

MCF example for luamplib(Lua \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(C) : molecular formula calculated by mcf2graph
MW(C) : molecular weight calculated by mcf2graph
MW(D) : molecular weight from literature data

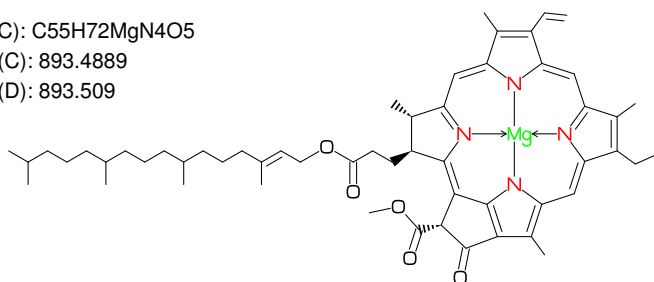
1.1 Chlorophyll a

```
beginfont("f:mcf_data_base","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(C): "&cal_FM,(0,h-5mm));  
    label.lrt("MW(C): "&cal_MW,(0,h-9mm));  
    label.lrt("MW(D): "&inf_MW,(0,h-13mm));)  
endfont
```

FM(C): C₅₅H₇₂MgN₄O₅

MW(C): 893.4889

MW(D): 893.509



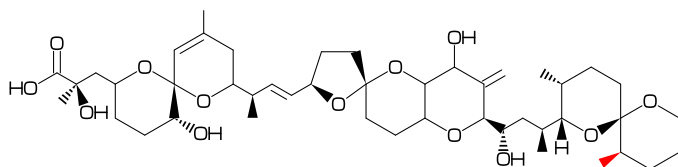
1.2 Dinophysistoxin-1

```
beginfont("f:mcf_data_base","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(C): "&cal_FM,(0,h-5mm));  
    label.lrt("MW(C): "&cal_MW,(0,h-9mm));  
    label.lrt("MW(D): "&inf_MW,(0,h-13mm));)  
endfont;
```

FM(C): C₄₅H₇₀O₁₃

MW(C): 819.0294

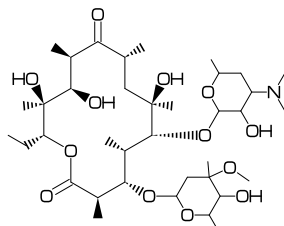
MW(D): 805.00



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

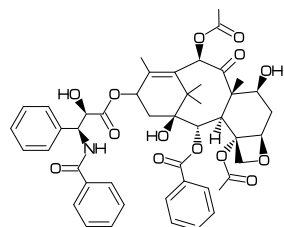
FM(C): C37H67NO13
MW(C): 733.9267
MW(D): 733.93



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

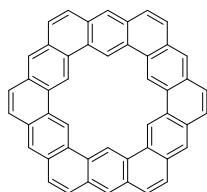
FM(C): C47H51NO14
MW(C): 853.9061
MW(D): 853.918



1.5 Kekulene

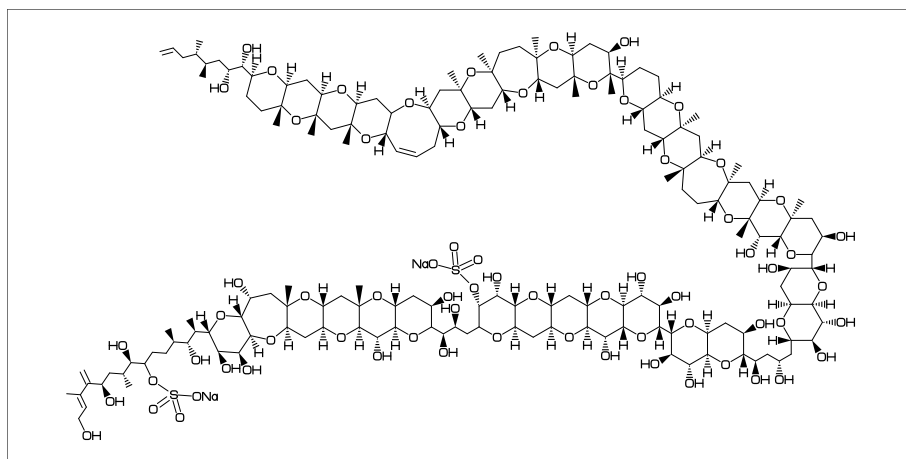
```
beginfont("EN:Kekulene","MW:600.7",
%-----
": <30,Ph,{3,-2,-3,-2,-3,-2,-3,-2,-3,-2}=?6,(-3,6)=?6[3],@-4,&6,      ",
": {8,12,14,16,18,22,24,26,28,32,34,36,38,42,44,46,48,52,54,56,58}=d1      ")
%-----
fsize:=(120mm,25mm);
if check(mc)=0: MC(scantokens(mc)) fi
endfont
```

