

Molecular Coding Format manual

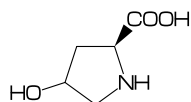
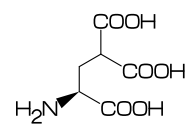
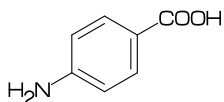
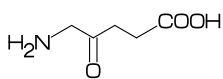
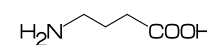
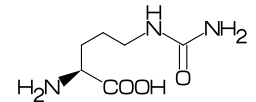
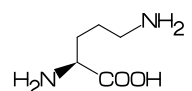
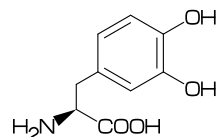
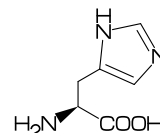
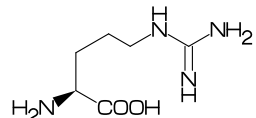
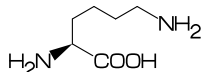
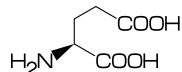
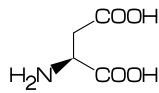
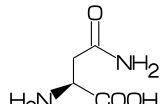
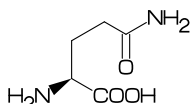
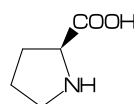
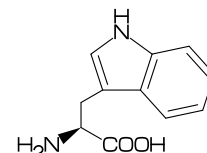
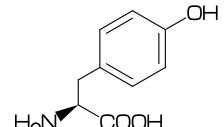
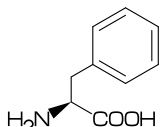
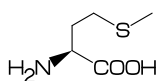
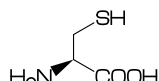
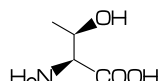
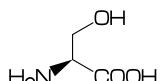
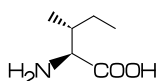
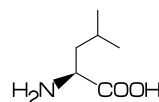
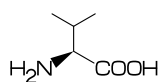
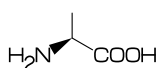
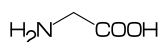
Akira Yamaji

May 15, 2023

mcf2graph version 5.01

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 programming technique such as operator, array, scope, macro, addressing, etc. mcf2graph convert from MCF to PNG, SVG, EPS, MOL file. It is also able to calculate molecular weight, exact mass, molecular formula.

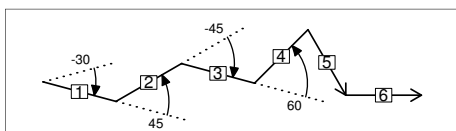
2 MCF syntax

2.1 Make bond

2.1.1 Chain

real number plus (+): counterclockwise
real number minus(-): clockwise
\$n (0<=n<360): absolute angle

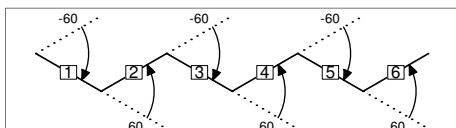
<10,-30,45,-45,60,\$300,\$0



2.1.2 Chain with !,!n

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

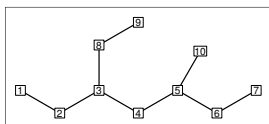
<-30,!6



2.1.3 Jump to atom

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

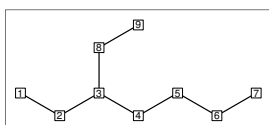
<-30,!6,@3,0,!,@5,-30



2.1.4 Branch bond

\ : 0

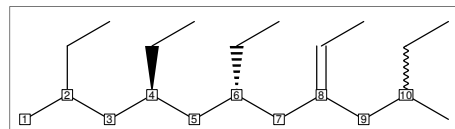
<-30,!6,@3,\,!



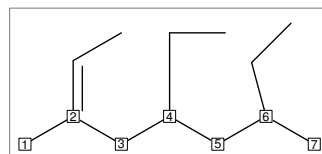
2.1.5 Branch modified bond

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

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



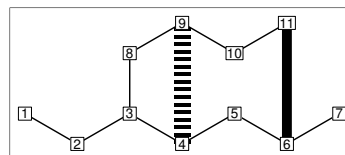
<30,!6,
\~dr,! : 0~dr,!
\^1.5,-90 : 0^1.5,-90
\^15,-60 : 0^15,-60



2.1.6 Connect atom

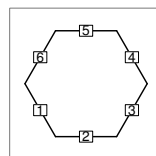
&n : Connect to An

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



2.1.7 Ring

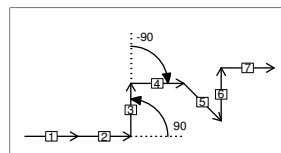
?n : n membered ring(3<=n<=20)
?6 : <-120,60,60,60,60,60,&1
?6



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

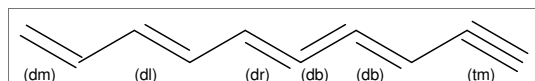
db : double left or right side

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 forward

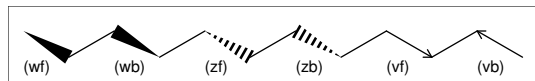
zb: hashed(zebra stripe) wedge backward

vf: vector forward

vb: vector backward

<-30,

!~wf, !, !~wb, !, !~zf, !, !~zb, !, !~vf, !~vb



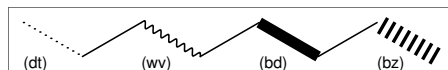
(Dotted, wave)

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_ : double left over line

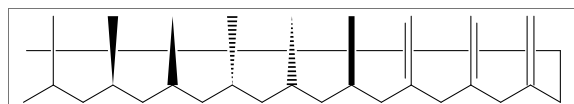
dr_ : double right over line

dm_ : double 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 forward (half width)

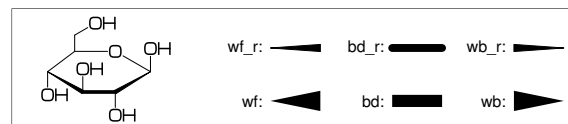
bd_r : broad (half width, rounded)

