

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

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

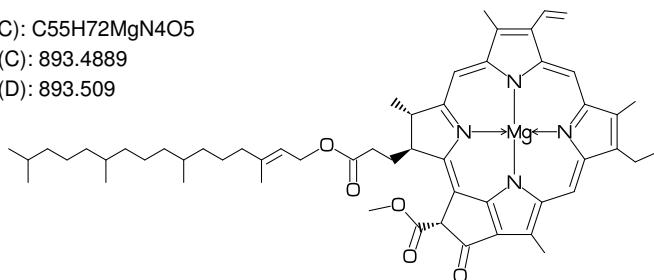
## 1 MCF example

use molecular data base file 'mcf\_exa\_data.mcf'  
FM(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")
  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
```

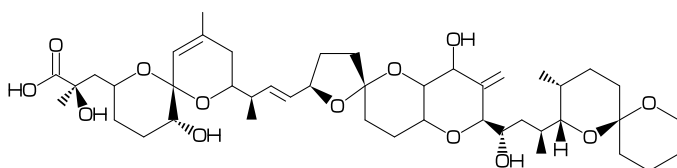
FM(C): C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>  
MW(C): 893.4889  
MW(D): 893.509



### 1.2 Okadaic acid

```
beginfont("f:mcf_data_base","t:EN","v:Okadaic acid")
  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;
```

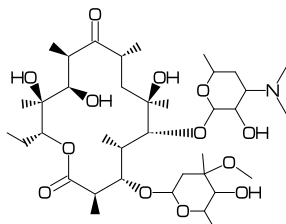
FM(C): C<sub>44</sub>H<sub>68</sub>O<sub>13</sub>  
MW(C): 805.0029  
MW(D): 805.00



## 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}:/_4:/OH,5^-35:/0!, ",
": @$5,\*^30'1.7,0,!,|,?6'.7,6:0,5:/_2:/OH,3:/N?! ")
%-----
fsize:=(120mm,30mm);
if check(mc)=0: MC(scantokens(mc)) fi
endfont;
```

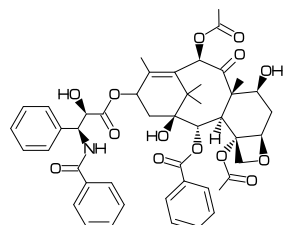
FM(C): C37H67NO13  
MW(C): 733.9267  
MW(D): 733.93



