Molecular Coding Format manual

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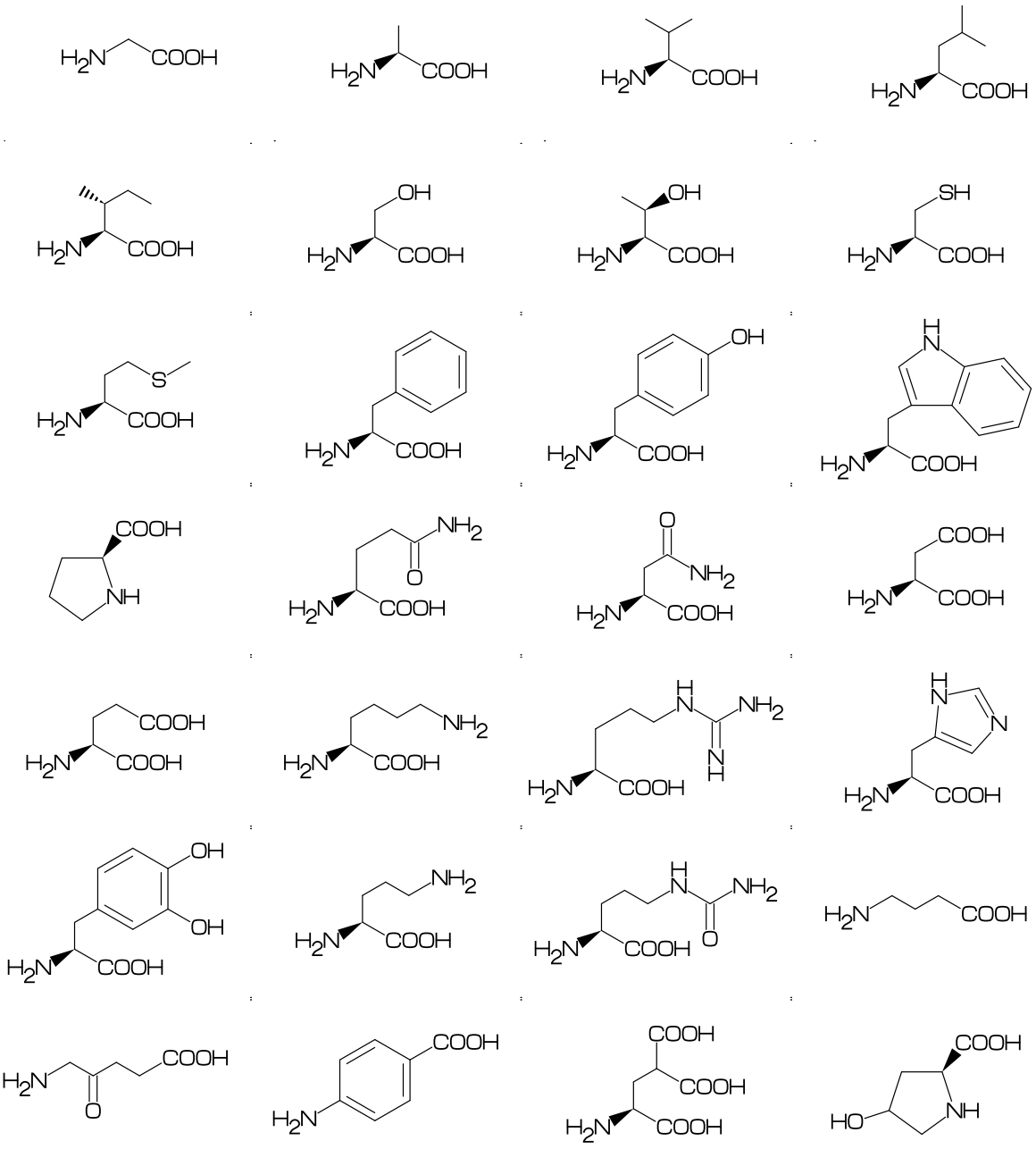
Located at http://www.ctan.org/pkg/mcf2graph

Suggestion or request mail to: mcf2graph@gmail.com



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1 Introduction

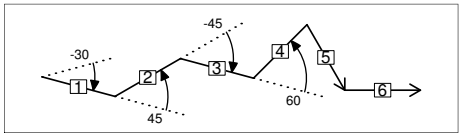
Molecular Coding Format(MCF) is new linear notation represent chemical structure diagrams. This Coding is named from programing technique such as operator, array, scope, macro, adressing, etc. mcf2graph convert from MCF to PNG, SVG, EPS, MOL file. It is also able to calculate molecular weight, exact mass, molecular formula.

2 MCF syntax

2.1 Make bond

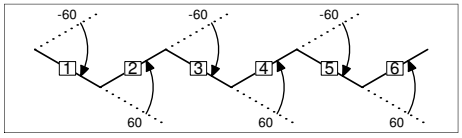
2.1.1 Chain

```
real number plus (+): counterclockwize
real number minus(-): clockwize
$n (0<=n<360): absolute angle

<10,-30,45,-45,60,$300,$0
```



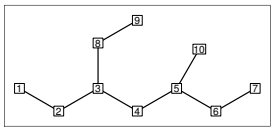
2.1.2 Chain with !,!n

```
!  : take value 60 or -60 depend on
     current angle and environment
!6 : !,!,!,!,!,!

<-30,!6
```



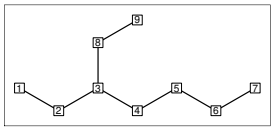
2.1.3 Jump to atom

```
@n : Jump to An
** An: atom number(-999<=n<=4095)

<-30,!6,@3,0,!,@5,-30
```



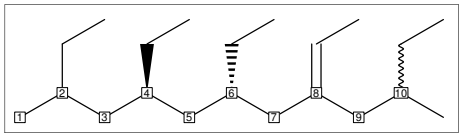
2.1.4 Branch bond

```
\ : 0

<-30,!6,@3,\,!
```

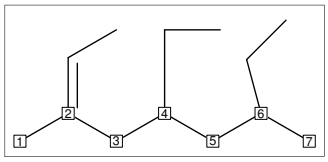


2.1.5 Branch modified bond

```
\   : 0
*\  : 0~wf
\*  : 0~zf
\\  : 0~dm
*\* : 0~wv

<30,!8,
@2,\,!,@4,*\,!,@6,\*,!,@8,\\,!,@10,*\*,!
```

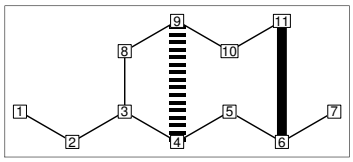



```
<30,!6,
\~dr,!,   : 0~dr,!
\`1.5,-90 : 0`1.5,-90
\^15,-60  : 0^15,-60
```



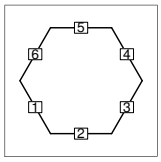
2.1.6 Connect atom

```
&n : Connect to An

<-30,!6,@3,\,!3,&6~bd,@9,&4~bz
```



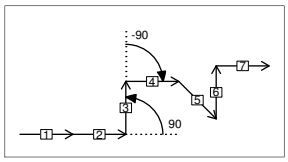
2.1.7 Ring

```
?n : n membered ring(3<=n<=20)
?6 : <-120,60,60,60,60,60,&1
?6
```



2.1.8 Rotate current angle

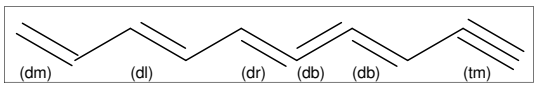
```
<angle : rotate current angle

0,0,<90,0,<-90,0,<$315,0,<$90,0,<$0,0
```



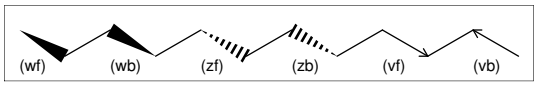
2.2 Change bond type

2.2.1 Double,triple,wedge,vector

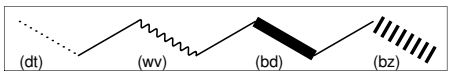
```
(Double,triple)
a~type : ~~type,a
dm  : double middle
dl  : double left side
dr  : double right side
db  : double left or right side
tm  : triple
!!  : !~db  / !!! : !~tm

<-30,!~dm,!,!~dl,!,!~dr,!~db,!~db,!,!~tm
<-30,!~dm,!,!~dl,!,!~dr,!!  ,!!  ,!,!!!
```




```
(Wedge,Vector)
wf: wedge forward
wb: wedge backward
zf: hashed(zebra stripe) wedge foward
zb: hashed(zebra stripe) wedge backward
vf:vector forward
vb:vector backward

<-30,
 !~wf,!,!~wb,!,!~zf,!,!~zb,!,!~vf,!~vb
```

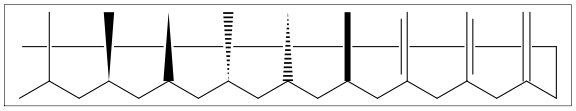



```
(Dotted,wave)
Bn=bond type : change bond type at Bn
dt : dotted   /  wv : wave
bd : broad    /  bz : broad dotted

<-30,!7,1=dt,3=wv,5=bd,7=bz
```



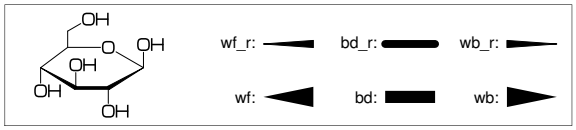
2.2.2 Over line

```
si_ : single over line
wf_ : wedge forward over line
wb_ : wedge backward over line
zf_ : hashed wedge forward over line
zb_ : hashed wedge backward over line
bd_ : broad over line
dl_ : duble left over line
dr_ : duble right over line
dm_ : duble over line

<30,!8,!,60,90`18,
{2~si_,4~wf_,6~wb_,8~zf_,10~zb_,
  12~bd_,14~dl_,16~dr_,18~dm_}:/_`2
```