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,

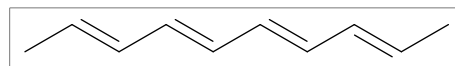
{1~\$-90, 2~\$90, 3~\$-90, 4~\$90}:/OH,



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

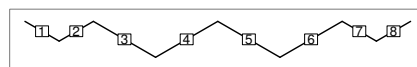


2.3 Change bond length

2.3.1 Chain length

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

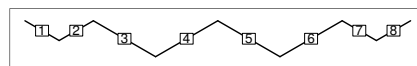
<-30, !2, !4`1.2, !2



#n : bond length=n

: reset bond length

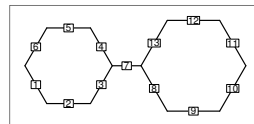
<-30, !2, #1.2, !4, ##, !2



2.3.2 Ring length

?n`length : change ring length

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

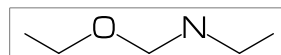


2.4 Change atom

2.4.1 Insert atom

Insert hetero atom

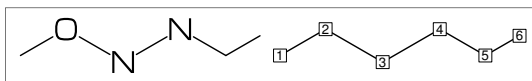
<-30, !2, 0, !2, N, !2



2.4.2 Addressed atom

2:0 : change A2 C to O
 {3,4}:N : change A3,A4 C to N

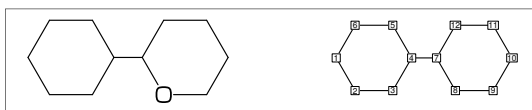
<30,14,2:0,{3,4}:N



2.4.3 Brock address

| : divide brock

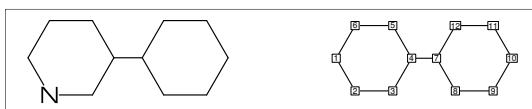
?6,@4,\,|,?6,2:0



2.4.4 Reset brock address

|| : reset brock address

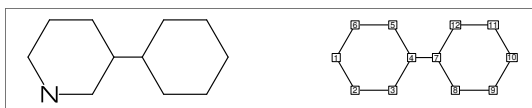
?6,@4,\,|,?6,||,2:N



2.4.5 Absolute address

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

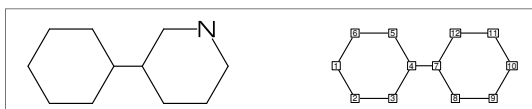
?6,@4,\,|,?6,\$2:N



2.4.6 Relative address

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

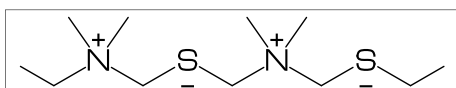
?6,@4,\,?6,-2:N



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_~180



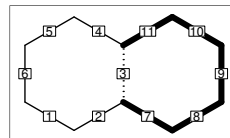
2.5 Fuse ring

(Attached 1 bond)

?6,3=?6 : fuse ?6 at B3

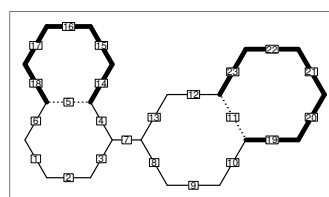
** Bn(n:-999<=n<=4095): bond number

?6,3=?6



** fused ring size depend on attached bond length

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

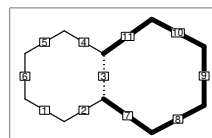


?6,3=?6[13] : fuse ?6[13] at B3

?6[13]: 6 membered ring scaled 13/10

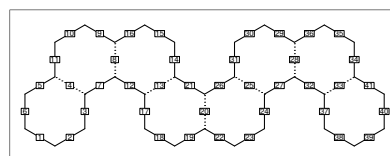
** ?m[n] (5<=m<=8,11<=n<=15)

?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

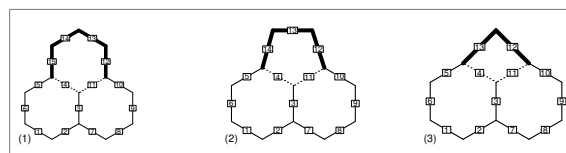
4--11=?5 : fuse 3/5 ring to B11..B4

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



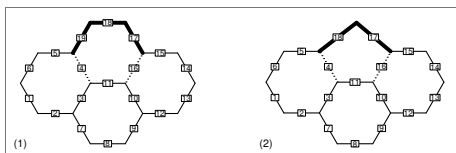
(Attached 3 bond)

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

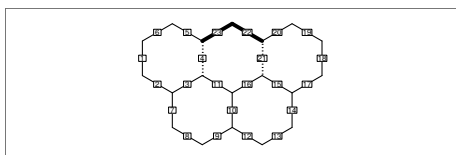
2:?6,{3,10}=?6,16---4=?5



(Attached 4 bond)

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

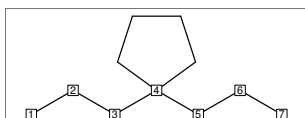
<-30,?6,{3,10,15,21----4}=?6



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

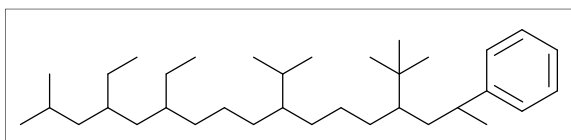
/?! : isopropyl

/??! : tert-butyl

/Ph : phenyl

<30,!/_,!2,/!,!2,/!2,!4,/?!,

!4,/??!,!2,/Ph^-60,!



2.7.2 Insert modified group

// : double (double middle)

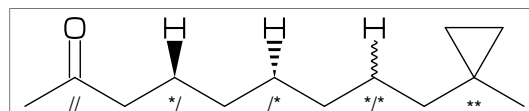
*/ : wedge forward

/* : hashed wedge forward

/ : wave

** : direct

<30,!//0,!2,*H,!2,*H,!2,*H,!2,**?3,!