## 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
```

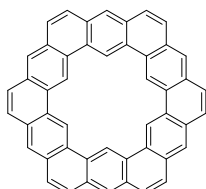
FM(C): C47H51NO14  
MW(C): 853.9061  
MW(D): 853.918



## 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 Vancomycin

% extract from molecular data base file 'mcf\_data\_base.mcf'

EN:Vancomycin;MW:1449.25

+

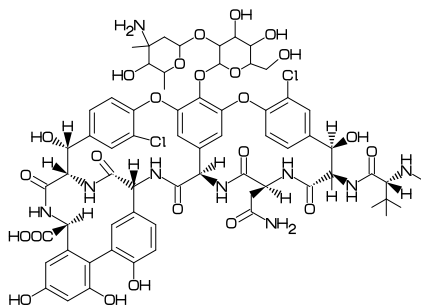
```
<-30,#1,!12,{1,3,12}=zf,7=wf,/H^-60,60,*/OH,60,  
  Ph,-4:/Cl,@-3,\,0,! ,Ph,@-4,\,0,! ,Ph,-1^15:/Cl,@-3,\,/*OH,*/H^-60,&1,  
  @7,&26,@$1,60,/0,60,NH,60,/*H,*/COOH^180,-60,  
  Ph,{-2,-4}:/OH,@-1,\,Ph,-5:/OH,@-2,&4,##,  
  {3^40,6,9,12}:/0,{2,5,8,11}:NH,{1,4^180}:*/H,{7^-60,10^60,14^60}:*/H,  
  @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
```

-----

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



## 1.7 Maitotoxin

% extract from molecular data base file 'mcf\_data\_base.mcf'

EN:Maitotoxin;MW:3425.86

+

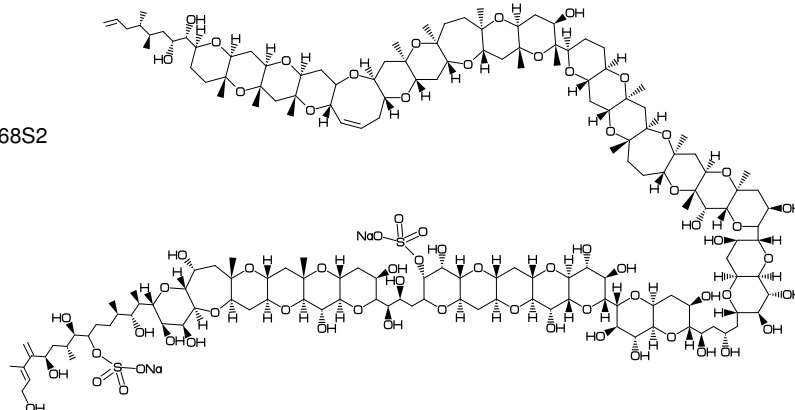
```
<55.8,?6,-4=?7 ,{-4,-3,-3,-3}=?6,@-3,\,!3,?6,{-4,-3,-3,-3}=?6,@-3,\,!3,60,<-30,?6,-3=?6,@-3,30,<30,?6,{-3,-3}=?6,-3=?7,{-4,-3,-3}=?6,  
  @-2,\,!3,60,-3=?6,-3=?7,{-3,-3}=?6,-3=?8,-3=d1,{-5,-3,-3,-3}=?6,  
  {5,7,15,16,23,24,32,40,41,48,49,58,59,72,73,82,83,90,91,99,  
    100,107,113,114,122,123,130,131,140,141,148,149}:0,  
  {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
```

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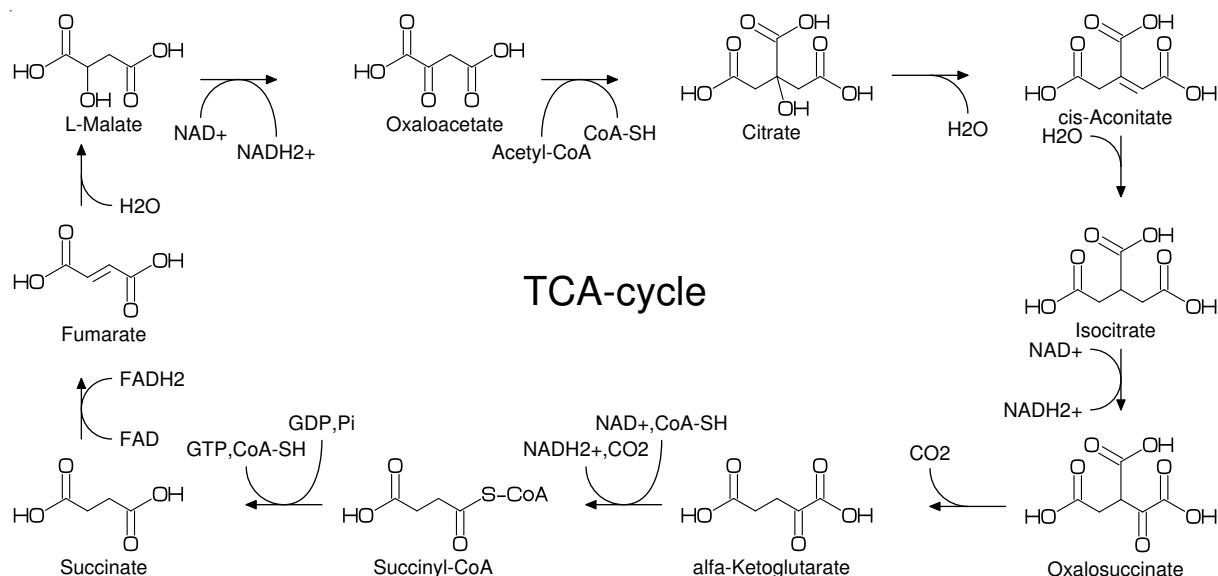
FM(C): C<sub>164</sub>H<sub>256</sub>Na<sub>2</sub>O<sub>68</sub>S<sub>2</sub>

MW(C): 3425.856

MW(D): 3425.86



## 1.8 TCA cycle



```

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

```