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



1.6 Maitotoxin

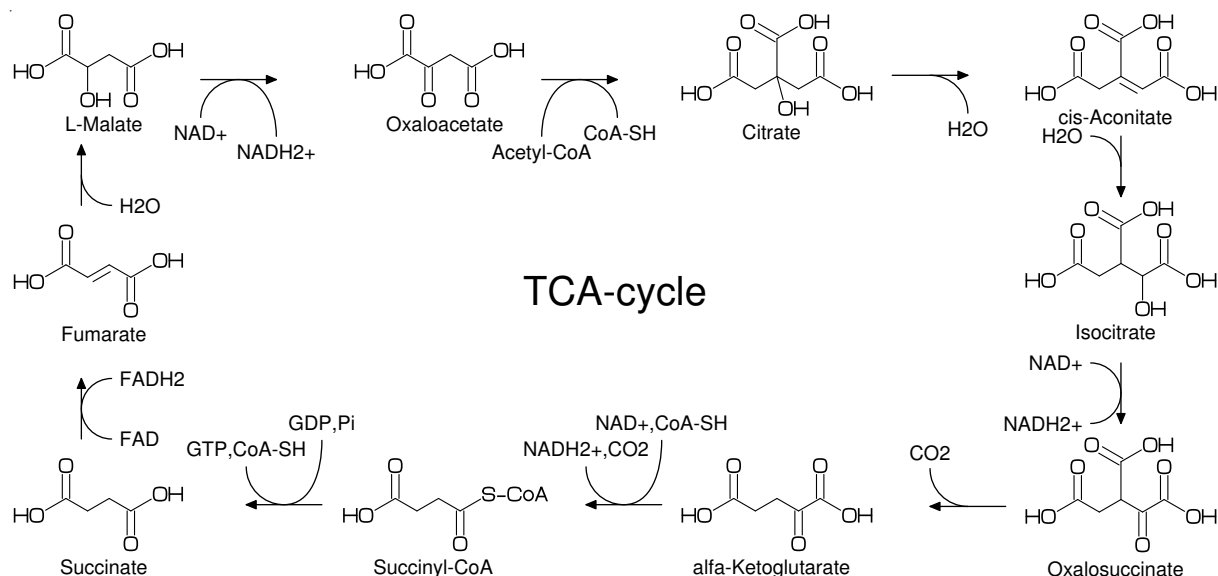
```
%-----
\begin{mplibcode}
  beginfont("f:mcf_data_base","t:EN","v:Maitotoxin")
    sw_output:=Info+Mcode+Temp;          %%%% output temp-info,temp-mc.aux %%%%
  endfont;
\end{mplibcode}
\verbatiminput{temp-mc.aux}              %%%% input temp-mc.aux %%%%
\begin{mplibcode}
  beginfont("f:mcf_data_base","t:EN","v:Maitotoxin")
    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(C):\MW \quad MW(D):\mw \quad FM(C):\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,{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
```

```
** EN:Maitotoxin MW(C):3425.86 MW(D):3425.856 FM(C):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

```