~ : change type

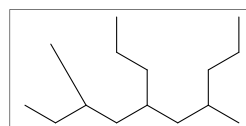
^ : change angle

` : change length

> : change environment

<-30,`^1,!,

/_`^2^30,!2,/!2>lr,!2,/!2>r1,!)

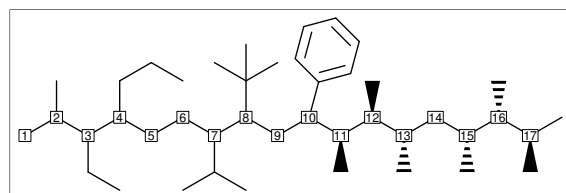


2.7.3 Add group

<30,!17,2:/_,3:/!,4:/!2,7:/iPr,

8:/tBu,10:/!(Ph^0.6)^-15,

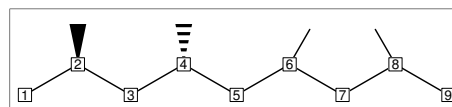
{11,12,13'}:*/_,{15,16,17'}:/*_



2.7.4 Add modified group

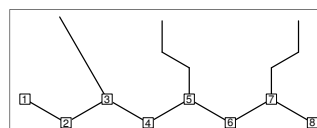
~,^,` : change type,angle,length

<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>r1

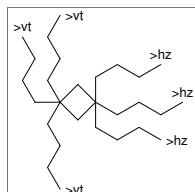


2.8 Chain environment

2.8.1 Horizontal,vertical

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

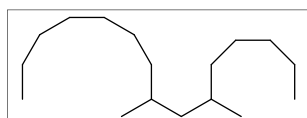
```
?4,  
{3^-90,3^-30,3^90}:/!3>hz,  
{1^-60,1,1^60}:/!3>vt
```



2.8.2 Left-right,right-left

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

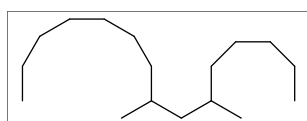
```
<-30,!6,  
{3^-30,3,3^30}:/!3>lr,  
{5^-30,5,5^30}:/!3>rl
```



2.8.3 Fixed rotate angle

>n : rotate n

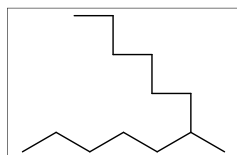
```
<30,!4,  
2:/!6>30, % 2:\,30,30,30,30,30,30  
4:/!4>-45 % 4:\,-45,-45,-45,-45
```



2.8.4 Multiple rotate angle

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

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

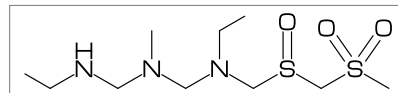


2.9 Miscellaneous

2.9.1 Abbreviated parts

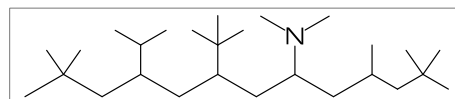
```
NH : N,/H~n1 N! : N,/_ N!2 : N,/!  
SO : S,//0 SOO : S,//0^35,/^-35
```

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



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

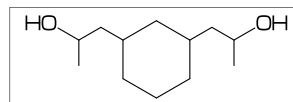
```
<30,!9^1,?!,! ,?!,! ,2:??,4:??,6:??!,8:/N?!
```



2.9.2 Parts definition

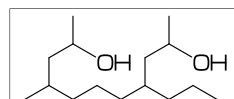
'(..) : user defined parts

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



2.9.3 Parts inline definition

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



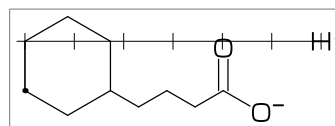
2.9.4 Move position

@(x,y) : Move l*(x,y) from current position

@\$(x,y) : Move l*(x,y) from origin(@l)

** l=bond length of ring

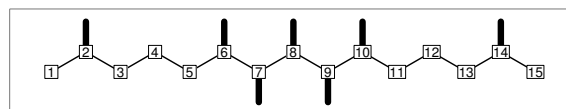
```
<30,?6,@3,!4,//0,! ,0,n_^60,@$(6,1),H,p_^15
```



2.9.5 Serial number

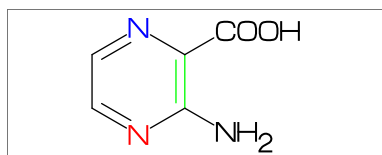
```
6:10 : 6,7,8,9,10
```

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



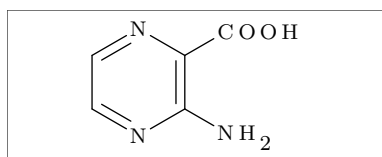
2.9.6 Change color

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

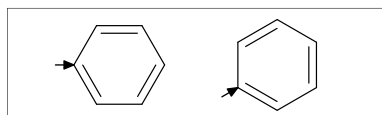


3 Option parameter

3.1 Angle parameter

mangle=0 ** default

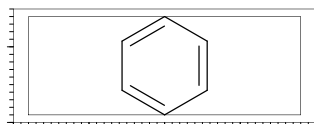
```
cvat(0.2,0.5)(Ph)
mangle:=30;
cvat(0.8,0.5)(Ph)
```



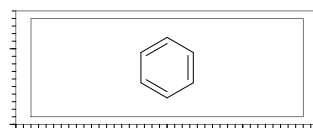
3.2 Size/Ratio parameter

3.2.1 Bond length

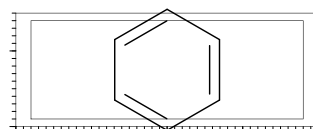
(fit to figure size)
blength=0 ** default



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

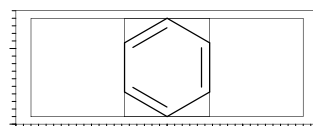


(bond length)
blength=9mm
** (blength>1) ignore msize(w,h)

