Molecular Coding Format manual

Akira Yamaji

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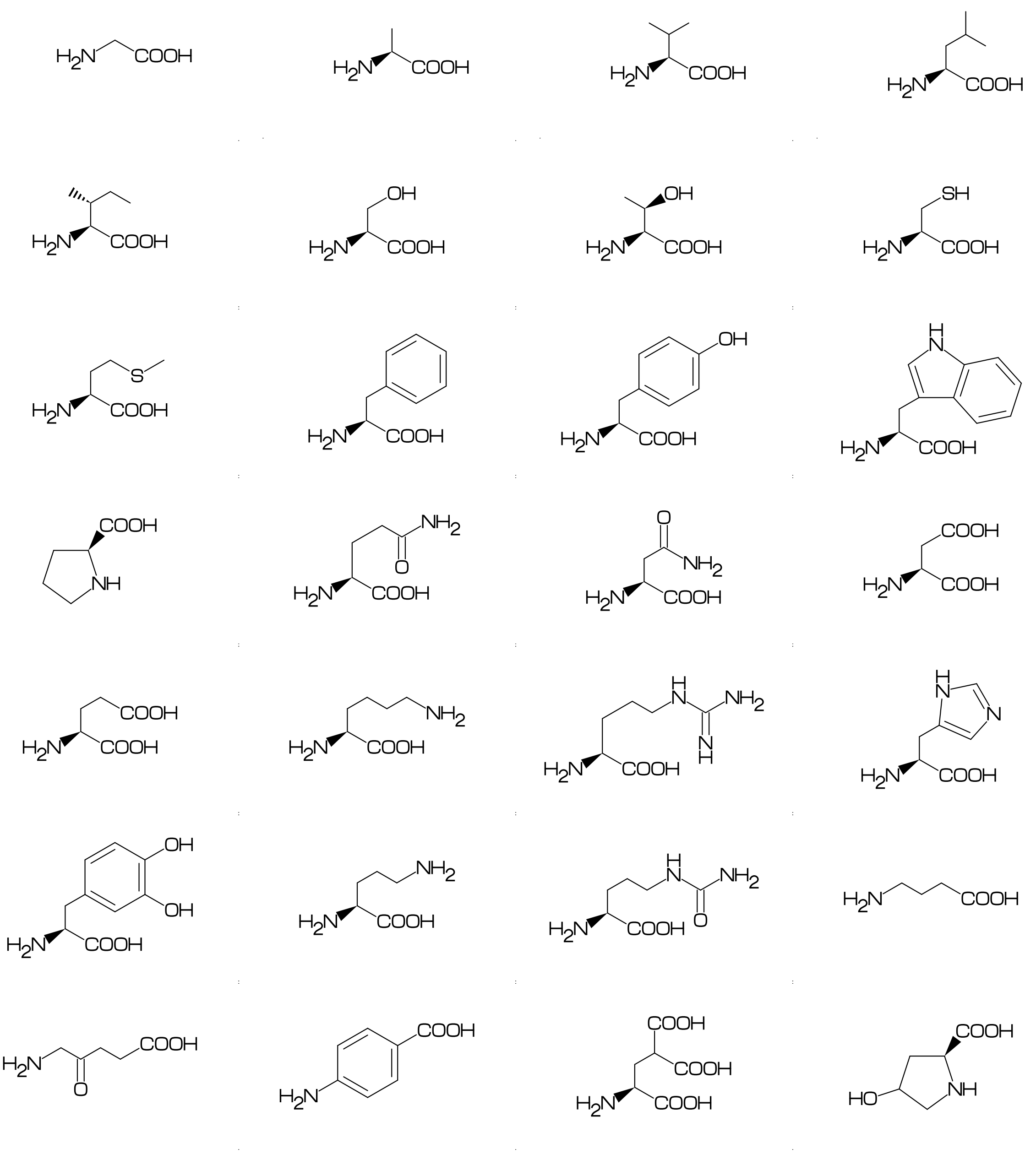
mcf2graph version 5.03

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

Suggestion or request mail to: mcf2graph@gmail.com



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1 Introduction

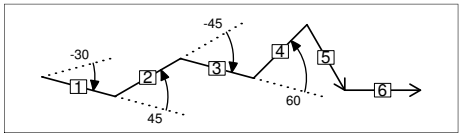
Molecular Coding Format(MCF) is new linear notation represent chemical structure diagrams. This Coding is named from programing technique such as operator, array, scope, macro, adressing, etc. mcf2graph convert from MCF to PNG, SVG, EPS, MOL file. It is also able to calculate molecular weight, exact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

2 MCF syntax

2.1 Make bond

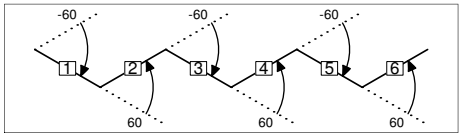
2.1.1 Chain

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

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



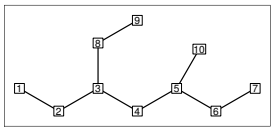
2.1.2 Chain with !,!n

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

<-30,!6
```



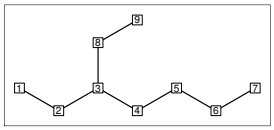
2.1.3 Jump to atom

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

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



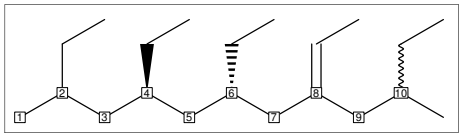
2.1.4 Branch bond

```
\ : 0

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

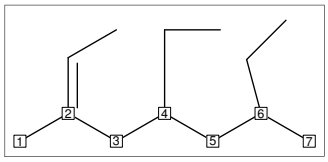


2.1.5 Branch modified bond

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

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

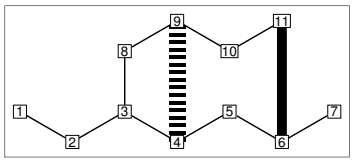



```
<30,!6,
\~dr,!,   : 0~dr,!
\`1.5,-90 : 0`1.5,-90
\^15,-60  : 0^15,-60
```



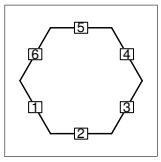
2.1.6 Connect atom

```
&n : Connect to An

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



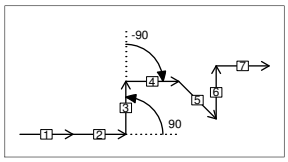
2.1.7 Ring

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



2.1.8 Rotate current angle

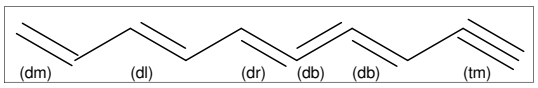
```
<angle : rotate current angle

