12^-35}:/OH,      ",
": @$3,\*,0,30~zb,|,?6'.7,6:0,#.5,{5~wf,3^35}:/_,4:/OH,3^-35:/O!,##, ",
": @$5,\*^30'1.7,0,!~zb,|,?6'.7,6:0,#.5,5:/*_ ,2:/OH,3:/N?!      ")
%-----
fsize:=(120mm,30mm);
if check(mc)=0: MC(scantokens(mc)) fi
endfont;
```

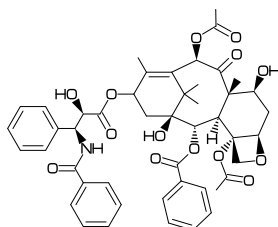
fm: C37H67NO13  
mw: 733.9267  
MW: 733.93



## 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>lr      ")
%-----
fsize:=(120mm,30mm);
if check(mc)=0: MC(scantokens(mc)) fi
endfont
```

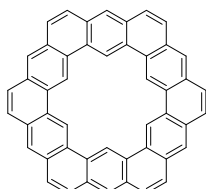
fm: C47H51NO14  
mw: 853.9061  
MW: 853.918



## 1.5 Kekulene

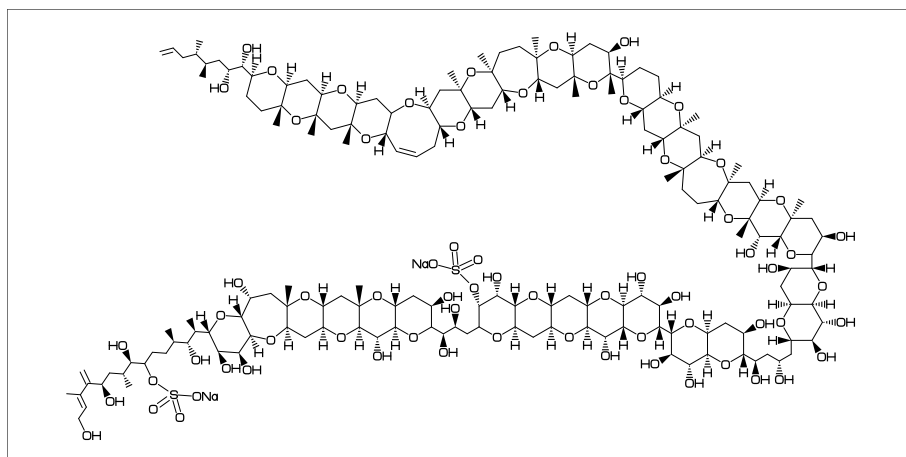
```
beginfont("EN:Kekulene","MW:600.7",
%-----
": <30,?6,{3,-3,-2,-3,-2,-3,-2,-3,-2,-3,(-2',5'),(5',-4')}=?6,      ",
": {1,5',7,9,11,13,17,19,21,23,27,29,31,33,37,39,41,43,47,49,51,53,57,60}=d1 ")
%-----
fsize:=(120mm,25mm);
if check(mc)=0: MC(scantokens(mc)) fi
endfont
```