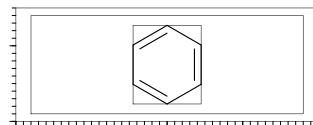


3.2.2 Molecular size

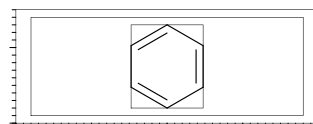
msize=(1,1) ** default



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

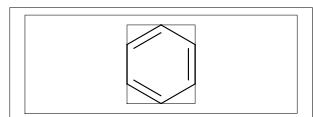


msize=(11mm,11mm)



3.2.3 Molecular position

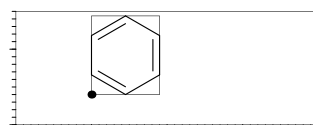
mposition=(0.5,0.5) ** default



mposition=(1,0)



mposition=(10mm,4mm)

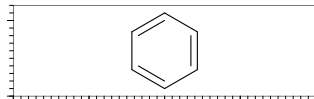


3.3 Size parameter

3.3.1 Figure size

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

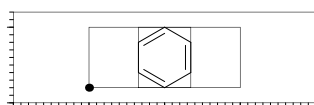
fsize=(40mm,15mm)



3.3.2 Figure margin

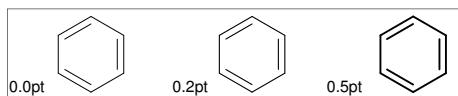
fmargin=(margin left right,top bottom)
** default: (0.4mm,0.4mm)

fmargin=(10mm,2mm)



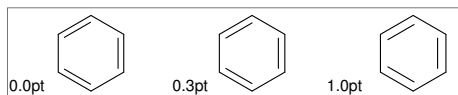
3.3.3 Offset thickness of bond

default: offset_thickness=0.2pt



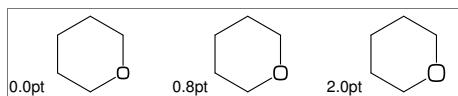
3.3.4 Offset of double bond gap

default: offset_bond_gap=0.3pt



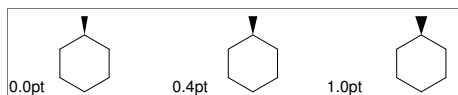
3.3.5 Offset of atom width

default: offset_atom=0.8pt



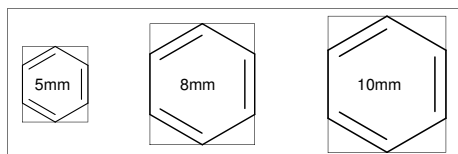
3.3.6 Offset of wedge width

default: offset_wedge=0.4pt



3.3.7 Max bond length

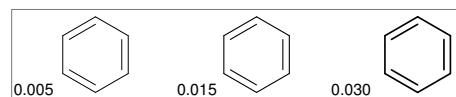
default: max_blength=10mm



3.4 Ratio parameter

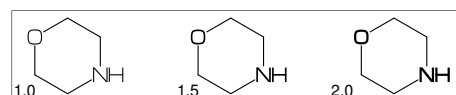
3.4.1 Thickness/bond length

default: ratio_thickness_bond=0.015



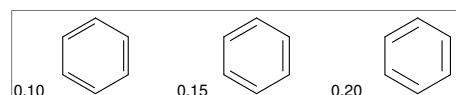
3.4.2 Char/bond thickness

default: ratio_char_bond=1.5



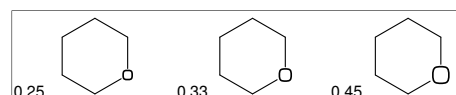
3.4.3 Bond gap/bond length

default: ratio_bondgap_bond= 0.15



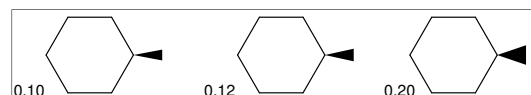
3.4.4 Atom/bond length

default: ratio_atom_bond= 0.36



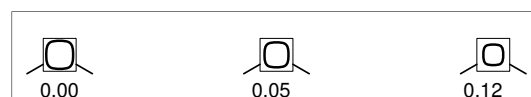
3.4.5 Wedge/bond length

default: ratio_wedge_bond=0.12



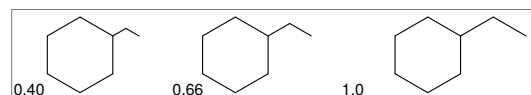
3.4.6 Figure atom gap/atom length

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

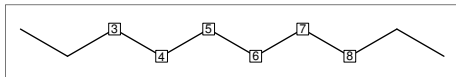


3.5 Drawing mode

3.5.1 Numbering atom

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

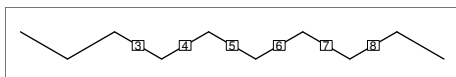
```
sw_numbering:=Atom;
cv(<-30,!9)
```



3.5.2 Numbering bond

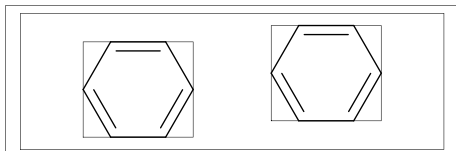
```
sw_numbering=Bond
numbering_start:=3;
numbering_end:=8;
default: sw_numbering=0
```

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

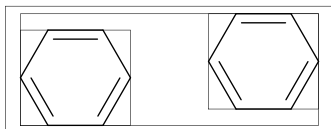


3.5.3 Trimming mode

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

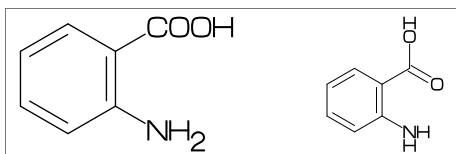


```
sw_trimming:=1;
cvat(0.2,0.3)(Ph)
cvat(0.8,0.7)(Ph)
```