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



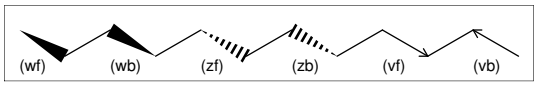
2.2 Change bond type

2.2.1 Double,triple,wedge,vector

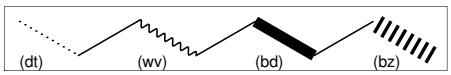
```
(Double,triple)
a~type : ~~type,a
dm  : double middle
dl  : double left side
dr  : double right side
db  : double left or right side
tm  : triple
!!  : !~db  / !!! : !~tm

<-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
```

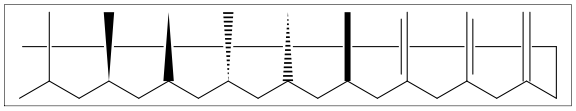



```
(Dotted,wave)
Bn=bond type : change bond type at Bn
dt : dotted   /  wv : wave
bd : broad    /  bz : broad dotted

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



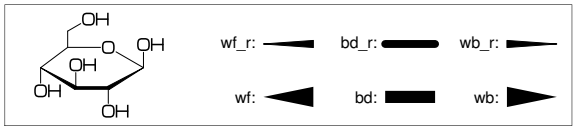
2.2.2 Over line

```
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
```



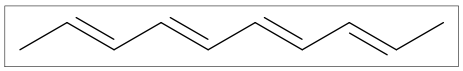
2.2.3 Steric ring

```
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

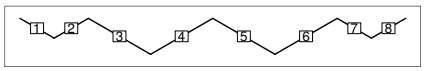
```
{2,4,6,8'}=dl : 2=dl,4=dl,6=dl,8=dr

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



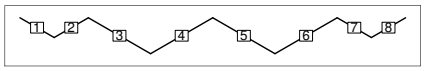
2.3 Change bond length

2.3.1 Chain length

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

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

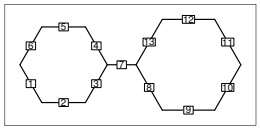



```
#n : bond length=n
## : reset bond length

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



2.3.2 Ring length

```
?n`length : change ring length

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



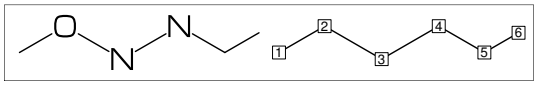
2.4 Change atom

2.4.1 Insert atom

```
Insert hetero atom

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

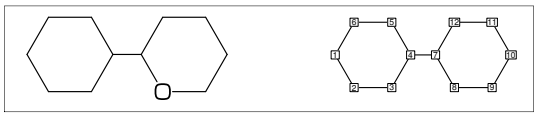
2.4.2 Addressed atom

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

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



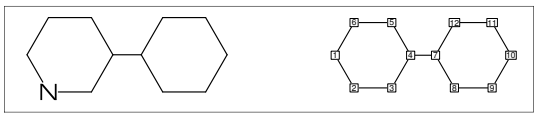
2.4.3 Brock address

```
| : divide brock

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



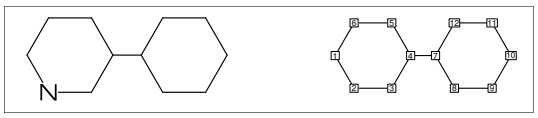
2.4.4 Reset brock address

```
|| : reset brock adress

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



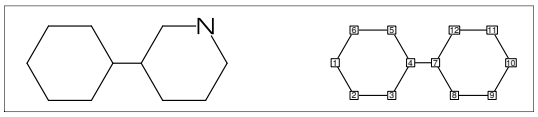
2.4.5 Absolute address

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

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



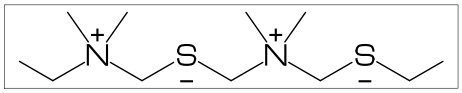
2.4.6 Relative address

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

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



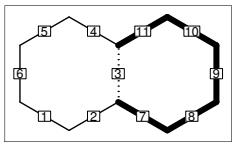
2.4.7 Charged atom

```
p_ : positive / n_ : negative

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

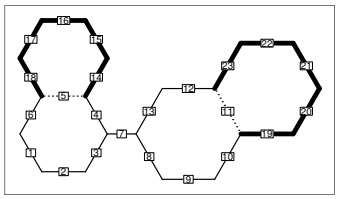


2.5 Fuse ring

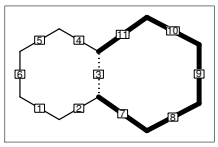
```
(Attached 1 bond)

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

?6,3=?6
```



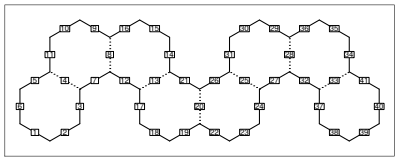
```
** fused ring size depend on
attached bond length

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



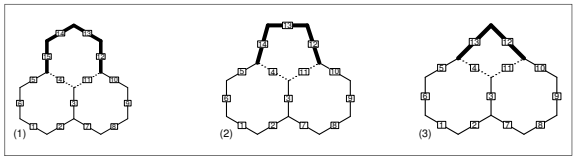
```
?6,3=?6[13] : fuse ?6[13] at B3
?6[13]: 6 membered ring scaled 13/10
** ?m[n] (5<=m<=8,11<=n<=15)

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



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

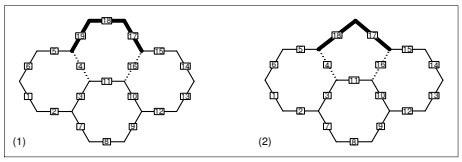


```
(Attached 2 bond)

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
```



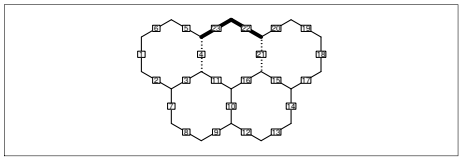
(Attached 3 bond)

```
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
```



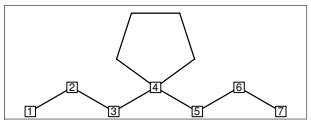
(Attached 4 bond)

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

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



2.6 Spiro ring

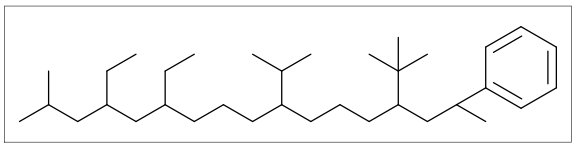
```
@4,?5 : add ?5 at A4