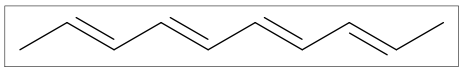
2.2.3 Steric ring

```
wf_r : wedge foward (half width)
bd_r : broad (half width, rounded)
wb_r : wedge backward (half width)

#1.25,-30~wf_r,30~bd_r`1,30~wb_r,
 120,0,30,&1,##,#.5,6^$90:/!OH,
 {1^$-90,2^$90,3^$-90,4^$90}:/OH,
```



2.2.4 Change multiple bond type

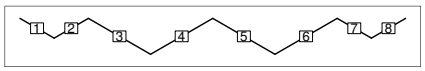
```
{2,4,6,8'}=dl : 2=dl,4=dl,6=dl,8=dr

<30,!7,{2,4,6,8'}=dl
```



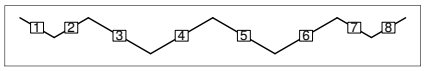
2.3 Change bond length

2.3.1 Chain length

```
(!,!n)`length : change length of !,!n

<-30,!2,!4`1.2,!2
```

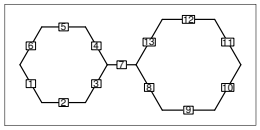



```
#n : bond length=n
## : reset bond length

<-30,!2,#1.2,!4,##,!2
```



2.3.2 Ring length

```
?n`length : change ring length

?6,@4,\,?6`1.2
```



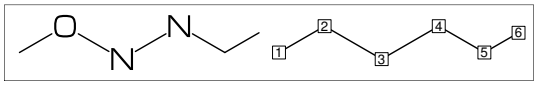
2.4 Change atom

2.4.1 Insert atom

```
Insert hetero atom

<-30,!2,O,!2,N,!2
```

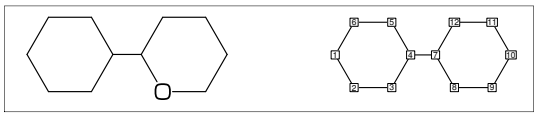
2.4.2 Addressed atom

```
2:O : change A2 C to O
{3,4}:N : change  A3,A4 C to N

<30,!4,2:O,{3,4}:N
```



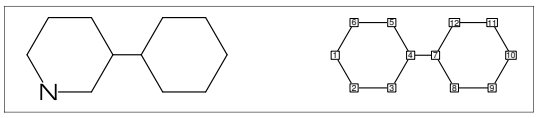
2.4.3 Brock address

```
| : divide brock

?6,@4,\,|,?6,2:O
```



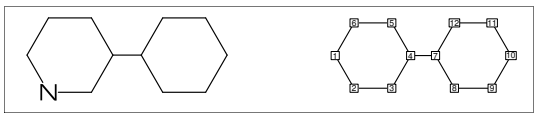
2.4.4 Reset brock address

```
|| : reset brock adress

?6,@4,\,|,?6,||,2:N
```



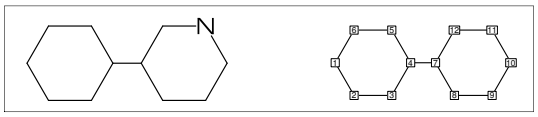
2.4.5 Absolute address

```
$2:N : change A$2 C to N  **1<=n<=3095

?6,@4,\,|,?6,$2:N
```



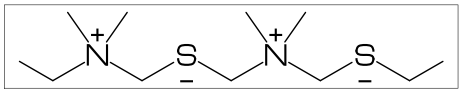
2.4.6 Relative address

```
-2:N : change A(-2) C to N **-999<=n<=-1

?6,@4,\,?6,-2:N
```



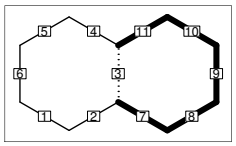
2.4.7 Charged atom

```
p_ : positive / n_ : negative

<-30,!2,N,??,p_,!2,S,n_^180,
!6,7:N,7:??,9:S,7:n_,9:n_^180
```

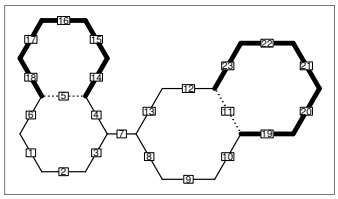


2.5 Fuse ring

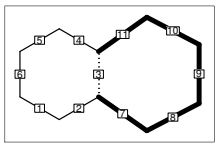
```
(Attached 1 bond)

?6,3=?6 : fuse ?6 at B3
** Bn(n:-999<=n<=4095): bond number

?6,3=?6
```



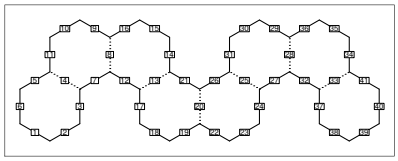
```
** fused ring size depend on
attached bond length

?6,@4,\,?6`1.2,5=?6,11=?6
```



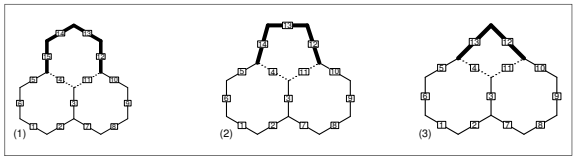
```
?6,3=?6[13] : fuse ?6[13] at B3
?6[13]: 6 membered ring scaled 13/10
** ?m[n] (5<=m<=8,11<=n<=15)

?6,3=?6[13]
```



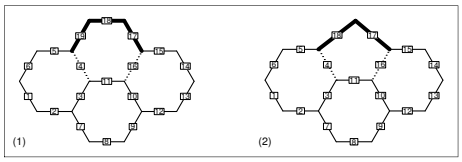
```
?6,{-3,-4,-4,-2,-2,-4,-4}=?6
?6,{4,8,13,20,25,28,33}=?6
```



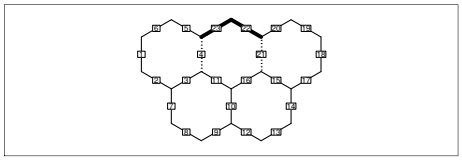
```
(Attached 2 bond)

4--11=?6 : fuse 4/6 ring to B11..B4
4--11=?5 : fuse 3/5 ring to B11..B4
4--11=?4 : fuse 2/4 ring to B11..B4

1:<30,?6,3=?6,11--4=?6
2:<30,?6,3=?6,11--4=?5
3:<30,?6,3=?6,11--4=?4
```



```
(Attached 3 bond)

16---4=?6 : fuse 3/6 ring to B16..B4
16---4=?5 : fuse 2/5 ring to B16..B4

1:?6,{3,10,16---4}=?6
2:?6,{3,10}=?6,16---4=?5
```

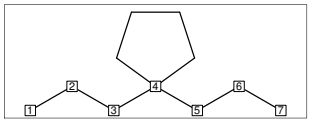



```
(Attached 4 bond)

21----4=?6 : fuse 2/6 ring to B21..B4

<-30,?6,{3,10,15,21----4}=?6
```



2.6 Spiro ring

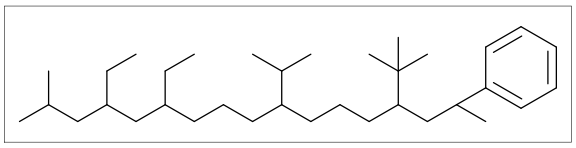
```
@4,?5 : add ?5 at A4

<30,!6,@4,?5
```



2.7 Group

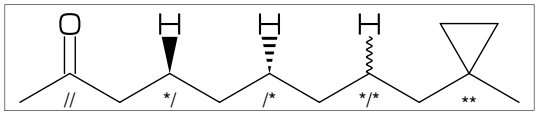
2.7.1 Insert group

```
/ : group start single bond

/_   : methyl
/!   : ethyl
/!2  : propyl
/?!  : isopropyl
/??! : tert-butyl
/Ph  : phenyl

<30,!,/_,!2,/!,!2,/!2,!4,/?!,
 !4,/??!,!2,/Ph^-60,!
```

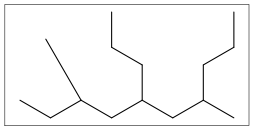


2.7.2 Insert modified group

```
//  : double (double middle)
*/  : wedge forward
/*  : hashed wedge forward
*/* : wave
**  : direct

<30,!,//O,!2,*/H,!2,/*H,!2,*/*H,!2,**?3,!
```

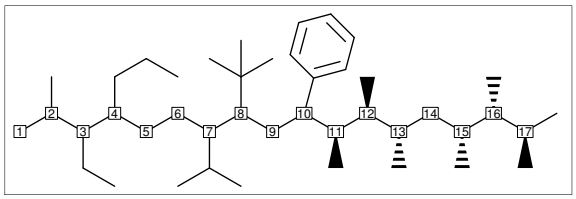



```
~ : change type
^ : change angle
` : change length
> : change environment

<-30,``1,!,
  /_`2^30,!2,/!2>lr,!2,/!2>rl,!)
```



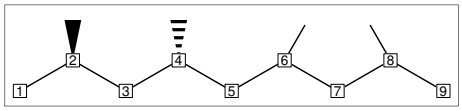
2.7.3 Add group

```
<30,!17,2:/_,3:/!,4:/!2,7:/iPr,
 8:/tBu,10:/'(Ph`0.6)^-15,
 {11,12,13'}:*/_,{15,16,17'}:/*_
```