3.5.4 Expand mode

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

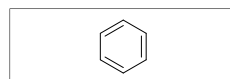
```
** default: sw_abbreviate=Bond
```



3.6 Frame

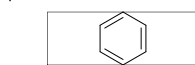
3.6.1 Figure frame

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



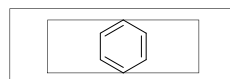
(Frame inside margin)

```
sw_frame=Inside
```



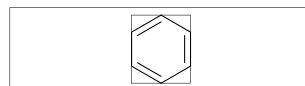
(Draw both frame)

```
sw_frame=Bothside=Inside+Outside
```



3.6.2 Molecular frame

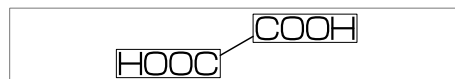
```
sw_frame=Mol
** default:sw_frame=0
```



3.6.3 Atom frame

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

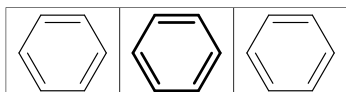
```
cv(<30,COOH,! ,COOH)
```



3.7 Parameter setting

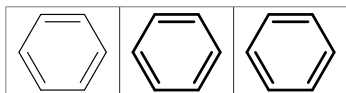
3.7.1 Local parameter setting

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



3.7.2 Global parameter setting

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



4 Command

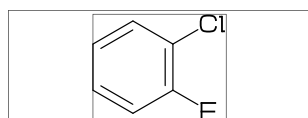
4.1 cv()

(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 height/figure height
c: x axis position
d: y axis position

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

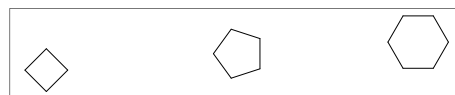


4.2 cvat()

(Draw molecule at mposition)

```
cvat(c,d)(....) :
  mposition:=(c,d); cv(....)
  c: x axis position / d: y axis position
```

```
cvat(0 ,0 )(?4)
cvat(0.5,0.5)(?5)
cvat(1 ,1 )(?6)
```



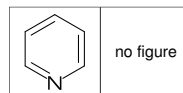
4.3 checkm()

(immediately compile)

```
beginfigm cv(<30,Ph,2:N) endfigm
```

(check mcf and compile)

```
beginfigm
  readm("<30,Ph,}2:N") % ** extra '}'
  if checkm(mc)=0: cv(scantokens(mc)) fi
endfigm
** checkm(mc) : error count
```



4.4 getm()

```
getm(number): number=numeric
ucount: figure count
```

```
for i=1 upto ucount:
  beginfigm
    getm(i);          % get data unit no=i
    putm;             % put figure
  endfigm
endfor
```

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

```
loadm("EN<>*");
beginfigm
  getm("Adenine"); % get data EN="Adenine"
  putm;           % put figure
endfigm
```

4.5 putm

putm: put figure

```
if op_row>=1: scantokens(op) fi
if mc_row>=1:
  if checkm(mc)=0: cv(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)

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

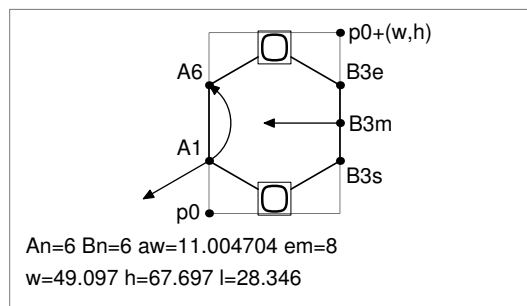
plus : '+' circled
minus : '-' circled
 circlediam = 0.6aw (default)
 circlepen = 0.2bp (default)

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

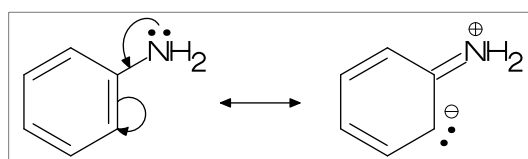
** : scaled
<< : rotated
a /* b : point b of a

```
beginfigm
  fsize:=(70mm,40mm);
  sw_frame:=sw_frame+Atom+Mol;
  max_blength:=10mm;
  msize:=(.91,.9);
  cvat(.5,.85)(<30,?6,{2,5}:0)
  add(
    defaultscale:=.8;
    labeloffset:=.3aw;
    dotlabel.lft("p0",p0);
    dotlabel.rt("p0+(w,h)",p0+(w,h));
    dotlabel.ulft("A1",A1);
    drawarrow A1..A1+__*1<<A1ang;
    dotlabel.lrt("B3s",B3s);
    dotlabel.rt("B3m",B3m);
    drawarrow B3m..B3m+__*1<<(B3ang+90);
    dotlabel.ulft("A6",A6);
```

```
drawarrow A1{A1down}..A6;
dotlabel.urrt("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
  fsize:=(60mm,20mm);
  msize:=(1,0.85);
  %-----
  cvat(0,0)(<30,Ph,3=d1,4://NH2)
  %-----
  add(
    labeloffset:=.7aw;
    label.top(lonpair 90,A7);
    drawarrow
      (A7+up**1.2aw){A7left}
      ..{B7right}B7/*0.3;
    drawarrow
      B3m..A3+B2up**1.5aw..{A3down}A3;
  )
  %-----
  cvat(1,0)(<30,?6,{1,5}=d1,4://NH2)
  %-----
  add(
    labeloffset:=.7aw;
    label.top(plus,A7);
    label.urrt(minus,A3);
    label(lonpair A3ang,A3+A3up**0.7aw);
  )
  %-----
  ext(drawdblarrow (.4w,.4h)..(.55w,.4h));
  %-----
endfigm
```



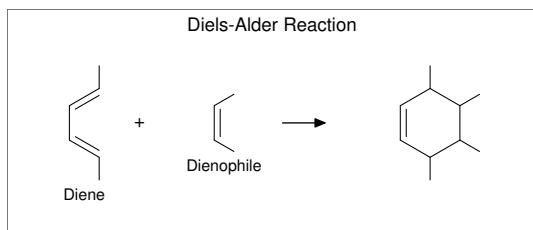
4.7 ext()

(Extra label to figure)

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

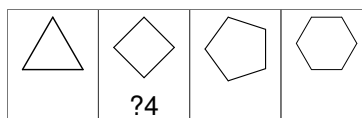
n:      molecular number
p[m]:   molecular origin position
w[m]:   molecular width
h[m]:   molecular height

ratio_thickness_char:
pen thickness / char width
%-----
beginfigm
  fsize:=(70mm,30mm);
  blength:=0.065;
  %-----
  cvat(0.1,0.5)(
    <-210,60`1,60`1,60`1,{1,3}=d1,
    1:/R1,4:/R2~-60
  )
  add(
    defaultscale:=0.6;
    label.bot("Diene",p0+(0.5w,0));
  )
  cvat(0.4,0.5)(
    <-30,-60`1,1=d1,1:/R3,2:/R4^60
    add(defaultscale:=0.6;
      label.bot("Dienophile",p0+(.5w,0));
    )
  )
  cvat(0.9,0.5)(
    <30,?6,6=d1,2:/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
```