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



2.7 Group

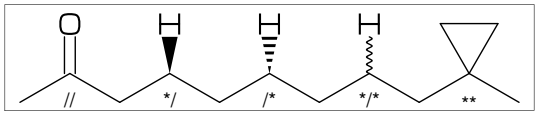
2.7.1 Insert group

```
/ : group start single bond

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

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

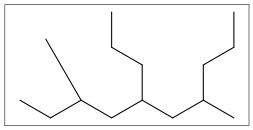


2.7.2 Insert modified group

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

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

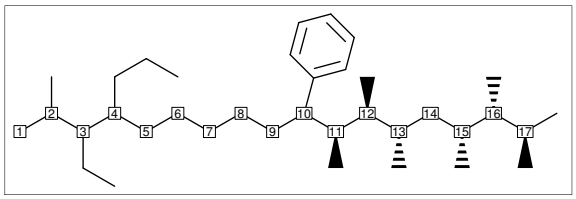



```
~ : change type
^ : change angle
` : change length
> : change environment

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



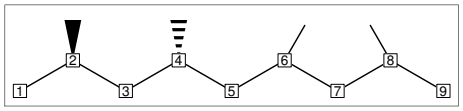
2.7.3 Add group

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

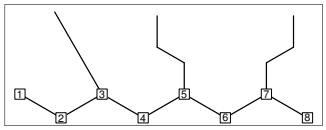


2.7.4 Add modified group

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

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



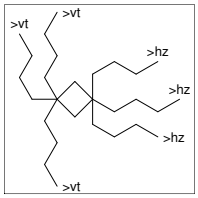
```
^,`,> : change angle,length,environment

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



2.8 Chain environment

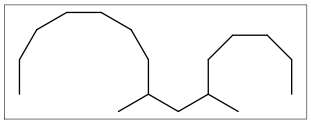
2.8.1 Horizontal,vertical

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

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



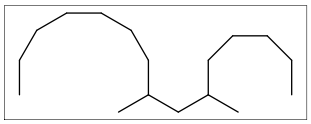
2.8.2 Left-right,right-left

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

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



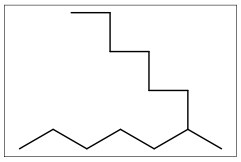
2.8.3 Fixed rotate angle

```
>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

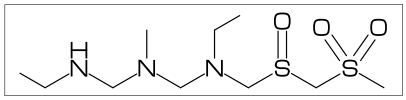
```
>'(90,-90,...) : rotate 90,-90,...

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



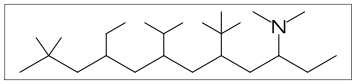
2.9 Miscellaneous

2.9.1 Abbreviated parts

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

<-30,!2,NH,!2,N?,!2,N?2,S?O,!2,S?O?O,!
```

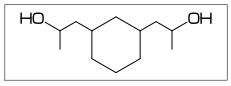



```
??   : /_^35,/_-35  /?!  : isopropyl
/??! : tert-butyl   /N?! : dimethylamino

<30,!11`1,2:??,4:/!,6:/?!,8:/??!,10:/N?!
```



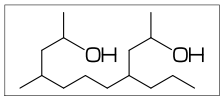
2.9.2 User definition

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

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



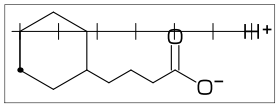
2.9.3 Inline definition

```
a+b : '(a,b)

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



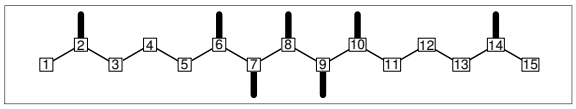
2.9.4 Move position

```
@(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
```



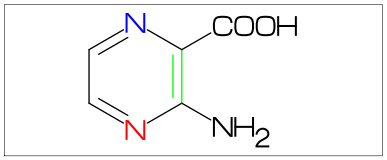
2.9.5 Serial number

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



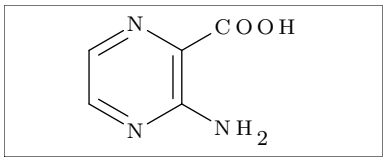
2.9.6 Change color

```
beginfigm
  \(
    <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

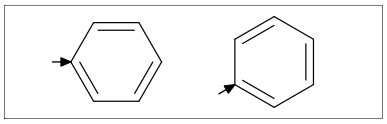
```
beginfigm
  %----------------
  atomfont:="cmr8";
  %----------------
  \(<30,Ph,{2,5}:N,3:/NH2,4:/COOH)
endfigm
```



3 Option parameter

3.1 Angle parameter

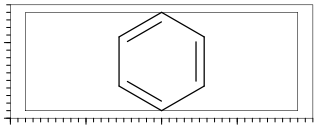
```
mangle=0    ** default

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



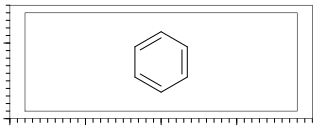
3.2 Size/Ratio parameter

3.2.1 Bond length [|=()]

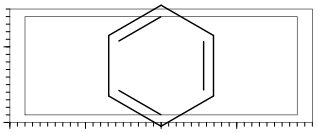
```
|=(n) : abbreviated form of blength:=n;

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



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

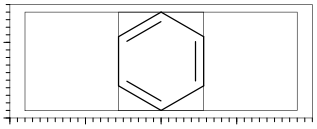


```
(bond length)
blength=9mm
** (blength>1) ignore msize(w,h)
```

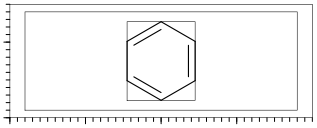


3.2.2 Molecular size

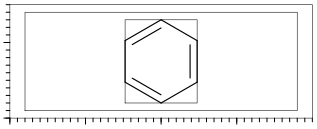
```
##(1,1) : msize=(1,1)   ** default
## p : abbreviated form of msize:=p;
```



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

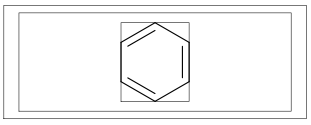


```
##(11mm,11mm) : msize=(11mm,11mm)
```

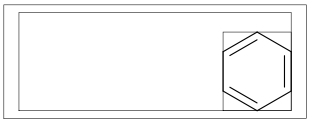


3.2.3 Molecular position

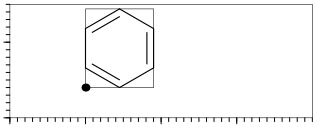
```
@(0.5,0.5) : mposition=(0.5,0.5)   **default
```



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



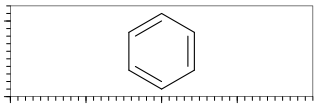
```
@(10mm,4mm) : mposition=(10mm,4mm)
```



3.3 Size parameter

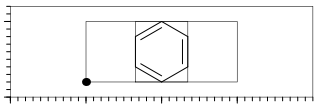
3.3.1 Figure size [#()]

```
fsize=(figure width,figure height)
** default: (30mm,20mm)
# p : abbreviated form of fsize:=p;

#(40mm,15mm) : fsize=(40mm,15mm)
```