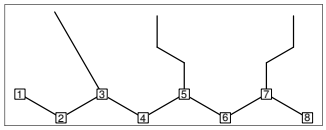


2.7.4 Add modified group

```
~,^,` : change type,angle,length

<30,!6,{2~wf,4~zf,6^-30,8^$120}:/_
```



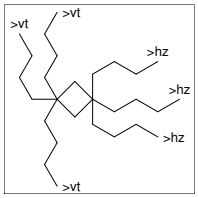
```
^,`,> : change angle,length,environment

<-30,!7`1,3:/_`2^30,5:/!2>lr,7:/!2>rl
```



2.8 Chain environment

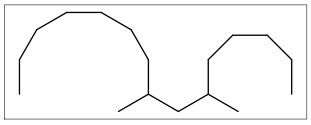
2.8.1 Horizontal,vertical

```
>hz : horizontal environment (default)
>vt : vertical environment

?4,
{3^-90,3^-30,3^90}:/!3>hz,
{1^-60,1,1^60}:/!3>vt
```



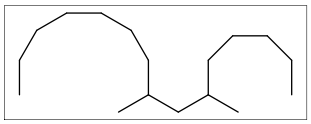
2.8.2 Left-right,right-left

```
>lr : left-right environment
>rl : right-left environment

<-30,!6,
{3^-30,3,3^30}:/!3>lr,
{5^-30,5,5^30}:/!3>rl
```



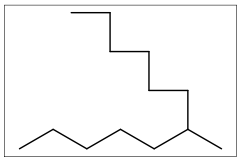
2.8.3 Fixed rotate angle

```
>n : rotate n

<30,!4,
2:/!6>30,  % 2:\,30,30,30,30,30,30
4:/!4>-45  % 4:\,-45,-45,-45,-45
```



2.8.4 Multiple rotate angle

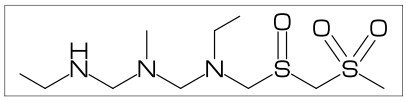
```
>'(90,-90,...) : rotate 90,-90,...

<30,!6,6>'(90,-90,90,-90,90):/!5
```



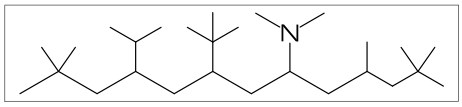
2.9 Miscellaneous

2.9.1 Abbreviated parts

```
NH  : N,/H~nl    N! : N,/_     N!2 : N,/!
SO  : S,//O    SOO : S,//O^35,//^-35

<-30,!2,NH,!2,N!,!2,N!2,SO,!2,SOO,!
```

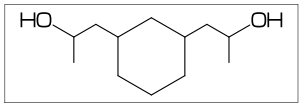



```
?!   : /_,!           ??   : /_^35,/_-35
/?!  : isopropyl      /??! : tert-butyl
/N?! : dimethylamino

<30,!9`1,?!,!,??,!,2:??,4:/??,6:/??!,8:/N?!
```



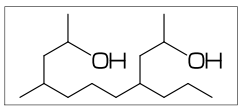
2.9.2 Parts definition

```
'(..) : user defined parts

iBuOH:='(!,/_,!,OH);
MC(<30,?6,{4,6}:/iBuOH)
```



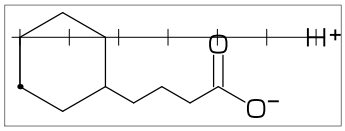
2.9.3 Parts inline definition

```
<30,!8,{2,6}:/'(!,/_,!,OH)
```



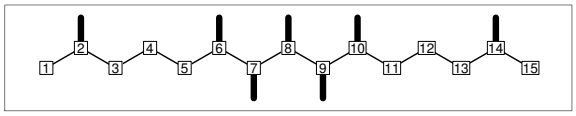
2.9.4 Move position

```
@(x,y) : Move l*(x,y) from current position
@$(x,y): Move l*(x,y) from origin(@1)
         ** l=bond length of ring

<30,?6,@3,!4,//O,!,O,n_^60,@$(6,1),H,p_^15
```



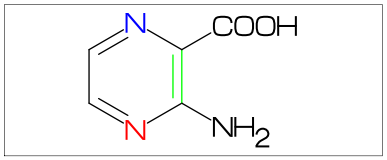
2.9.5 Serial number

```
6:10 : 6,7,8,9,10
<30,!14,{2,6:10,14}:/_~bd_r`0.5
```



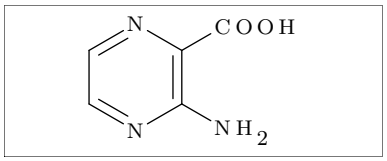
2.9.6 Change color

```
beginfigm()
  MC(
    <30,Ph,{2,5}:N,3:/NH2,4:/COOH,
     %---------------------
     2:red,      % red   A2
     5:blue,     % blue  A5
     3=green     % green B3
     %---------------------
  )
endfigm
```



2.9.7 Change font

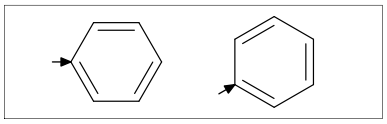
```
beginfigm()
  %----------------
  atomfont:="cmr8";
  %----------------
  MC(<30,Ph,{2,5}:N,3:/NH2,4:/COOH)
endfigm
```



3 Option parameter

3.1 Angle parameter

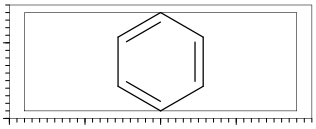
```
mangle=0    ** default

MCat(0.2,0.5)(Ph)
mangle:=30;
MCat(0.8,0.5)(Ph)
```



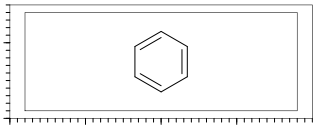
3.2 Size/Ratio parameter

3.2.1 Bond length

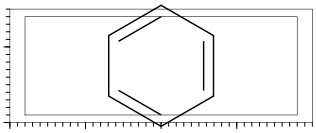
```
(fit to figure size)
blength=0    ** default
```



```
(ratio bond/figure width)
blength=0.1   ** (0<blength<=1)
blength=60mm(width)*0.1=6mm
```

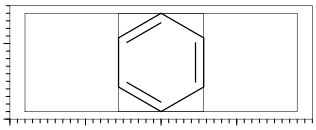


```
(bond length)
blength=9mm
** (blength>1) ignore msize(w,h)
```

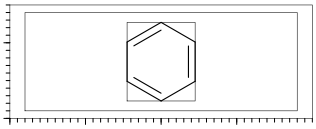


3.2.2 Molecular size

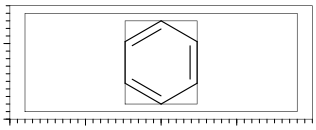
```
msize=(1,1)   ** default
```



```
msize=(0.25,1)
msize=40mm-4mm*0.25=9mm
```

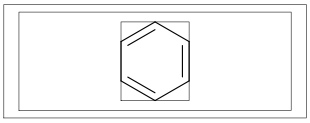


```
msize=(11mm,11mm)
```



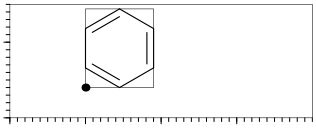
3.2.3 Molecular position

```
mposition=(0.5,0.5) ** default
```



```
mposition=(1,0)
```

```
mposition=(10mm,4mm)
```

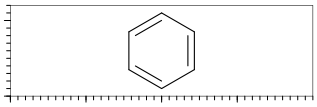


3.3 Size parameter

3.3.1 Figure size

fsize=(figure width,figure height)
** default: (30mm,20mm)

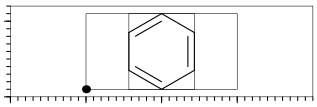
fsize=(40mm,15mm)



3.3.2 Figure margin

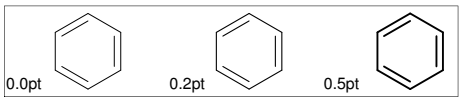
fmargin=(margin left rigth,top bottom)
** default: (0.4mm,0.4mm)

fmargin=(10mm,2mm)



