

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(fm) : molecular formula (calculated)

MW(mw) : molecular weight (calculated)

1.1 Erythromycin

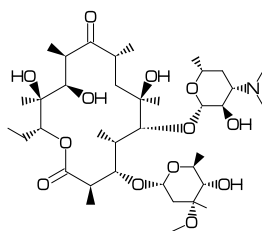
(pass mcf to MC())

```
beginfigm("EN:Erythromycin","MW:733.93")
  fsize:=(120mm,30mm);
  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',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:/*!,##,
    @$5,\*^30'1.7,0,!~zb,|,?6'.7,6:0,#.5,5:/*_,2:*/OH,3:/*N?!))
  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));)
endfigm;
```

fm: C₃₇H₆₇NO₁₃

mw: 733.9267

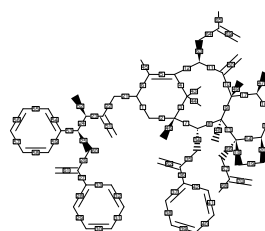
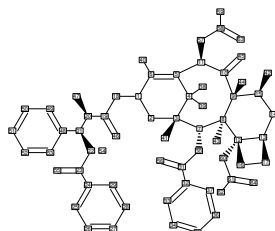
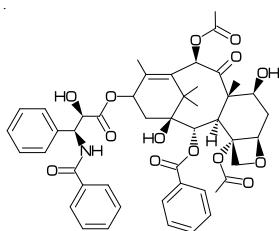
MW: 733.93



1.2 Paclitaxel

(pass mcf to beginfigm())

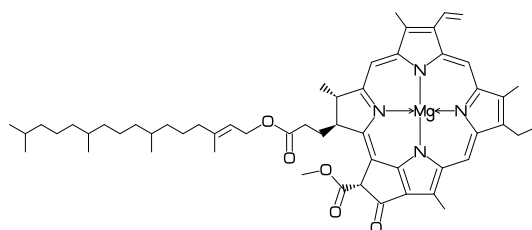
```
beginfigm("EN:Paclitaxel","MW:853.918",
  %-----
  ": ?6,5=d1,@3,#1,36,45,45,45,45,##,&5,-4=?6,-4=?4,-1=wb,-3=wf,-1:0, ",
  ": 4:??,6:/_,{3~60,15}:*/OH,8:/*H~60,9:*/_~60,10://0, ",
  ": @1,\,0,!,//0,!,*OH,!/Ph,60~wf,NH,-60,//0,60,Ph, ",
  ": @7,\*,0,-45,//0,60,Ph,11:/*OC0!>r1,12:/*OC0!~15>lr ")
  %-----
  fsize:=(140mm,30mm);
  if check(mc)=0:       MCat(0,0.5)(scantokens(mc))
    sw_numbering:=Atom; MCat(0.6,0.5)(scantokens(mc))
    sw_numbering:=Bond; MCat(1,0.5)(scantokens(mc))
  fi
endfigm
```



1.3 Chlorophyll a

(read data-base file)

```
beginfigm("f:mcf_data_base.mcf","t:EN","v:Chlorophyll a","N0:-")
  sw_output:=Fig+Calc+Mcode;          %%% output temp-mc.aux %%%
  fsize:=(100mm,30mm);
  if check(mc)=0:
    MC(scantokens(mc))
    VerbatimTeX("\gdef\EN{"&inf_EN&"}\gdef\MW{"&inf_MW&"}");
    VerbatimTeX("\gdef\mw{"&cal_MW&"}\gdef\fm{"&cal_FM&"}");
  fi
endfigm
\end{mplibcode}
\verbatiminput{temp-mc.aux}           %%% input temp-mc.aux %%%
{\tt ** EN:\EN \quad mw:\MW \quad MW:\mw \quad fm:\fm}%
```



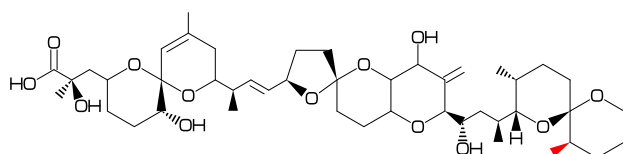
```
<-36,#1,?5,@3,\,54,?5,@-2,\,54,?5,@-2,\,54,?5,@-2,\,&5,@6,22,70,&8,##,
{4,6,8,10,14,16,18,21,23,27}=dl,@4,\,1.48~vf,Mg,&17~vb,@11,&27,@27,&23,
{4,11,17,23}:N,{1~zf,9,15,21}:/_ ,14:/!,20:/!!,25:/*COO!,26://0,
@2,*\^-6,!2,//0,!0,!2,!! ,!13,{1,5,9,13}:/_
```

** EN:Chlorophyll a mw:893.509 MW:893.4889 fm:C55H72MgN4O5

1.4 Dinophysistoxin-1

(read data-base file + pass mcf to beginfigm())

```
beginfigm("t:EN","v:Okadaic acid","EN:Dinophysistoxin-1",
  "MW:819",",38:*/_,65=red") %%% add methyl group (color red) %%%
  sw_output:=Fig+Calc+Mcode;          %%% output temp-mc.aux %%%
  fsize:=(120mm,20mm);
  if check(mc)=0: MC(scantokens(mc))
    VerbatimTeX("\gdef\EN{"&inf_EN&"}\gdef\MW{"&inf_MW&"}");
    VerbatimTeX("\gdef\mw{"&cal_MW&"}\gdef\fm{"&cal_FM&"}");
  fi
endfigm;
\end{mplibcode}
\verbatiminput{temp-mc.aux}           %%% input temp-mc.aux %%%
{\tt ** EN:\EN \quad mw:\MW \quad MW:\mw \quad fm:\fm}%
```