4.7.1 Local ext() setting

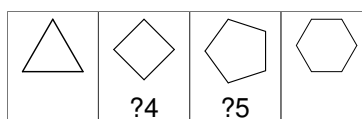
```
beginfigm
  EN:="?3";
  cvat(0.5,1)(<30,?3)
endfigm
beginfigm
  EN:="?4";
  cvat(0.5,1)(?4)
  %-----
  ext(label.top(EN,(0.5w,0));)
  %-----
endfigm
beginfigm
  EN:="?5";
  cvat(0.5,1)(?5)
endfigm
beginfigm
  EN:="?6";
  cvat(0.5,1)(?6)
endfigm
```



4.7.2 Global ext() setting

ext_clear: reset global ext()

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

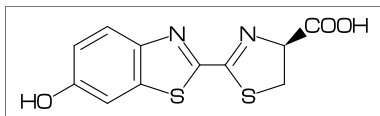


5 Example

5.1 cv() example

(Luciferin)

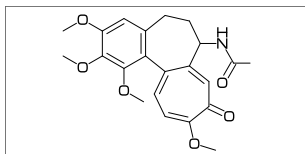
```
beginfigm
  fsize:=(50mm,15mm);
  cv(<30,Ph,3=?5,@8,\,?5,{9,16}=d1,{9,14}:N,{7,11}:S,1:/OH,-2:*/COOH)
endfigm
```



5.2 readm() example

(Colchicine)

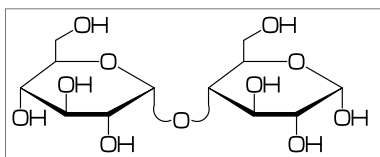
```
beginfigm
  readm(
    "<30,Ph,{1,2,6}:/O!,{-4,-5}=?7, ",
    " {-1,-4,-6}=d1,-2://0,-3:/O!, ",
    " @9,\,NH,!//0,! " )
  fsize:=(40mm,20mm);
  putm;
endfigm
```



(Maltose)

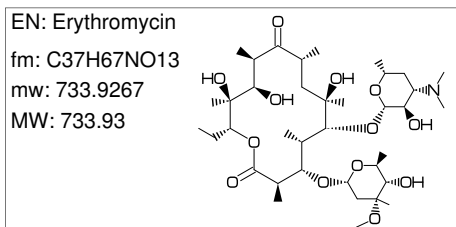
(bond type for glycan)
arc_lb : arc left > bottom
arc_br : arc bottom right

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



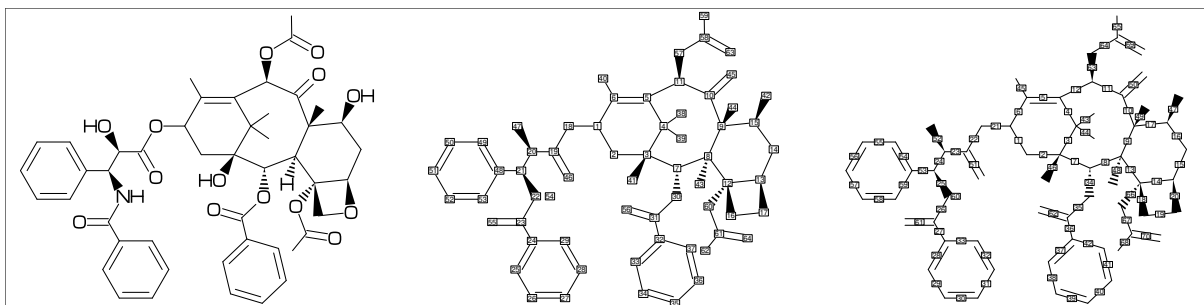
(Erythromycin)

```
beginfigm
EN:="Erythromycin"; MW:="733.93";
fsize:=(60mm,30mm); mposition:=(1,0.5);
readm(
%-----
"<30,#1,<-120,60,60,60,-60,60,60,-60,60,60,60,-60,60,60,##,&1,      ",
" 14:0,13:/*Et,{1,9}://0,                                          ",
" {2',4,6^-35,8,10',12^35}:/*_,                                  ",
" {6^35,11,12^-35}:*/OH,                                          ",
" @$3,\*,0,30~zb,|,?6`.7,6:0,#.5,{5~wf,3^35}:/_4:/*OH,3^-35:/*0!,##, ",
" @$5,\*^30^1.7,0,!~zb,|,?6`.7,6:0,#.5,5:/*_,2:*/OH,3:/*N?!      ")
%-----
putm;
ext(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",
readm(
%-----
"?6,5=d1,@3,#1,36,45,45,45,45,##,&5,-4=?6,-4=?4,-1=wb,-3=wf,-1:0, ",
" 4:??,6:/_,{3^-60,15}:*/OH,8:/*H^-60,9:/*/_^60,10://0,          ",
" @1,\,0,!//0,!,*OH,!/,Ph,60~wf,NH,-60,//0,60,Ph,              ",
" @7,\*,0,-45,//0,60,Ph,11:*/OCO!>r1,12:*/OCO!^-15>1r          ")
%-----
fsize:=(140mm,30mm);
if checkm(mc)=0:
cvat(0,0.5)(scantokens(mc))
sw_numbering:=Atom;
cvat(0.6,0.5)(scantokens(mc))
sw_numbering:=Bond;
cvat(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=d1,10:0,7://0,@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=d1,8:N,{15,17}:0,"
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,-1:0,-1=zb,"
row[3] [4]="@7,60~wf`0.75,70~si_`1.3,45,N!,&9~wb,15=d1,6:/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}:0,@4,\,!!,,!!,,!!,,//0,!,?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=d1,10:0,7://0,@9,\,Ph,{2,6,14,15}:/OH"
row[1] [5]=":"

** default sw_comment=0
```