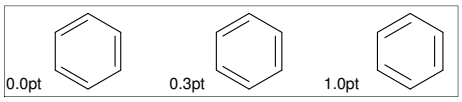
3.3.3 Offset thickness of bond

default: offset_thickness=0.2pt



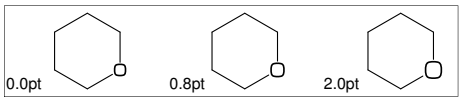
3.3.4 Offset of double bond gap

default: offset_bond_gap=0.3pt



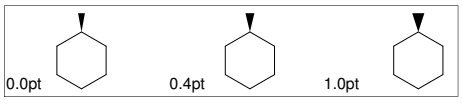
3.3.5 Offset of atom width

default: offset_atom=0.8pt



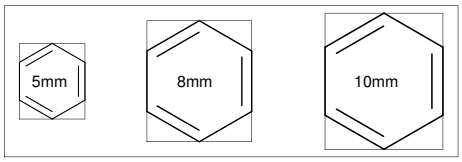
3.3.6 Offset of wedge width

default: offset_wedge=0.4pt



3.3.7 Max bond length

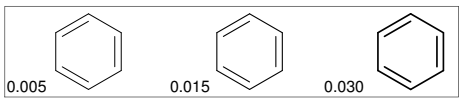
default: max_blength=10mm



3.4 Ratio parameter

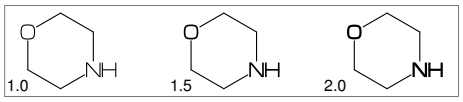
3.4.1 Thickness/bond length

default: ratio_thickness_bond=0.015



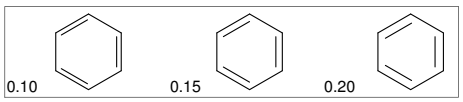
3.4.2 Char/bond thickness

default: ratio_char_bond=1.5



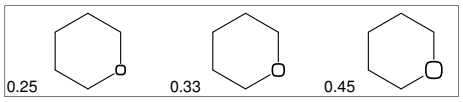
3.4.3 Bond gap/bond length

default: ratio_bondgap_bond= 0.15



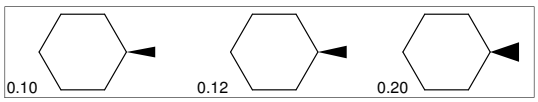
3.4.4 Atom/bond length

default: ratio_atom_bond= 0.36



3.4.5 Wedge/bond length

default: ratio_wedge_bond=0.12

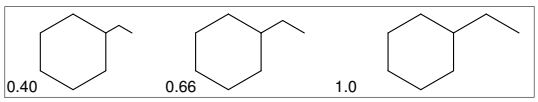


3.4.6 Figure atom gap/atom length

default: ratio_atomgap_atom= 0.050

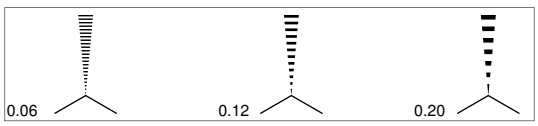
3.4.7 Chain/ring length

default: ratio_chain_ring= 0.66



3.4.8 Hash gap/bond length

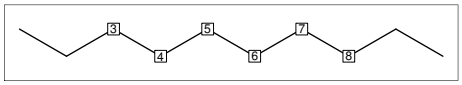
default: ratio_hashgap_bond=0.12



3.5 Drawing mode

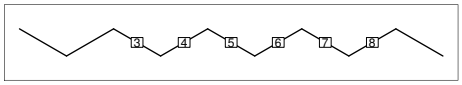
3.5.1 Numbering atom

```
sw_numbering=Atom
numbering_start:=3;
numbering_end:=8;
default: sw_numbering=0

sw_numbering:=Atom;
MC(<-30,!9)
```



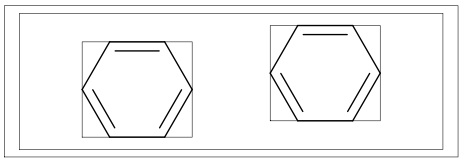
3.5.2 Numbering bond

```
sw_numbering=Bond
numbering_start:=3;
numbering_end:=8;
default: sw_numbering=0

sw_numbering:=Bond;
MC(<-30,!9)
```

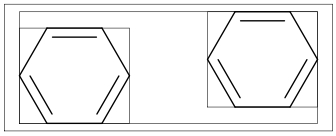


3.5.3 Trimming mode

```
sw_trimming:=0;  ** default
msize:=(1,0.7);
MCat(0.2,0.3)(Ph)
MCat(0.8,0.7)(Ph)
```

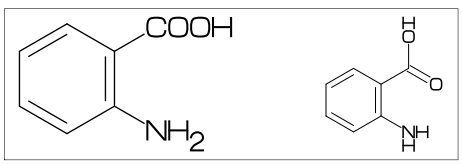


```
sw_trimming:=1;
MCat(0.2,0.3)(Ph)
MCat(0.8,0.7)(Ph)
```



3.5.4 Expand mode

```
MCat(0, .5)(<30,Ph,4:/COOH,3:/NH2)
sw_expand:=1;
MCat(1, .5)(<30,Ph,4:/COOH,3:/NH2)
** default: sw_expand=0
```



3.5.5 Abbreviate group

```
** default: sw_abbreviate=Group
```

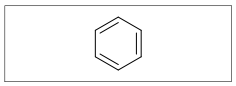
3.5.6 Abbreviate bond type

```
** default: sw_abbreviate=Bond
```

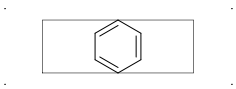
3.6 Frame

3.6.1 Figure frame

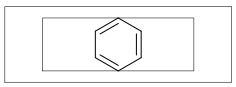
```
** default:sw_frame=0
(Draw figure frame)
fmargin:=(5mm,2mm);
sw_frame=Outside
```



```
(Frame inside margin)
sw_frame=Inside
```

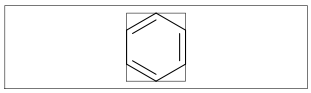


```
(Draw both frame)
sw_frame=Bothside=Inside+Outside
```



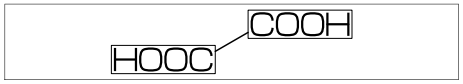
3.6.2 Molecular frame

```
sw_frame=Mol
** default:sw_frame=0
```



3.6.3 Atom frame

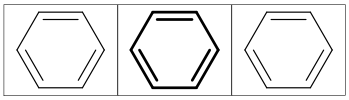
```
sw_frame=Atom
** default: sw_frame=0

MC(<30,COOH,!,COOH)
```



3.7 Parameter setting

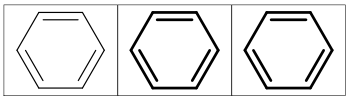
3.7.1 Local parameter setting

```
beginfigm()
  MC(Ph)
endfigm
beginfigm()
  %-------------------------
  ratio_thickness_bond:=0.05;
  %-------------------------
  MC(Ph)
endfigm
beginfigm()
  MC(Ph)
endfigm
```



3.7.2 Global parameter setting

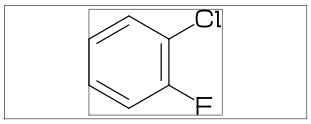
```
beginfigm()
  MC(Ph)
endfigm
%-------------------------
ratio_thickness_bond:=0.05;
%-------------------------
beginfigm()
  MC(Ph)
endfigm
beginfigm()
  MC(Ph)
endfigm
```



4 Function

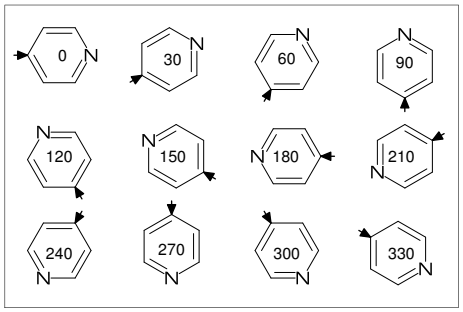
4.1 Function MC()

```
(Draw molecule)

msize=(a,b)         **default (1,1)
mposition=(c,d)     **default (0.5,0.5)

a: ratio molecular width/figure width
b: ratio molecular hight/figure hight
c: x axis position
d: y axis position

beginfigm()
  MC(<30,Ph,3:/F,4:/Cl)
endfigm
```



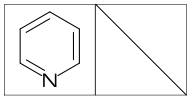
4.2 Function MCat()

```
(Draw molecule at mposition)

MCat(c,d)(....) :

mposition:=(c,d); MC(....)

c: x axis position
d: y axis position

defaultsize:=5bp;
fsize:=(60mm,40mm); fmargin:=(3mm,3mm);
blength:=0.07; sw_frame:=Outside;
mangle:=0;
for i=1 step -0.5 until 0:
  for j=0 step 0.33 until 1:
    MCat(j,i)(Ph,4:N)
    add(drawarrow((A1+A1up**aw)..A1);
        label(decimal(mangle),
              p0+(0.5w,0.5h));
    )
    mangle:=mangle+30;
  endfor
endfor
```



4.3 Function mc_check()

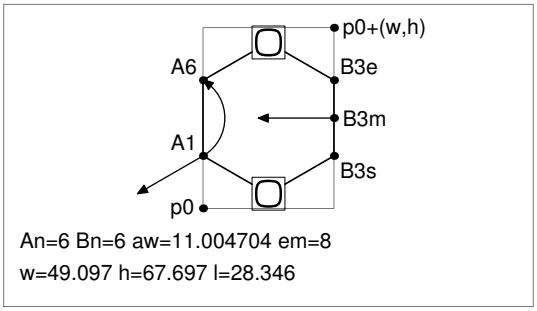
```
(immediately compile)

beginfigm("EN:Pyridine")
  MC(<30,Ph,2:N)
endfigm

(check mcf and compile)

** mc_check(mc) : error count

beginfigm("EN:Pyridine",
  ":<30,Ph,}2:N") % ** extra '}'
  if mc_check(mc)=0: MC(scantokens(mc)) fi
endfigm
```



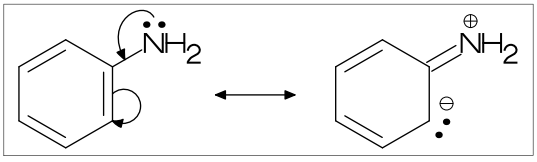
```
mc_check(mc)=0   mc_check(mc)>=1
```