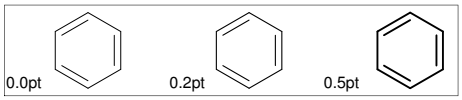
3.3.2 Figure margin [#@()]

```
fmargin=(margin left rigth,top bottom)
** default: (0.4mm,0.4mm)
#@ p : abbreviated form of fmargin:=p;

#@(10mm,2mm) : fmargin=(10mm,2mm)
```



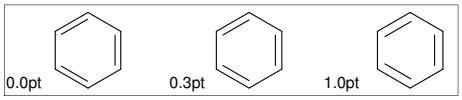
3.3.3 Offset thickness of bond

default: offset_thickness=0.2pt



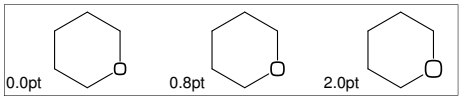
3.3.4 Offset of double bond gap

default: offset_bond_gap=0.3pt



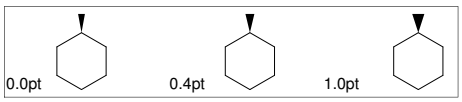
3.3.5 Offset of atom width

default: offset_atom=0.8pt



3.3.6 Offset of wedge width

default: offset_wedge=0.4pt



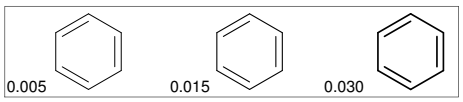
3.3.7 Max bond length [|<=()]

```
|<(n): abbreviated form of max_blength:=n;
default: max_blength=10mm
```

3.4 Ratio parameter

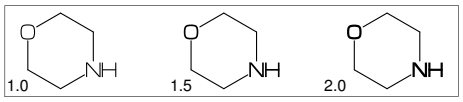
3.4.1 Thickness/bond length

default: ratio_thickness_bond=0.015



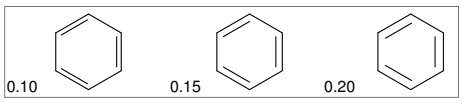
3.4.2 Char/bond thickness

default: ratio_char_bond=1.5



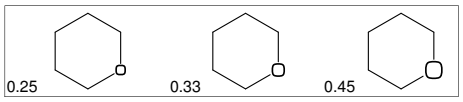
3.4.3 Bond gap/bond length

default: ratio_bondgap_bond= 0.15



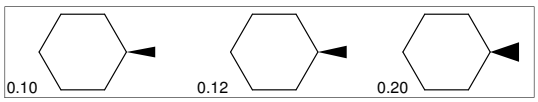
3.4.4 Atom/bond length

default: ratio_atom_bond= 0.36



3.4.5 Wedge/bond length

default: ratio_wedge_bond=0.12

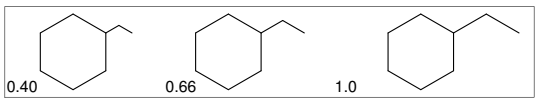


3.4.6 Figure atom gap/atom length

default: ratio_atomgap_atom= 0.050

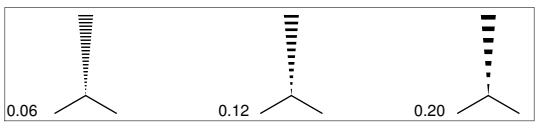
3.4.7 Chain/ring length

default: ratio_chain_ring= 0.66



3.4.8 Hash gap/bond length

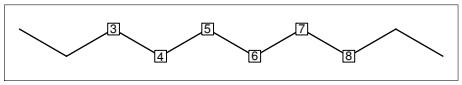
default: ratio_hashgap_bond=0.12



3.5 Drawing mode

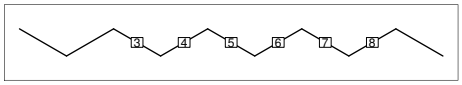
3.5.1 Numbering atom

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

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



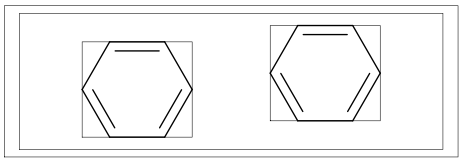
3.5.2 Numbering bond

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

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

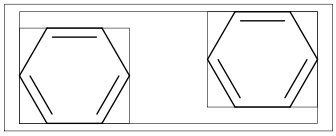


3.5.3 Trimming mode

```
sw_trimming:=0;  ** default
##(1,0.7)
@(0.2,0.3)\(Ph)
@(0.8,0.7)\(Ph)
```

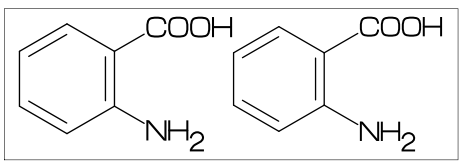


```
sw_trimming:=1;
@(0.2,0.3)\(Ph)
@(0.8,0.7)\(Ph)
```



3.5.4 Expand mode

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



3.5.5 Abbreviate group

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

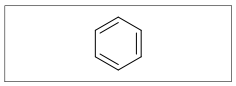
3.5.6 Abbreviate bond type

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

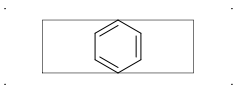
3.6 Frame

3.6.1 Figure frame

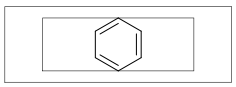
```
** default:sw_frame=0
(Draw figure frame)
fmargin:=(5mm,2mm);
sw_frame=Outside
```



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

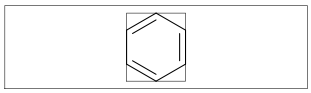


```
(Draw both frame)
sw_frame=Bothside=Inside+Outside
```



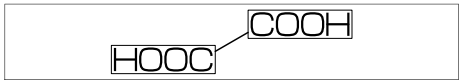
3.6.2 Molecular frame

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



3.6.3 Atom frame

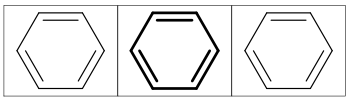
```
sw_frame=Atom
** default: sw_frame=0

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



3.7 Parameter setting

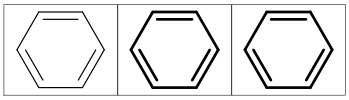
3.7.1 Local parameter setting

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



3.7.2 Global parameter setting

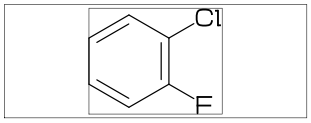
```
beginfigm
  \(Ph)
endfigm
%-------------------------
ratio_thickness_bond:=0.05;
%-------------------------
beginfigm
  \(Ph)
endfigm
beginfigm
  \(Ph)
endfigm
```



4 Command

4.1 drawm [\()]