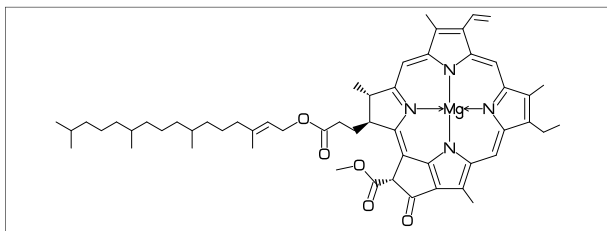
(Tag)

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
  getm("Chlorophyll a");
  sw_output:=Fig+Calc+Mcode;
  fsize:=(80mm,30mm);
  cv(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}%
```

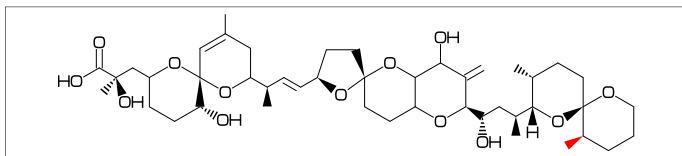


```
<-36,#1,?5,@3,\,54,?5,@-2,\,54,?5,@-2,\,54,?5,@-2,\,&5,@6,22,70,&8,##,
{4,6,8,10,14,16,18,21,23,27}=d1,@4,\`1.48~vf,Mg,&17~vb,@11,&27,@27,&23,
{4,11,17,23}:N,{1~zf,9,15,21}:/_ ,14: /!,20: /!!,25:/*COO!,26://0,
@2,*\^-6,!2, //0,!0,!2,!! ,!13,{1,5,9,13}:/_
```

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

(Dinophysistoxin-1)

```
beginfigm
  getm("Okadaic acid");
  readm(",38:*/_,65=red")          %%% add methyl group (color red) %%%
  sw_output:=Fig+Calc+Mcode;      %%% output temp-mc.aux %%%
  EN:"Dinophysistoxin-1"; MW:"819";
  fsize:=(90mm,20mm);
  if checkm(mc)=0: cv(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}%
```

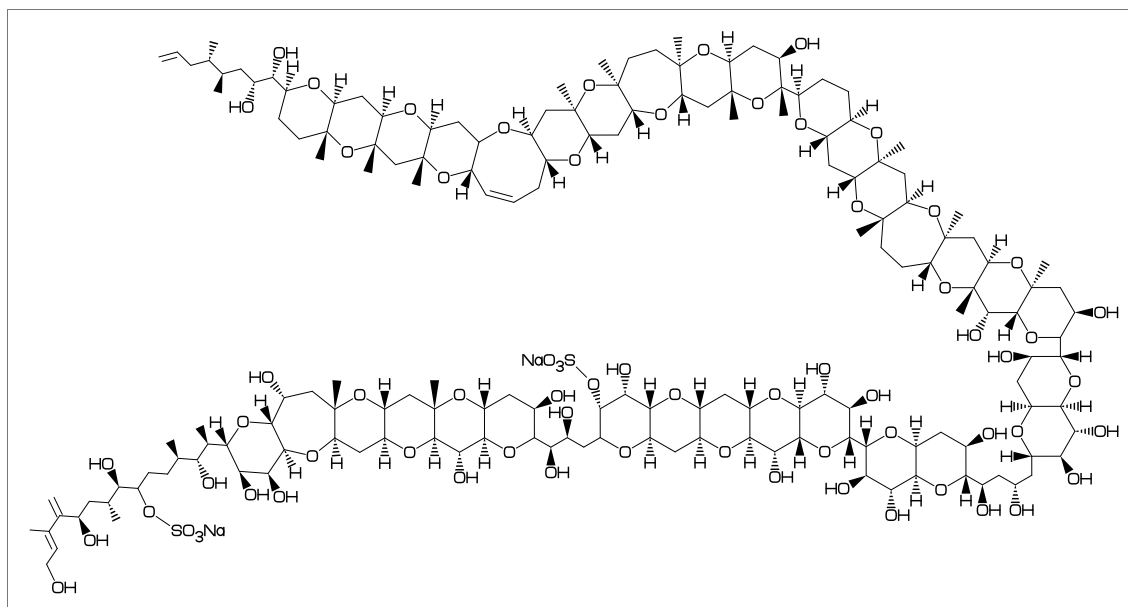