4.4 Function add()

```
(Add label to molecule)

w:       molecular width
h:       molecular height
aw:      atom font size
em:      label font size
p0:      origin of molecular structure
l:       bond length

An:      atom number
A[m]:    atom position
A[m]ang: branch angle of A[m]
A[m]up:    dir A[m]ang
A[m]left:  dir A[m]ang+90
A[m]right: dir A[m]ang-90
A[m]down:  dir A[m]ang+180

Bn:      bond number
B[m]:    bond(path)
B[m]s:   bond start position
B[m]m:   bond middle position
B[m]e:   bond end position
B[m]ang: bond angle
B[m]up:    dir B[m]ang
B[m]left:  dir B[m]ang+90
B[m]right: dir B[m]ang-90
B[m]down:  dir B[m]ang+180

plus  : '+' circled
minus : '-' circled
  circlediam = 0.6aw (default)
  circlepen =  0.2bp (default)

lonepair r: ':' rotated r
  lonepairdiam  = 0.3aw (default)
  lonepairspace = 0.7aw (default)

** : scaled
<< : rotated
a /* b : point b of a

beginfigm("EN:add() 1")
 fsize:=(70mm,40mm);
 sw_frame:=sw_frame+Atom+Mol;
 max_blength:=10mm;
 msize:=(.91,.9);
 MCat(.5,.85)(<30,?6,{2,5}:O)
 add(
  defaultscale:=.8;
  labeloffset:=.3aw;
  dotlabel.lft("p0",p0);
  dotlabel.rt( "p0+(w,h)",p0+(w,h));
  dotlabel.ulft("A1",A1);
  drawarrow A1..A1+__*l<<A1ang;
  dotlabel.lrt( "B3s",B3s);
  dotlabel.rt("B3m",B3m);
  drawarrow B3m..B3m+__*l<<(B3ang+90);
  dotlabel.ulft("A6",A6);
  drawarrow A1{A1down}..A6;
  dotlabel.urt( "B3e",B3e);
  label.rt(  "An="&decimal(An)&
           "  Bn="&decimal(Bn)&
           "  aw="&decimal(aw)&
           "  em="&decimal(em),
           p0+(-9em,-1.5em));
  label.rt(  "w="&decimal(w)&
    "  h="&substring (0,6)of decimal(h)&
    "  l="&substring (0,6)of decimal(l),
           p0+(-9em,-3em));
 )
endfigm
```

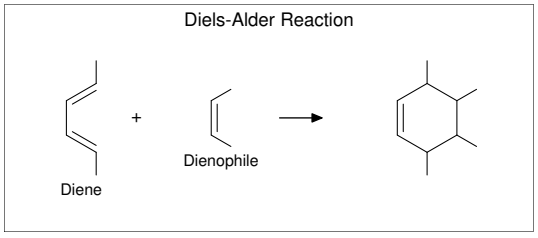



```
beginfigm("EN:add() 2")
 fsize:=(60mm,20mm);
 msize:=(1,0.85);
 %---------------------------------------
 MCat(0,0)(<30,Ph,3=dl,4:/NH2)
 %---------------------------------------
 add(
  labeloffset:=.7aw;
  label.top(lone_pair 90,A7);
  drawarrow
    (A7+up**1.2aw){A7left}
     ..{B7right}B7/*0.3;
  drawarrow
    B3m..A3+B2up**1.5aw..{A3down}A3;
 )
 %---------------------------------------
 MCat(1,0)(<30,?6,{1,5}=dl,4://NH2)
 %---------------------------------------
 add(
  labeloffset:=.7aw;
  label.top(plus,A7);
  label.urt(minus,A3);
  label(lonepair A3ang,A3+A3up**.7aw);
 )
 %---------------------------------------
 ext(drawdblarrow (.4w,.4h)..(.55w,.4h);)
 %---------------------------------------
endfigm
```



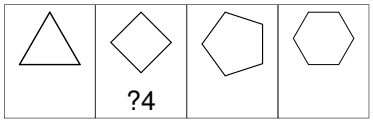
4.5 Function ext()

```
(Extra label to figure)

w:    figure width
h:    figure height
w0:   figure width-2xpart(fmargin)
h0:   figure height-2ypart(fmargin)
aw:   atom font size
em:   label font size
p0:   fmargin

n:    molecular number
p[m]: molecular origin position
w[m]: molecular width
h[m]: molecular height

ratio_thickness_char:
pen thickness / char width
%---------------------------------------
beginfigm()
 fsize:=(70mm,30mm;);
 blength:=0.065;
 %---------------------------------------
 MCat(0.1,0.5)(
   <-210,60`1,60`1,60`1,{1,3}=dl,
   1:/R1,4:/R2^-60
   )
 add(
     defaultscale:=0.6;
     label.bot("Diene",p0+(0.5w,0));
 )
 MCat(0.4,0.5)(
   <-30,-60`1,1=dl,1:/R3,2:/R4^60)
   add(defaultscale:=0.6;
   label.bot("Dienophile",p0+(.5w,0));
 )
 MCat(0.9,0.5)(
   <30,?6,6=dl,2:/R2,3:/R4,4:/R3,5:/R1
 )
 %---------------------------------------
 ext(
  drawarrow (.52w,.5h)..(.6w,.5h);
  defaultscale:=0.7;
  label("+",(0.25w,0.5h));
  ratio_thickness_char:=0.125;
  label.bot("Diels-Alder Reaction",
            (.5w,h));
 )
 %---------------------------------------
endfigm
```



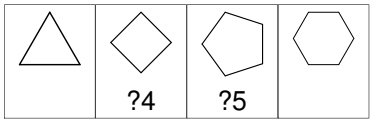
4.5.1 Local ext() setting

```
beginfigm("EN:?3")
  fsize:=(12mm,15mm);
  MCat(0.5,1)(<30,?3)
endfigm
beginfigm("EN:?4")
  fsize:=(12mm,15mm);
  MCat(0.5,1)(?4)
  %-------------------------------
  ext(label.top(inf_EN,(0.5w,0));)
  %-------------------------------
endfigm
beginfigm("EN:?5")
  fsize:=(12mm,15mm);
  MCat(0.5,1)(?5)
endfigm
beginfigm("EN:?5")
  fsize:=(12mm,15mm);
  MCat(0.5,1)(?6)
endfigm
```



4.5.2 Global ext() setting

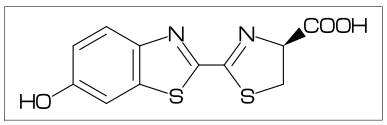
```
ext_clear: reset global ext()

beginfigm("EN:?3")
  fsize:=(12mm,15mm);
  MCat(0.5,1)(<30,?3)
endfigm
%-------------------------------
ext(label.top(inf_EN,(0.5w,0));)
%-------------------------------
beginfigm("EN:?4")
  fsize:=(12mm,15mm);
  MCat(0.5,1)(?4)
endfigm
beginfigm("EN:?5")
  fsize:=(12mm,15mm);
  MCat(0.5,1)(?5)
endfigm
%---------
ext_clear;
%---------
beginfigm("EN:?6")
  fsize:=(12mm,15mm);
  MCat(0.5,1)(?6)
endfigm
```



5 MCF example

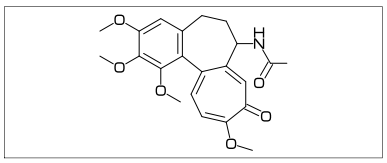
5.1 Luciferin

```
(use library file 'mcf_library')
beginfigm("f:mcf_library",
          "t:EN","v:Luciferin")
  fsize:=(50mm,15mm);
  if mc_check(mc)=0: MC(scantokens(mc)) fi
endfigm
```



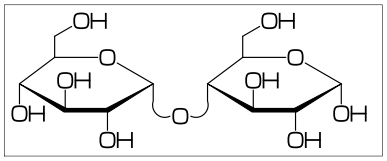
5.2 Colchicine

```
beginfigm("EN:Colchicine","MW:385.41",
  %-----------------------------------
  ": <30,Ph,{1,2,6}:/O!,{-4,-5}=?7,   ",
  ": {-1,-4,-6}=dl,-2://O,-3:/O!,     ",
  ": @9,\,NH,!,//O,!                  ")
  %-----------------------------------
  fsize:=(50mm,20mm);
  if mc_check(mc)=0: MC(scantokens(mc)) fi
endfigm
```



5.3 Maltose

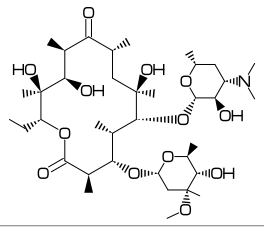
```
(bond type for glycan)
arc_lb : arc left > bottom
arc_br : arc bottom right

beginfigm("EN:Maltose","MW:342.3",
  %-------------------------------------------------------
  ": #1.25,-30~wf_r,30~bd_r`1,30~wb_r,120,O,30,&1,##,   ",
  ": #.5,{1^$-90,2^$90,3^$-90}:/OH,6^$90:/!OH,          ",
  ": @4,$-50~arc_lb`1,O,$50~arc_br`1,<$0,               ",
  ": |,#1.25,-30~wf_r,30~bd_r`1,30~wb_r,120,O,30,&1,##, ",
  ": #.5,{2^$90,3^$-90,4^$-90}:/OH,6^$90:/!OH           ")
  %-------------------------------------------------------
  fsize:=(50mm,20mm);
  if mc_check(mc)=0: MC(scantokens(mc)) fi
endfigm
```