```
(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
\(): abbreviated form of drawm()

  drawm(<30,Ph,3:/F,4:/Cl)
  \(<30,Ph,3:/F,4:/Cl)
```

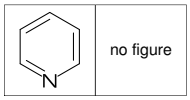


4.2 readm() [”()]

```
readm(string1,string2, ...);
** string = mcf code
'':() abbreviated form of readm()

(example)
''("<30,Ph,{1,2,6}:/O!,{-4,-5}=?7,",
   " {-1,-4,-6}=dl,-2://O,-3:/O!, ",
   " @9,\,NH,!,//O,!              ")
```

4.3 checkm() [*()]

```
\*(): abbreviated form of checkm()
(immediately compile)
beginfigm \(<30,Ph,2:N) endfigm

(check mcf and compile)
beginfigm
  ''("<30,Ph,2:") % ** '2:' missing arg
  if \*(mc)=0: \(scantokens(mc)) fi
endfigm
** \*(mc) : error count
```



4.4 getm() [$()]

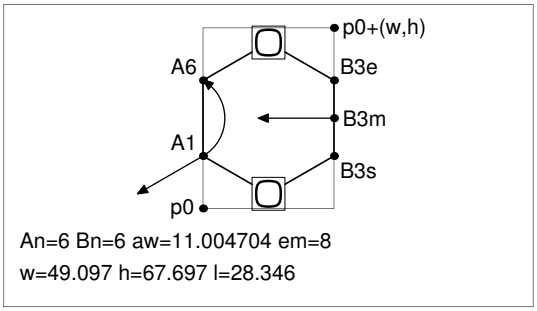
```
getm(number)
** number = numeric
** ucount = molecular data unit count
$() : abbreviated form of getm()

for i=1 upto ucount:
  beginfigm
    $(i)          % get data unit no=i
    \\            % put figure
  endfigm
endfor

getm("name"): "name"=string

beginfigm
  $("Adenine")    % get data EN="Adenine"
  \\              % put figure
endfigm
```

4.5 putm [\\ ]

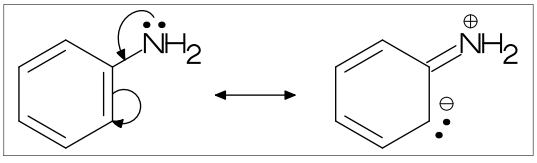
```
putm: put figure
\\ : abbreviated form of putm

  if op_row>=1: scantokens(op) fi
  if mc_row>=1:
    if checkm(mc)=0: drawm(scantokens(mc))
    fi
  fi
  if ad_row>=1: add(scantokens(ad)) fi
  if ex_row>=1: ext(scantokens(ex)) fi
```

4.6 add()

```
(Add label to molecule)

++(): add()
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
 #(70mm,40mm) ##(.91,.9) |<(10mm)
 sw_frame:=sw_frame+Atom+Mol;
 @(.5,.85)\(<30,?6,{2,5}:O)
 ++(
  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
```

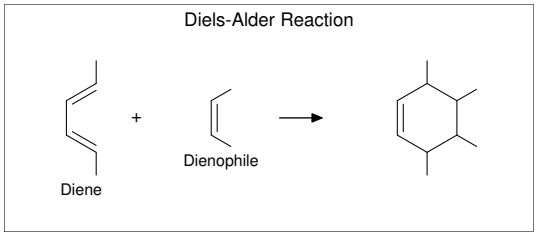



```
beginfigm
 #(60mm,20mm) ##(1,0.85)
 %---------------------------------------
 @(0,0)\(<30,Ph,3=dl,4:/NH2)
 %---------------------------------------
 ++(
  labeloffset:=.7aw;
  label.top(lone_pair 90,A7);
  drawarrow
    (A7+up#1.2aw){A7left}
     ..{B7right}B7/*0.3;
  drawarrow
    B3m..A3+B2up#1.5aw..{A3down}A3;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



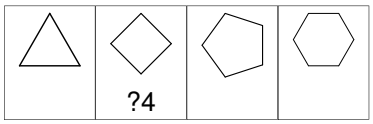
4.7 ext()

```
(Extra label to figure)

**(): ext()
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
 #(70mm,30mm) |=(0.065)
 %---------------------------------------
 @(0.1,0.5)\(
   <-210,60`1,60`1,60`1,{1,3}=dl,
   1:/R1,4:/R2^-60
   )
 ++(
     defaultscale:=0.6;
     label.bot("Diene",p0+(0.5w,0));
 )
 @(0.4,0.5)\(
   <-30,-60`1,1=dl,1:/R3,2:/R4^60)
   ++(defaultscale:=0.6;
   label.bot("Dienophile",p0+(.5w,0));
 )
 @(0.9,0.5)\(
   <30,?6,6=dl,2:/R2,3:/R4,4:/R3,5:/R1
 )
 %---------------------------------------
 **(
  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
```



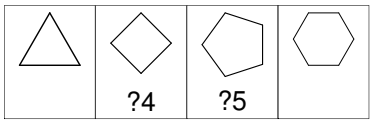
4.7.1 Local ext() setting

```
_s : abbreviated form of EN:=s;

beginfigm
  _"?3"@(0.5,1)\(<30,?3)
endfigm
beginfigm
  _"?4"@(0.5,1)\(?4)
  %------------------------------
  **(label.top(EN,(0.5w,0));)
  %------------------------------
endfigm
beginfigm
  _"?5"@(0.5,1)\(?5)
endfigm
beginfigm
  _"?6"@(0.5,1)\(?6)
endfigm
```



4.7.2 Global ext() setting

```
ext_clear: reset global ext()

beginfigm
  _"?3"@(0.5,1)\(<30,?3)
endfigm
%------------------------------
ext(label.top(EN,(0.5w,0));)
%------------------------------
beginfigm
  _"?4"@(0.5,1)\(?4)
endfigm
beginfigm
  _"?5"@(0.5,1)\(?5)
endfigm
%---------
ext_clear;
%---------
beginfigm
  _"?6"@(0.5,1)\(?6)
endfigm
```

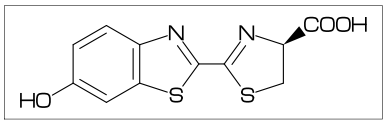


5 Example

5.1 drawm() example

(Luciferin)

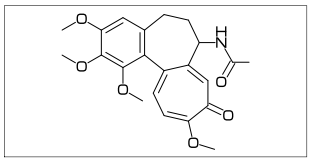
```
beginfigm
  #(50mm,15mm)
  \(<30,Ph,3=?5,@8,\,?5,{9,16}=dl,{9,14}:N,{7,11}:S,1:/OH,-2:*/COOH)
endfigm
```