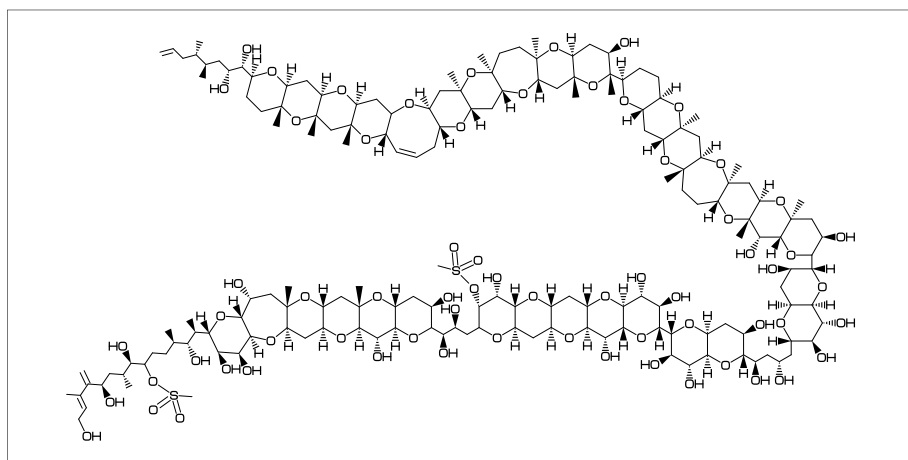
```
<30,?6,@4,?6,@-4,\,!3,<-12,?5,@-3,<-12,?6,-3=?6,@-3,*\,!3,
?6,@-4,?6,@6,\,!,/*_^-40,*OH^20,! ,//0,!1,OH,
3=wb,11=dl,15=dr,17=wf,19=wf,38=wb,{5,7,16,24,25,33,42}:0,
32:*/H^60,10:/_,{12,31,37'}:*/_,27://_,28:/OH,{3,29}:/*OH
,38:*/_,65=red
```

** EN:Dinophysistoxin-1 mw:819 MW:819.0294 fm:C45H70O13

1.5 Maitotoxin

(read data-base file)

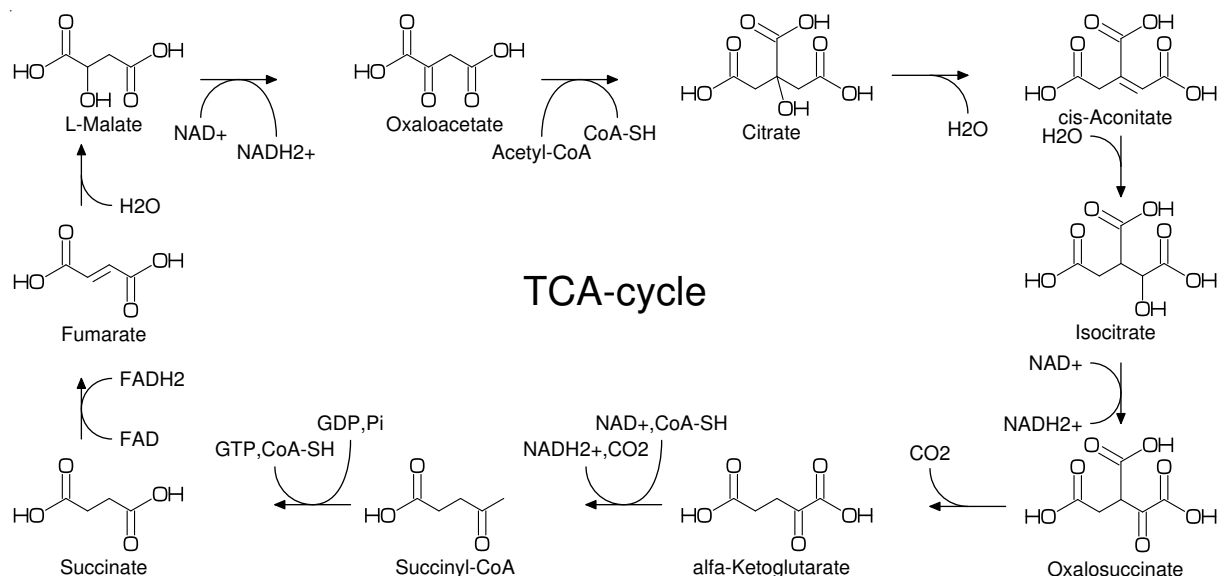
```
%-----
\begin{mplibcode}
  beginfigm("t:EN", "v:Maitotoxin")
    sw_output:=Fig+Calc+Mcode;          %%% output temp-mc.aux %%%
    fsize:=(120mm,60mm); fmargin:=(0,3mm); sw_frame:=Outside;
    if check(mc)=0: MC(scantokens(mc))
      VerbatimTeX("\gdef\EN{"&inf_EN&"}\gdef\MW{"&inf_MW&"}");
      VerbatimTeX("\gdef\mw{"&cal_MW&"}\gdef\fm{"&cal_FM&"}");
    fi
  endfigm
\end{mplibcode}
\verbatiminput{temp-mc.aux}             %%% input temp-mc.aux %%%
{\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,\,!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,
{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:3377.946 fm:C166H262O66S2

1.6 TCA cycle



```

beginfigmy"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));
)
endfigm

```