5.4 Erythromycin

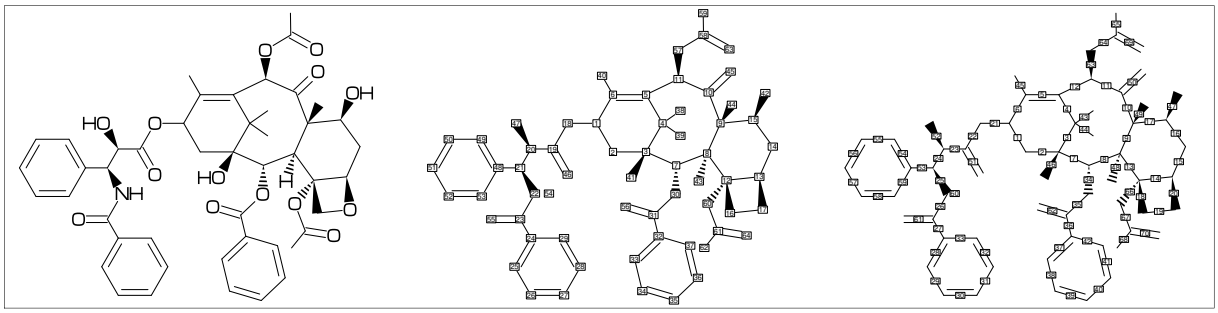
```
beginfigm("EN:Erythromycin","MW:733.93")
  fsize:=(120mm,30mm);
  MC(<30,#1,<-120,60,60,60,-60,60,60,-60,60,60,60,-60,60,60,##,&1,
      14:O,13:/*Et,{1,9}://O,
      {2',4,6^-35,8,10',12^35}:/*_,
      {6^35,11,12^-35}:*/OH,
      @$3,\*,O,30~zb,|,?6`.7,6:O,#.5,{5~wf,3^35}:/_,4:/*OH,3^-35:/*O!,##,
      @$5,\*^30`1.7,O,!~zb,|,?6`.7,6:O,#.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



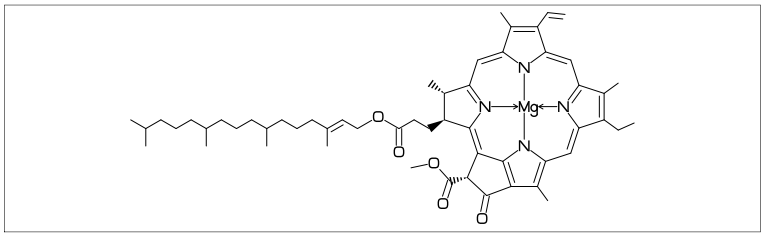
5.5 Paclitaxel

```
beginfigm("EN:Paclitaxel","MW:853.918",
  %-------------------------------------------------------------------------
  ": ?6,5=dl,@3,#1,36,45,45,45,45,##,&5,-4=?6,-4=?4,-1=wb,-3=wf,-1:O, ",
  ": 4:??,6:/_,{3^-60,15}:*/OH,8:/*H^-60,9:*/_^60,10://O,              ",
  ": @1,\,O,!,//O,!,*/OH,!,/Ph,60~wf,NH,-60,//O,60,Ph,                 ",
  ": @7,\*,O,-45,//O,60,Ph,11:*/OCO!>rl,12:/*OCO!^-15>lr               ")
  %-------------------------------------------------------------------------
  fsize:=(140mm,30mm);
  if mc_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
```



5.6 Chlorophyll a

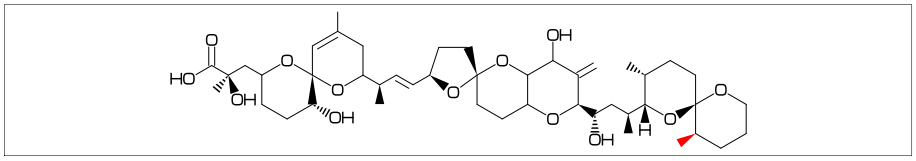
```
beginfigm("f:mcf_library.mcf","t:EN","v:Chlorophyll a","NO:-",
          "= sw_output:=Fig+Calc+Mcode;",
          "= fsize:=(100mm,30mm);")
  if op_row>=1: scantokens(op) fi
  if mc_check(mc)=0:
    MC(scantokens(mc))
    VerbatimTeX("\gdef\EN{"&inf_EN&"}\gdef\MW{"&inf_MW&"}");
    VerbatimTeX("\gdef\mw{"&cal_MW&"}\gdef\fm{"&cal_FM&"}");
  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://O,
 @2,*\^-6,!2,//O,!,O,!2,!!,|,!13,{1,5,9,13}:/_

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

5.7 Dinophysistoxin-1

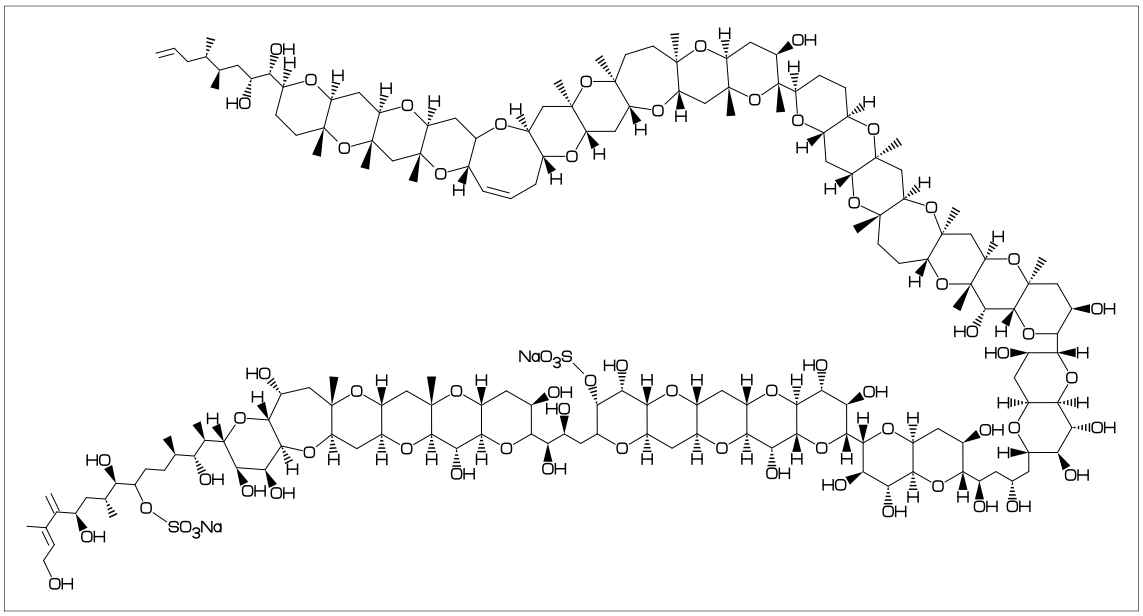
```
beginfigm("t:EN","v:Okadaic acid","EN:Dinophysistoxin-1",
          "MW:819",":,38:*/_,65=red")  %%%% add methyl group (color red) %%%%
  sw_output:=Fig+Calc+Mcode;           %%%% output temp-mc.aux %%%%
  fsize:=(120mm,20mm);
  if mc_check(mc)=0: MC(scantokens(mc))
    VerbatimTeX("\gdef\EN{"&inf_EN&"}\gdef\MW{"&inf_MW&"}");
    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,!,//O,!1,OH,
 3=wb,11=dl,15=dr,17=wf,19=wf,38=wb,{5,7,16,24,25,33,42}:O,
 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
```

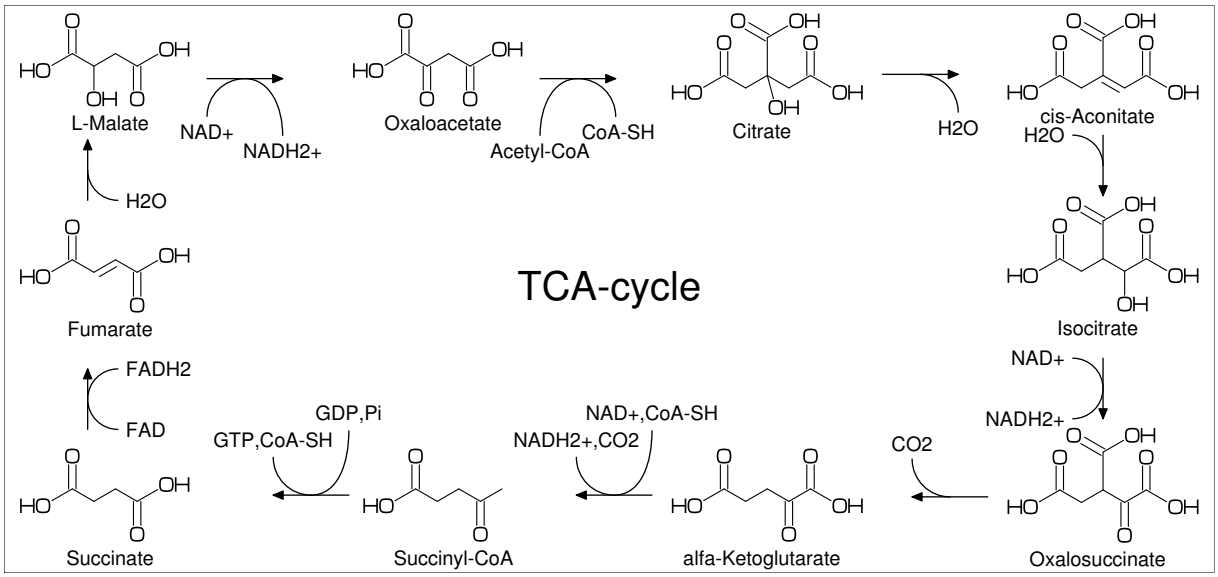
5.8 Maitotoxin

```
%-------------------------------------------------------------------------------
\begin{mplibcode}
  beginfigm("t:EN","v:Maitotoxin")
    sw_output:=Fig+Calc+Mcode;          %%% output temp-mc.aux %%%
    fsize:=(150mm,80mm);
    fmargin:=(3mm,3mm);
    sw_frame:=Outside;
    if mc_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,\,?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=dl,{-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}:O,
 {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,\,O,30,SO3Na,
 @$36,-45~zf,O,30,SO3Na,
 @$150,\,|,!7,{1,2}:/*OH,4:*/_,5:/*_,7=dl

** EN:Maitotoxin  mw:3425.86  MW:3425.856  fm:C164H256Na2O68S2
```