5.2 readm() example

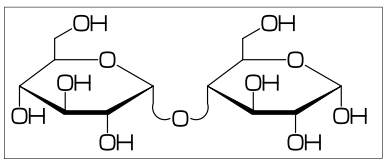
(Colchicine)

```
beginfigm
  ''(
  "<30,Ph,{1,2,6}:/O!,{-4,-5}=?7, ",
  " {-1,-4,-6}=dl,-2://O,-3:/O!,  ",
  " 9:/NH!+?O!                    ")
  #(40mm,20mm) \\
endfigm
```



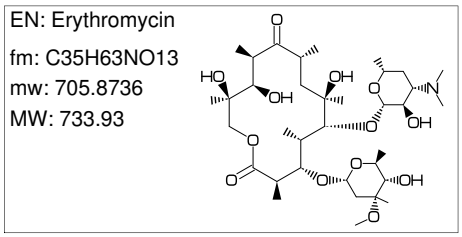
(Maltose)

```
(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           ")
  %-----------------------------------------------------
  #(50mm,20mm) \\
endfigm
```



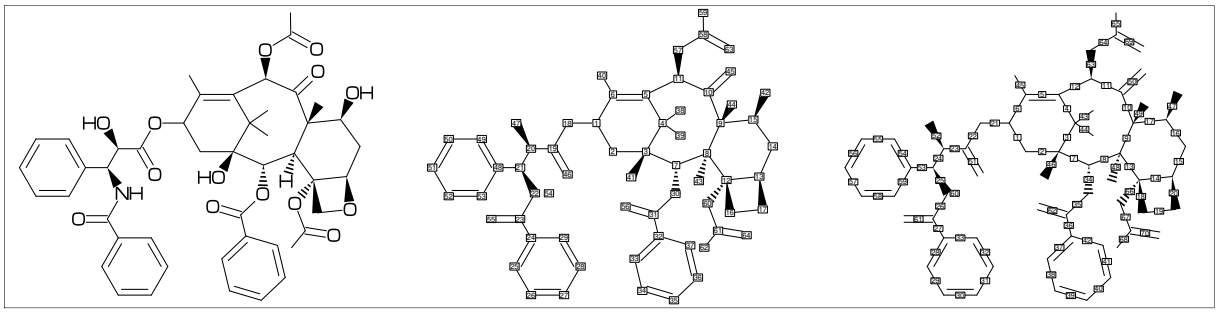
(Erythromycin)

```
beginfigm
  _"Erythromycin" MW:="733.93";
  #(60mm,30mm) @(1,0.5)
  ''(
  %-------------------------------------------------------------------------
    "<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?!           ")
  %-------------------------------------------------------------------------
  \\
  **(defaultscale:=0.8;
      label.lrt("EN: "&EN,(0,h));
      label.lrt("fm: "&fm,(0,h-5mm));
      label.lrt("mw: "&mw,(0,h-9mm));
      label.lrt("MW: "&MW,(0,h-13mm));
  )
endfigm;
```



(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>rl,12'^-15>lr}:*/O!+?O!               ")
  %-------------------------------------------------------------------
  #(140mm,30mm)
  if \*(mc)=0:
    @(0,0.5)\(scantokens(mc))
    sw_numbering:=Atom;
    @(0.6,0.5)\(scantokens(mc))
    sw_numbering:=Bond;
    @(1,0.5)\(scantokens(mc))
  fi
endfigm
```



5.3 loadm() example

(Example)

```
loadm("CAT=biological","MW>=285","MW<=288","a:EN");
```

(output)

```
* jobname=mcf_exa_soc
* numbersystem=double
* output report file
* file name=mcf_exa_soc-report.txt)
* mcf_template 2023.05.07
* Input  : main_lib.mcf [525]
* Output : ucount [4]
* Filter(1): CAT =biological
* Filter(2): MW >= 285
* Filter(3): MW <= 288
* Sort key : EN (ascending)
[1]:Luteolin
[2]:Lycorine
[3]:Morphine
[4]:Piperine )

row[1][1]="CAT:biological;EN:Luteolin;MW:286.24;EXA:-"
row[1][2]=":"
row[1][3]="<30,Ph,3=?6,9=dl,10:O,7://O,@9,\,Ph,{2,6,14,15}:/OH"
row[1][4]=";"
row[2][1]="CAT:biological;EN:Lycorine;MW:287.315;EXA:1"
row[2][2]=":"
row[2][3]="<30,Ph,{-4,-2}=?6,{6,9--12}=?5,13=dl,8:N,{15,17}:O,"
row[2][4]="{9'^180,10^60}:*/H,{13,14'}:*/OH"
row[2][5]=";"
row[3][1]="CAT:biological;EN:Morphine;MW:285.343;EXA:1"
row[3][2]=":"
row[3][3]="<30,Ph,{2,-4}=?6,1---12=?5,-1:O,-1=zb,"
row[3][4]="@7,60~wf`0.75,70~si_`1.3,45,N!,&9~wb,15=dl,6:/OH,8^180:*/H,12:/*OH"
row[3][5]=";"
row[4][1]="CAT:biological;EN:Piperine;MW:285.343;EXA:1"
row[4][2]=":"
row[4][3]="<30,Ph,-1=?5,{-1,-3}:O,@4,\,!!,!,!!,!,//O,!,?6,-6:N"
row[4][4]=";"
```

(sw_comment)

```
sw_comment=1:

row[1][1]="%-------------------------------------------------------------------------"
row[1][2]="CAT:biological;EN:Luteolin;MW:286.24;EXA:-"
row[1][3]=":"
row[1][4]="<30,Ph,3=?6,9=dl,10:O,7://O,@9,\,Ph,{2,6,14,15}:/OH"
row[1][5]=";"