fm: C48H24  
mw: 600.7041  
MW: 600.7



## 1.6 Maitotoxin

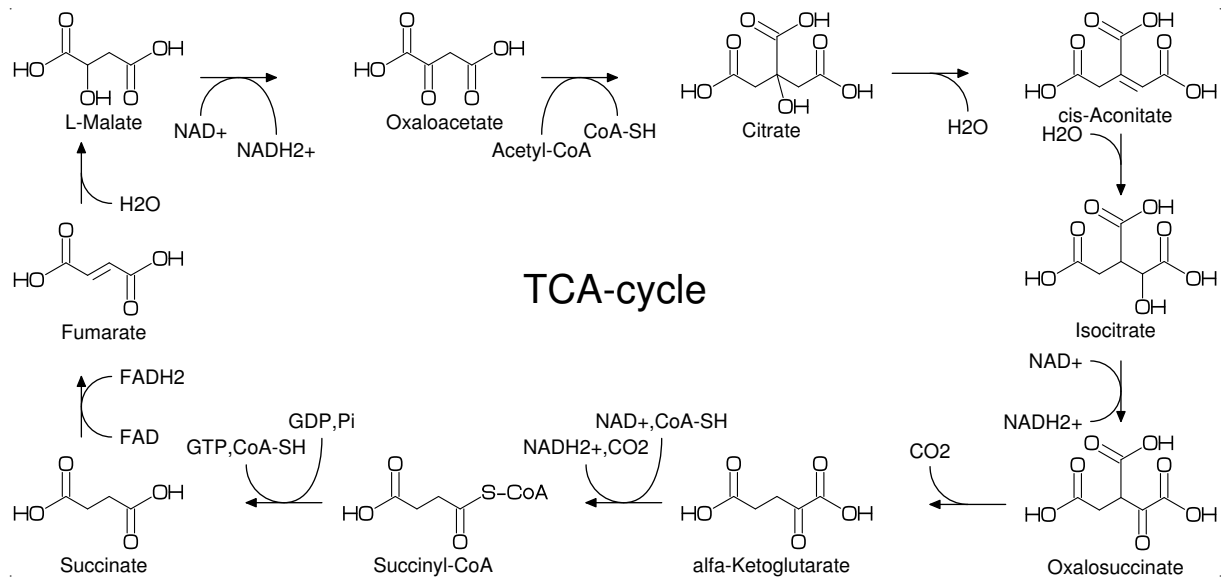
```
%-----
\begin{mplibcode}
  beginfont("t:EN", "v:Maitotoxin")
    sw_output:=Info+Mcode+Temp;          %%% output temp-info,temp-mc.aux %%%
  endfont;
\end{mplibcode}
\verbatiminput{temp-mc.aux}              %%% input temp-mc.aux %%%
\begin{mplibcode}
  beginfont("t:EN", "v:Maitotoxin")
    fsize:=(120mm,60mm); fmargin:=(0,3mm); sw_frame:=Outside;
    if check(mc)=0: MC(scantokens(mc)) fi %%% output font %%%
  endfont
\end{mplibcode}
%-----
\newread\auxfile%
\openin\auxfile=temp-info.aux           %%% input temp-info.aux %%%
\read\auxfile to \info%
\infotovar{\info}                       %%% info to variables %%%
\closein\auxfile%
{\tt ** EN:EN \quad mw:\MW \quad MW:\mw \quad fm:\fm}%
%-----
```



```
<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,
{3,8,13,17,21,33,38,42,56,70,84,92,101,106,111,128,138,142,146,150}:/*H^-60,
{4,14,22,34,39,43,47',57',71',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}:*/_^-60'1,{80,88,97,108',115,120,124}:/*_^-60'1,
@$6,\,|,!11,60~dr,-60,60,OH,{2',7,10}:*/OH,{1,3,8'}:*/_,11://_,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
```

```
** EN:Maitotoxin mw:3425.86 MW:3425.856 fm:C164H256Na2068S2
```

## 1.7 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) % Oxaloacetate
MCat(0.66, 1)(<30,HOCO,!,4,COOH,@-4'1,\,COOH,4:/OH~-165) % Citrate
MCat(1, 1)(<30,HOCO,!,2,!~dr,!,COOH,@-4'1,\,COOH) % cis-Aconitate
MCat(1, 0.58)(<30,HOCO,!,4,COOH,@-4,\ '1,COOH,5:/OH) % Isocitrate
MCat(1, 0.05)(<30,HOCO,!,3,/0,!,COOH,@-4,\ '1,COOH) % Oxalosuccinate
MCat(0.66,0.05)(<30,HOCO,!,3,/0,!,COOH) % alfa-Ketoglutarate
MCat(0.33,0.05)(<30,HOCO,!,3,/0,!, "{S-CoA}") % Succinyl-CoA
MCat(0, 0.05)(<30,HOCO,!,3,COOH) % Succinate
MCat(0, 0.55)(<30,HOCO,!,!~dr,!,COOH) % Fumarate
MCat(0, 1)(<30,HOCO,!,3,COOH,3:/OH) % L-Malate
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

```