5.9 TCA cycle




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

6 Example to use mcf2graph

6.1 MetaPost souce file

```
%-------------------------------------------------------------------------
input mcf2graph;                                          > input main macro
%-------------------------------------------------------------------------
sw_output:=Info;      % aux(information) file output on > global setting
%%%% sw_output:=Report;                                 > report output
%%%% sw_output:=MOL2k;                                  > MOL file output
fsize:=(60mm,40mm);   %  (figure width,figure height)   >
tag1:="J";                                                > jobname
tag2:="C";                                                > char No
tag3:="mw";           % calculated molecular weight     >
tag4:="fm";           % calculated molecular formula    >
outputformat:="png"; hppp:=vppp:=0.1;                     > PNG output
outputtemplate:="c%3c-%{EN_}.png";                        >
%-------------------------------------------------------------------------
beginfigm("EN:Ampicillin","MW:349.405")                   > information
  MC(<45,?4,-3=?5,2:N,7:S,                                > immediately compile
    3^45:/*H,1://O^15,5:/*COOH^-18,6:??,                  >
    @4,*\^15,NH,!,//O,!,/*NH2,!,Ph)                       >
endfigm                                                   >
%-------------------------------------------------------------------------
beginfigm("EN:Cholesterol","MW:386.65",                   >information
  %--------------------------------------               >
  ": <30,?6,{-4,-2}=?6,-4=?5,7=dl,      ",                > mc1
  ": 10:/*H^180,11:/*H^-60,17:/*H^-54,  ",                > mc2
  ": {4,12}:*/_^60,                     ",                > mc3
  ": @-1,18,/*_,-60,!3,?!               ")                > mc4
  %--------------------------------------               >
  if mc_check(mc)=0: MC(scantokens(mc)) fi                   > mc=mc1 - mc4
endfigm                                                   >
%-------------------------------------------------------------------------
beginfigm("f:mcf_library.mcf","t:EN","v:Adenine")         > from mcf_library.mcf
  if mc_check(mc)=0: MC(scantokens(mc)) fi                   > select EN="Adenine"
endfigm                                                   >
%-------------------------------------------------------------------------
beginfigm("t:EN","v:Guanine")                             > select EN="Guanine"
  if mc_check(mc)=0: MC(scantokens(mc)) fi
endfigm
%-------------------------------------------------------------------------
beginfigm("t:EN","v:Cytosine")                            > select EN="Cytosine"
  if mc_check(mc)=0: MC(scantokens(mc)) fi                   >
endfigm                                                   >
%-------------------------------------------------------------------------
beginfigm("t:n","v+:4")                                   > v+:4 = select No.4
  if mc_check(mc)=0: MC(scantokens(mc)) fi                >        keep file open
endfigm                                                   >
%-------------------------------------------------------------------------
forever:
%%%%%%%%%%  beginfigm("f:mcf_library","v+:*")             > select all
  beginfigm("f:mcf_library","t:EXA","v+:1")               > 'v+:1'= select EXA=1
    if f_EOF=0: if mc_check(mc)=0: MC(scantokens(mc)) fi fi >   keep file open
  endfigm                                                 >
  exitif f_EOF=1;                                         > exit if file end
endfor
%-------------------------------------------------------------------------
bye
```

6.2 Molecular library file

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% molecular library file    mcf_library.mcf   by Akira Yamaji   2022.10.10
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%  tag1:var1;tag2:var2;tag3:var3 .....
%  first character of line "%" comment out
%  first character of line ":"  start MCF
%  first character of line ";"  stop MCF
%  first character of line "="  start parameter setting
%  first character of line "*"  start ext(...)
%  first character of line "+"  start add(...)
%  Cat = Category,EN = Name,MW = Molecular weight
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
Cat:Category;EN:Example;MW:100.00;EXA:%
=
 sw_frame:=Atom;
:
<30,?6,3=?5,{1,3,5,9}=dl,{2,6,9}:N,5:/NH2,7:NH
*
 defaultscale:=.5;
 label.bot(decimal(fig_num)&":"&inf_EN,(.5w,0));
+
 defaultscale:=.3;
 label.bot("A2",A2) withcolor red;
 label.top("A6",A6) withcolor red;
 label.top("A9",A9) withcolor red;
;
%=============================================================================
Cat:biological;EN:Adenine;MW:135.13;EXA:1
:
<30,?6,3=?5,{1,3,5,9}=dl,{2,6,9}:N,5:/NH2,7:NH
;
%-----------------------------------------------------------------------------
Cat:biological;EN:Guanine;MW:151.13;EXA:1
:
<30,?6,3=?5,{1,3,9}=dl,{2,9}:N,{6,7}:NH,5://O,1:/NH2
;
%-----------------------------------------------------------------------------
Cat:biological;EN:Cytosine;MW:111.10;EXA:1
:
<30,?6,{4,6}=dl,4:N,3://O,2:NH,5:/NH2
;
%-----------------------------------------------------------------------------
Cat:biological;EN:Thymine;MW:126.11;EXA:1
:
<30,?6,3=dl,{2,6}:NH,{1,5}://O,4:/_
;
%-----------------------------------------------------------------------------
Cat:biological;EN:Uracil;MW:112.09;EXA:1
:
<30,?6,6=dl,{3,5}://O,{2,4}:NH
;
%== Amino acid ===============================================================
Cat:biological;EN:Glycine;MW:75.07;EXA:-
:
<30,NH2,!2,COOH
;
%-----------------------------------------------------------------------------
```

6.3 Function mc_query()

(Example)

```
%--------------------------------------------------------------
% mc_query()
%
% "f:filename" : input file name  (default "mcf_library.mcf")
% "o:filename" : output file name (default "temp.mcf")
%
% "a:sort-key" : sort by sort-key ascending
% "d:sort-key" : sort by sort-key descending
%
% operator  :  = , <> , <= , >= , < , >
%
% filter 1  : Cat=biological
% filter 2  : MW>=285
% filter 3  : MW<=295
%
%--------------------------------------------------------------
mc_query("Cat=biological","MW>=285","MW<=290","a:EN");
%--------------------------------------------------------------
```

(output)

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Input  : mcf_library.mcf [506]
% Output : temp.mcf [5]
% Filter(1): Cat =biological
% Filter(2): MW >= 285
% Filter(3): MW <= 290
% Sort key : EN (ascending)
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
Cat:biological;EN:Atoropin;MW:289.375;EXA:1
:
<30,O,!,//O,!2,Ph,@$1,\~zb^-60,|,?7`1.1,@6,*\^190`1.25,N!,&3~wb,$3:/!OH~wv
;
Cat:biological;EN:Luteolin;MW:286.24;EXA:-
:
<30,Ph,3=?6,9=dl,10:O,7://O,@9,\,Ph,{2,6,14,15}:/OH
;
Cat:biological;EN:Lycorine;MW:287.315;EXA:1
:
<30,Ph,{-4,-2}=?6,{6,(9,12)}=?5,13=dl,8:N,{15,17}:O,
 {9'^180,10^60}:*/H,{13,14'}:*/OH
;
Cat:biological;EN:Morphine;MW:285.343;EXA:1
:
<30,Ph,{2,-4}=?6,(1,12)=?5[2],-1:O,-1=zb,
 @7,60~wf`0.75,70~si_`1.3,45,N!,&9~wb,15=dl,6:/OH,8^180:*/H,12:/*OH
;
Cat:biological;EN:Piperine;MW:285.343;EXA:1
:
<30,Ph,-1=?5,{-1,-3}:O,@4,\,!!,!,!!,!,//O,!,?6,-6:N
;
```

6.4 Information aux file output

(Option parameter setting)

```
  sw_output:=Info;        %% tag1:var1;tag2:var2
  sw_output:=Info+Table;  %% tag1;tag2 var1;var2
```

(Command line)

```
  >mpost -s ahlength=1 FILENAME  (sw_output=Info)
  >mpost -s ahlength=2 FILENAME  (sw_output=Info+Table)
```

(Sourse)

```
beginfigm("EN:Ampicillin")    .... endfigm
beginfigm("EN:Cholesterol")   .... endfigm
beginfigm("EN:Limonin")       .... endfigm
beginfigm("EN:beta-Carotene") .... endfigm
```

(Setting)

```
tag1:="J"; tag2:="C"; tag3:="mw"; tag4:="fm"; tag5:="EN";
```

(Output)

```
(sw_output=Info)
F:mcf_man_soc;C:1;mw:349.40462;fm:C16H19N3O4S;EN:Ampicillin
F:mcf_man_soc;C:2;mw:386.6532;fm:C27H46O;EN:Cholesterol
F:mcf_exa_soc;C:3;mw:470.5113;fm:C26H30O8;EN:Limonin
F:mcf_exa_soc;C:4;mw:536.8722;fm:C40H56;EN:beta-Carotene

(sw_output=Info+Table)
F;C;mw;fm
mcf_man_soc;1;349.40462;C16H19N3O4S;Ampicillin
mcf_man_soc;2;386.6532;C27H46O;Cholesterol
mcf_exa_soc;3;470.5113;C26H30O8;Limonin
mcf_exa_soc;4;536.8722;C40H56;beta-Carotene

(aux_delimiter="/")
F:mcf_man_soc/C:1/mw:349.40462/fm:C16H19N3O4S/EN:Ampicillin
F:mcf_man_soc/C:2/mw:386.6532/fm:C27H46O/EN:Cholesterol
F:mcf_exa_soc/C:3/mw:470.5113/fm:C26H30O8/EN:Limonin
F:mcf_exa_soc/C:4/mw:536.8722/fm:C40H56/EN:beta-Carotene
```