** default sw_comment=0
```

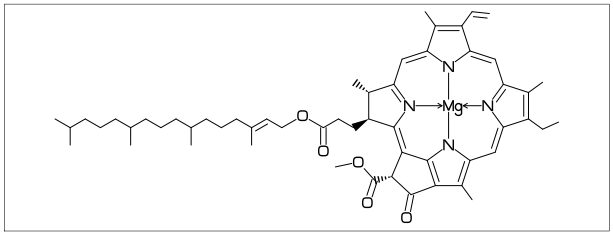
(Tag)

```
J   : jobname                          CAT : category
EN  : english name                     JN  : japanese name
FM  : formula from data                MW  : molecular weight from data
MI  : monoisotopic mass from data      USE : the use
```

5.4 getm() example

(Chlorophyll a)

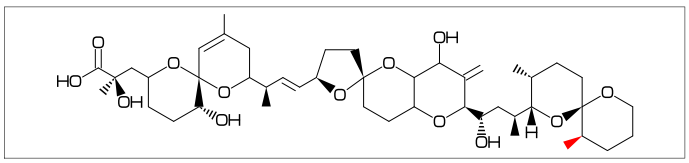
```
beginfigm
  $("Chlorophyll a")
  sw_output:=Fig+Calc+Mcode;
  #(80mm,30mm)
  \(scantokens(mc))
  VerbatimTeX("\gdef\EN{"&EN&"}\gdef\MW{"&MW&"}");
  VerbatimTeX("\gdef\mw{"&mw&"}\gdef\fm{"&fm&"}");
endfigm
\end{mplibcode}
\verbatiminput{temp-mc.aux}            %%%% input temp-mc.aux %%%%
{\tt ** EN:\EN \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:/*?O!+O!,26://O,
 @2,*\^-6,!2,?O!,O!2,!!,|,!13,{1,5,9,13}:/_

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

(Dinophysistoxin-1)

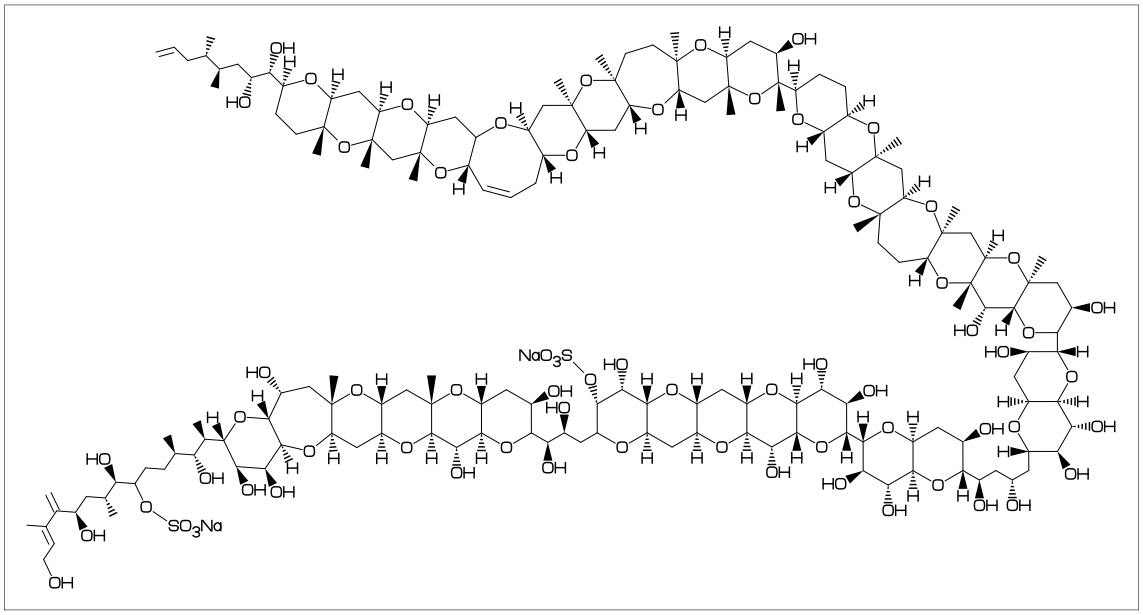
```
beginfigm
  $("Okadaic acid")
  ''(",38:*/_,65=red")                 %%%% add methyl group (color red) %%%%
  sw_output:=Fig+Calc+Mcode;           %%%% output temp-mc.aux %%%%
  _"Dinophysistoxin-1" #(90mm,20mm)
  MW:="819";
  if \*(mc)=0: \(scantokens(mc))
    VerbatimTeX("\gdef\EN{"&EN&"}\gdef\MW{"&MW&"}");
    VerbatimTeX("\gdef\mw{"&mw&"}\gdef\fm{"&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!,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
```

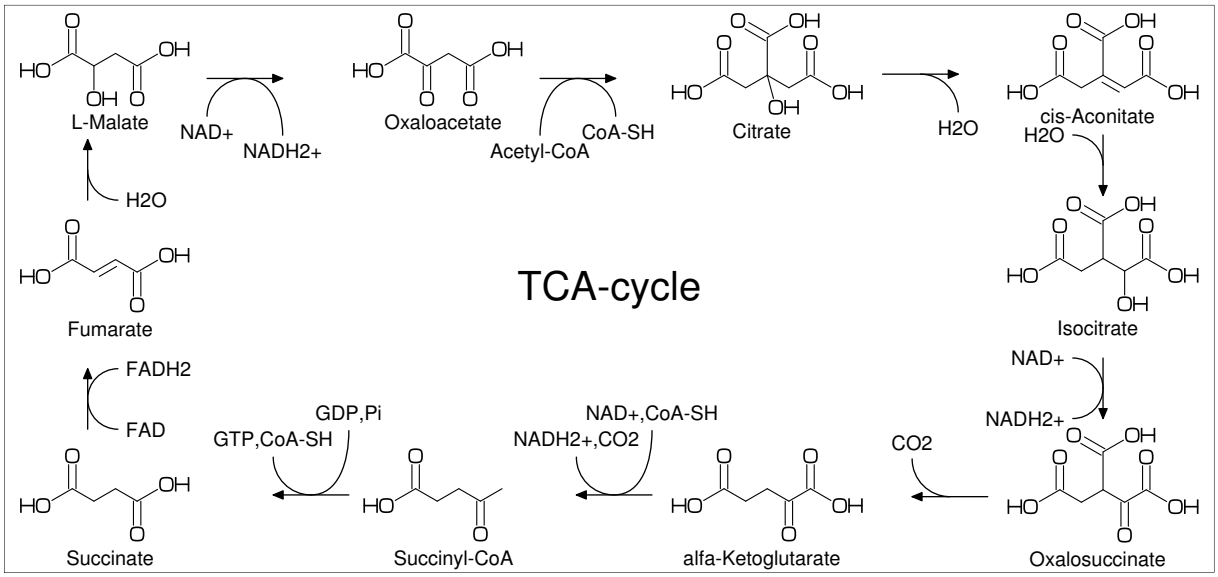
(Maitotoxin)

```
%-------------------------------------------------------------------------------
\begin{mplibcode}
  beginfigm
    $("Maitotoxin") #(150mm,80mm) #@(3mm,3mm)
    sw_output:=Fig+Calc+Mcode;          %%%% output temp-mc.aux %%%%
    sw_frame:=Outside;
    if \*(mc)=0: \(scantokens(mc))
      VerbatimTeX("\gdef\EN{"&EN&"}\gdef\MW{"&MW&"}");
      VerbatimTeX("\gdef\mw{"&mw&"}\gdef\fm{"&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
```

5.5 User define parts example




```
beginfigm
#(160mm,75mm) |<(5mm)
COOH:='(//O,!,OH);      % define COOH
HOCO:='(OH,!,//O,);     % define HOCO
@(0.33,   1)\(<30,HOCO,!,//O,!2,COOH)                    % Oxaloacetate
@(0.66,   1)\(<30,HOCO,!4,COOH,@-4`1,\,COOH,4:/OH^-165)  % Citrate
@(1,      1)\(<30,HOCO,!2,!~dr,!,COOH,@-4`1,\,COOH)      % cis-Aconitate
@(1,   0.58)\(<30,HOCO,!4,COOH,@-4,\`1,COOH,5:/OH)       % Isocitrate
@(1,   0.05)\(<30,HOCO,!3,//O,!,COOH,@-4,\`1,COOH)       % Oxalosuccinate
@(0.66,0.05)\(<30,HOCO,!3,//O,!,COOH)                    % alfa-Ketoglutarate
@(0.33,0.05)\(<30,HOCO,!3,//O,!,"{S-CoA}")               % Succinyl-CoA
@(0,   0.05)\(<30,HOCO,!3,COOH)                          % Succinate
@(0,   0.55)\(<30,HOCO,!,!~dr,!,COOH)                    % Fumarate
@(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:=MOL2000;                                 > MOL file output
#(60mm,40mm);   %  (figure width,figure height)          >
outputformat:="png"; hppp:=vppp:=0.1;                     > PNG output
outputtemplate:="c%3c-%{EN_}.png";                        >
%-------------------------------------------------------------------------------
beginfigm
  % EN:Ampicillin  MW:349.405
  \(<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
  ''(                                                     > read Mcode
  "<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
  \\                                                      > put figure
endfigm                                                   >
%-------------------------------------------------------------------------------
loadm("EN<>*");                                           > load all unit
beginfigm
  $("Adenine")                                            > get EN=Adenine
  \\                                                      > ** put figure
endfigm                                                   >
%-------------------------------------------------------------------------------
beginfigm
  $(4)                                                    > select No.4
  \\                                                      > put figure
endfigm                                                   >
%-------------------------------------------------------------------------------
for i=1 upto ucount:                                      > figure count
  beginfigm
    $(i)                                                  > select No.i
    \\                                                    > put figure
  endfigm
endfor
%-------------------------------------------------------------------------------
bye
```

6.2 Molecular library file

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% molecular library file    main_lib.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:-;EN:-;MW:0;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)&":"&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 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)

```
%-------------------------------------------------------------------------
%%  "EN:Vancomycin
\begin{mplibcode}
  beginfigm
    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
```

6.4 Report output

(Option parameter setting)

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

(Command line)

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

(Output)

```
================================================================================
 No[5],Name<Cytosine>,Category<biological>,File<main_lib.mcf>
--------------------------------------------------------------------------------
<30,?6,{4,6}=db,4:N,3://O,2:NH,5:/NH2
--------------------------------------------------------------------------------
 Row[1],Length[37],Block[7],Code pair[59],Warning[0]
--------------------------------------------------------------------------------
 =[1] :[4] ?[1] <[1]
--------------------------------------------------------------------------------
 Width[30.92419],Height[42.36527], Shift x[-1.77635],Shift y[-12.9921]
 Bond length[11.33855],Atom size[4.881881]
--------------------------------------------------------------------------------
 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 ,         -1 )    3
 A3     C        (         2 ,          0 )    4
 A4     N        (         2 ,          1 )    3
 A5     C        (         1 ,          1 )    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)0.660000 (       7)
 B8     2 ->   8 (  1)     270 (   -90)0.359999 (       4)
 B9     5 ->   9 (  1)      90 (    90)0.660000 (       7)
--------------------------------------------------------------------------------
<atom>( atom wt )[ mi wt   ]  < cnt > < sum wt   >[ sum mi wt  ]
 C    (  12.0107)[       12] *        4    48.0428[          48]
 H    (1.0079400)[1.0078250] *        5    5.03969[5.0391251611]
 N    (  14.0067)[14.003074] *        3    42.0200[42.009222013]
 O    (  15.9994)[15.994914] *        1    15.9994[15.994914619]
 Molecular Weight [Mono Isotopic] =       111.1019[  111.043261]
--------------------------------------------------------------------------------
 Weight Calc: 111.1019 - Input: 111.10 = 0.0019999
 Fomula Calc: C4H5N3O
================================================================================
```

6.5 MOL file output

(Option parameter setting)

```
  sw_output:=MOL2000;   % MOL(V2000)
  sw_output:=MOL3000;   % 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
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

6.6 LuaTeX file example

```
\documentclass{article}
\usepackage{luamplib}%
\usepackage[T1]{fontenc}%
\usepackage{textcomp}%
\mplibcodeinherit{enable}%
\mplibverbatim{enable}%
\mplibnumbersystem{double}%
\begin{mplibcode}
\end{mplibcode}
\begin{document}
\noindent%
%-----------------------------------------------------------------------
\begin{mplibcode}
  input mcf2graph;
  sw_output:=Fig;
  max_blength:=4.5mm;
  defaultfont:="uhvr8r";
  defaultsize:=8bp;
  defaultscale:=1;
  %-------------------------------------------------------
  EN:="Limonin";
  MW="470.51";
  beginfigm
    #(50mm,50mm)
    ''(
    %---------------------------------------
    "<30,?6,{-3,-4}=?6,                    ",
    " -5=?3,-2=wf,-1=wb,6=?5,-4=?6,-5=wf, ",
    " {13,15,17,20}:0,{3,12,21}://0,       ",
    " {4~wf^60,8~zf^60,18^35,18^-35}:/_,   ",
    " {1^60,5^180,16^60}:/*H,              ",
    " @14,\*,|,?5,{1,4}=dl,3:0             ")
    %---------------------------------------
    \\
  endfigm
\end{mplibcode}\\
%-----------------------------------------------------------------------
\begin{mplibcode}
  EN:="beta-carotene";
  MW:="536.87";
  beginfigm
    #(80mm,50mm)
    ''(
    %---------------------------------------
    "<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}:/_           ")
    %---------------------------------------
    \\
  endfigm
\end{mplibcode}\\
%-----------------------------------------------------------------------
\end{document}
```

Index

!, 3
!!, 4
!!!, 4
', 7
'', 11
**, 6, 12
**(), 13
*/, 6
/, 6
*\, 3
**, 3
+, 7
++(), 12
--, 5
---, 5
----, 6
/, 6
/*, 6, 12
//, 6
:, 5
?, 3
?!, 7
??, 7
??!, 7
@, 3
@(), 7
#, 4
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