(Tag)

```
J   : jobname
C   : char number
NO  : serial number
EN  : english name
JN  : japanese name
FM  : formula from literature data
MW  : molecular weight from literature data
MI  : monoisotopic mass from literature data
USE : the use
mw  : molecular weight calculated
mi  : monoisotopic mass calculated
fm  : molecular formula calculated
w   : figure width
h   : figure height
```

6.5 MCF aux file output

(Option parameter setting)

```
sw_output:=Mcode;          %% output 'temp-mc.aux'
```

(Command line)

```
  >mpost -s ahlength=3 FILENAME  (sw_output=Info+Mcode)
```

(Output mcf file)

```
sw_output=Mcode            %% file name = 'temp-mc.aux'

(result)
<30,?6,3=?5,{1,3,5,9}=dl,{2,6,9}:N,5:/NH2,7:NH
```

(Output library file)

```
sw_output=Info+Mcode       %% file name = 'jobname-lib.aux'

(result)
Cat:biological;EN:Adenine;MW:135.13;EXA:1
+
<30,?6,3=?5,{1,3,5,9}=dl,{2,6,9}:N,5:/NH2,7:NH
+-------------------------------------------------
```

(LuaLaTeX example)

```
%-------------------------------------------------------------------------
\begin{mplibcode}
  beginfigm("t:EN","v:Vancomycin")
    sw_output:=Mcode;      %%%% output temp-mc.aux %%%%
  endfigm;
\end{mplibcode}
%-------------------------------------------------------------------------
\verbatiminput{temp-mc.aux}
%-------------------------------------------------------------------------

(result)
file name = 'temp-mc.aux'

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

6.6 Report output

(Option parameter setting)

```
  sw_output:=Report;        %% file name = 'jobname-report.aux'
```

(Command line)

```
  >mpost -s ahlength=7 FILENAME
```

(Output)

```
================================================================================
 No[3],Name<Cytosine>,Category<biological>,File<mcf_library.mcf>
--------------------------------------------------------------------------------
<30,?6,{4,6}=dl,4:N,3://O,2:NH,5:/NH2
--------------------------------------------------------------------------------
 Row[1],Length[37],Commands[7],&Code[59],Warning[0]
--------------------------------------------------------------------------------
 =[1]({}=[1]), :[4]({}:[0]), '()[0]
 @[0],&[0],<[1],~[0],^[0],`[0],>[0],|[0],||[0],#[0],##[0]
--------------------------------------------------------------------------------
 Width[30.92432],Height[42.36536], Shift x[0],Shift y[-12.99213]
 Bond length[11.33856],Atom size[4.8819]
--------------------------------------------------------------------------------
 Atom[9],Bond[9],Ring[1],Hide H[2]
< NO. ><atom(s) >(  x axis   ,   y axis   )<bond><hideH><chg>
 A1     C        (         0 ,          0 )    3     1
 A2     N        (         1 ,          0 )    3
 A3     C        (         2 ,          0 )    4
 A4     N        (         2 ,          1 )    3
 A5     C        (         1 ,          2 )    4
 A6     C        (         0 ,          1 )    3     1
 A7     O        (         3 ,          0 )    2
 A8     H        (         1 ,         -1 )    1
 A9     NH2      (         1 ,          2 )    1
--------------------------------------------------------------------------------
< NO. ><  bond   (sdt)><angle +(  +-  )><length (   pt   )>
 B1     1 ->   2 (  1)     330 (   -30)       1 (      11)
 B2     2 ->   3 (  1)      30 (    30)       1 (      11)
 B3     3 ->   4 (  1)      90 (    90)       1 (      11)
 B4     4 ->   5 (  2)     150 (   150)       1 (      11)
 B5     5 ->   6 (  1)     210 (  -150)       1 (      11)
 B6     6 ->   1 (  2)     270 (   -90)       1 (      11)
 B7     3 ->   7 (  2)     330 (   -30)    0.66 (       7)
 B8     2 ->   8 (  1)     270 (   -90)    0.36 (       4)
 B9     5 ->   9 (  1)      90 (    90)    0.66 (       7)
--------------------------------------------------------------------------------
<atom>( atom wt )[ mi wt   ]  < cnt > < sum wt   >[ sum mi wt  ]
 C    (  12.0107)[       12] *    4       48.04279[          48]
 H    (  1.00793)[  1.00783] *    5        5.03967[     5.03914]
 N    (  14.0067)[ 14.00307] *    3        42.0201[     42.0092]
 O    (  15.9994)[ 15.99492] *    1        15.9994[    15.99492]
 Molecular Weight [Mono Isotopic] =       111.1019[   111.04326]
--------------------------------------------------------------------------------
 Weight  Calc: 111.1019 / Input: 111.10 / weight gap= 0.00195
 Fomula  Calc: C4H5N3O / Input:
================================================================================
```

6.7 MOL file output

(Option parameter setting)

```
sw_output:=MOL2k;     % MOL(V2000)
sw_output:=MOL3k;     % MOL(V3000)
```

(Command line)

```
>mpost -s ahlength=5  FILENAME     % MOL(V2000)
>mpost -s ahlength=6  FILENAME     % MOL(V3000)
```

(Output)

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
  -MCFtoMOL- EN:Caffeine

 14 15  0  0  0  0  0  0  0  0999 V2000
        0         0         0 C   0  0  0  0
   0.86603      -0.5         0 N   0  0  0  0
   1.73206         0         0 C   0  0  0  0
   1.73206         1         0 C   0  0  0  0
   0.86603       1.5         0 C   0  0  0  0
        0         1         0 N   0  0  0  0
    2.6831  -0.30902         0 N   0  0  0  0
   3.27089       0.5         0 C   0  0  0  0
    2.6831   1.30902         0 N   0  0  0  0
   0.86603  -1.36383         0 C   0  0  0  0
  -0.76894   1.44394         0 C   0  0  0  0
  -0.76894  -0.44394         0 O   0  0  0  0
   0.86603   2.36383         0 O   0  0  0  0
   2.95299    2.1396         0 C   0  0  0  0
  1  2  1  0     0  0
  2  3  1  0     0  0
  3  4  2  0     0  0
  4  5  1  0     0  0
  5  6  1  0     0  0
  6  1  1  0     0  0
  3  7  1  0     0  0
  7  8  2  0     0  0
  8  9  1  0     0  0
  9  4  1  0     0  0
  2 10  1  0     0  0
  6 11  1  0     0  0
  1 12  2  0     0  0
  5 13  2  0     0  0
  9 14  1  0     0  0
M  END
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

6.8 LuaTeX file example

```
\documentclass{article}
\usepackage{luamplib}%
\usepackage[T1]{fontenc}%
\usepackage{textcomp}%
\mplibcodeinherit{enable}%
\mplibverbatim{enable}%
\mplibnumbersystem{double}%
\everymplib{%
  if unknown Ph1: input mcf2graph; fi
  sw_output:=Fig; max_blength:=4.5mm;
  defaultfont:="uhvr8r"; defaultsize:=8bp; defaultscale:=1;
}%
\begin{document}
\noindent%
%-----------------------------------------------------------------------
\begin{mplibcode}
  fsize:=(50mm,50mm);
  beginfigm("NO:1","EN:Limonin","MW:470.51",
    %---------------------------------------
    ": <30,?6,{-3,-4}=?6,                  ",
    ": -5=?3,-2=wf,-1=wb,6=?5,-4=?6,-5=wf, ",
    ": {13,15,17,20}:O,{3,12,21}://O,      ",
    ": {4~wf^60,8~zf^60,18^35,18^-35}:/_,  ",
    ": {1^60,5^180,16^60}:/*H,             ",
    ": @14,\*,|,?5,{1,4}=dl,3:O            ")
    %---------------------------------------
  if mc_check(mc)=0: MC(scantokens(mc)) fi
  endfigm
\end{mplibcode}\\
%-----------------------------------------------------------------------
\begin{mplibcode}
  fsize:=(80mm,50mm);
  beginfigm("NO:2","EN:beta-carotene","MW:536.87",
    %---------------------------------------
    ": <30,?6,3=dl,{3,5^35,5^-35}:/_,         ",
    ": @4,\,|,!18,{1,3,5,7,9,11,13,15,17}=dr, ",
    ": {3,7,12,16}:/_,                        ",
    ": |,?6,6=dl,{6,2^35,2^-35}:/_            ")
    %---------------------------------------
  if mc_check(mc)=0: MC(scantokens(mc)) fi
  endfigm
\end{mplibcode}\\
%-----------------------------------------------------------------------
\begin{mplibcode}
  fsize:=(50mm,50mm);
  beginfigm("NO:3","EN:Gibberellin A3","MW:346.37",
    %-----------------------------------
    ": <18,?5,3=?7,5=?6[12],           ",
    ": @8,160`1.3,&3,13=dl,6=wf,8=wb,  ",
    ": @5,40~zf`1,O,60,//O^180,&14~zb, ",
    ": 2:/COOH,7://_,13:*/OH,8:/*OH,   ",
    ": 14:*/_,{1^60,4^60}:*/H          ")
    %-----------------------------------
  if mc_check(mc)=0: MC(scantokens(mc)) fi
endfigm;
%-----------------------------------------------------------------------
\end{mplibcode}\\
\end{document}
```

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