```
<30,?6,@4,?6,@-4,\,!3,<-12,?5,@-3,<-12,?6,-3=?6,@-3,*\,!3,
?6,@-4,?6,@6,\,!,/*\^-40,* /OH^20,! ,//0,!1,OH,
3=wb,11=d1,15=dr,17=wf,19=wf,38=wb,{5,7,16,24,25,33,42}:0,
32:*/H^60,10:/_ ,{12,31,37'}:*/_,27://_,28:/OH,{3,29}:/*OH,
38:*/_,65=red
```

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

(Maitotoxin)

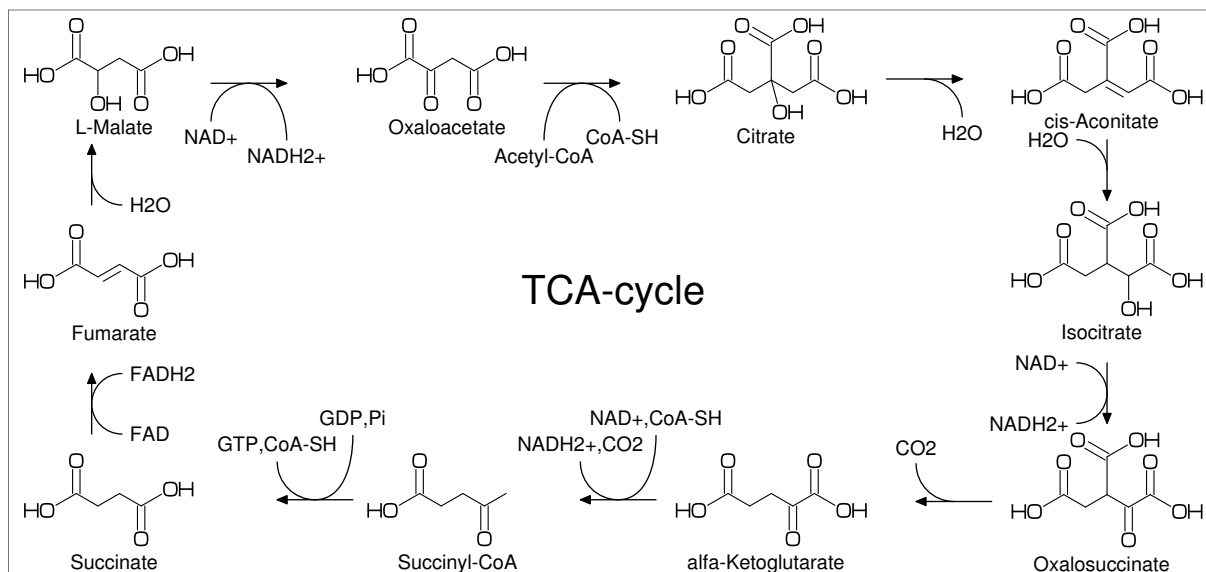
```
%-----  
\begin{mplibcode}  
  beginfigm  
    getm("Maitotoxin");  
    sw_output:=Fig+Calc+Mcode;          %%% output temp-mc.aux %%%  
    fsize:=(150mm,80mm);  
    fmargin:=(3mm,3mm);  
    sw_frame:=Outside;  
    if checkm(mc)=0: cv(scantokens(mc))  
      VerbatimTeX("\gdef\EN{"&EN&"}\gdef\MW{"&MW&"}");  
      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=d1,{-5,-3,-3,-3}=?6,  
{5,7,15,16,23,24,32,40,41,48,49,58,59,72,73,82,83,90,91,99,  
100,107,113,114,122,123,130,131,140,141,148,149}:0,  
{1^60,2,26,28,29,51,54,61,63,68,75^60,78,109}:*/OH,  
{11,20,35,45,52,55,65,69,86}:/*OH,  
{3,8,13,17,21,33,38,42,56,70,84,92,101,106,111,128,138,142,146,150}:/*H^-60,  
{4,14,22,34,39,43,47',57',71',81,89,98,102,116,121,125,129,133}:*/H^60,  
{6,46,50,53,60,67,74}:*/H^-60,  
{9,18,85,93,112,139,143,147}:*/_^-60^1,{80,88,97,108',115,120,124}:/*_^-60^1,  
@$6,\,|,\,!11,60~dr,-60,60,OH,{2',7,10}:*/OH,{1,3,8'}:*/_ ,11://_ ,12:/_ ,  
@6,\,0,30,S03Na,  
@$36,-45~zf,0,30,S03Na,  
@$150,\,|,\,!7,{1,2}:/*OH,4:*/_ ,5:/*_ ,7=d1
```

```
** EN:Maitotoxin mw:3425.86 MW:3425.856 fm:C164H256Na2068S2
```

5.5 cvat() example



```

beginfigm
fsize:=(160mm,75mm);
max_blength:=5mm;
COOH:=' (/0,!,OH); HOCO:=' (OH,!,//0,);
cvat(0.33, 1)(<30,HOCO,!,//0,!2,COOH) % Oxaloacetate
cvat(0.66, 1)(<30,HOCO,!4,COOH,@-4`1,\,COOH,4:/OH~-165) % Citrate
cvat(1, 1)(<30,HOCO,!2,!~dr,!,COOH,@-4`1,\,COOH) % cis-Aconitate
cvat(1, 0.58)(<30,HOCO,!4,COOH,@-4,\`1,COOH,5:/OH) % Isocitrate
cvat(1, 0.05)(<30,HOCO,!3,//0,!,COOH,@-4,\`1,COOH) % Oxalosuccinate
cvat(0.66,0.05)(<30,HOCO,!3,//0,!,COOH) % alfa-Ketoglutarate
cvat(0.33,0.05)(<30,HOCO,!3,//0,!,{"S-CoA"}) % Succinyl-CoA
cvat(0, 0.05)(<30,HOCO,!3,COOH) % Succinate
cvat(0, 0.55)(<30,HOCO,!,!~dr,!,COOH) % Fumarate
cvat(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 source 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
fsize:=(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
  cv(<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
  readm(    > read Mcode
    ": <30,?6,{-4,-2}=?6,-4=?5,7=d1,    ",    > mc1
    ": 10:/*H^180,11:/*H^-60,17:/*H^-54,    ",    > mc2
    ": {4,12}:*/_^60,    ",    > mc3
    ": @-1,18,*_,-60,!3,?!    ")    > mc4
  putm;    > put figure
endfigm    >
%-----
loadm("EN<>*");    > load all unit
beginfigm
  getm("Adenine");    > get EN=Adenine
  putm;    > ** put figure
endfigm    >
%-----
beginfigm
  getm(4);    > select No.4
  putm;    > put figure
endfigm    >
%-----
for i=1 upto ucount:    > figure count
  beginfigm
    getm(i);    > select No.i
    putm;    > 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}=d1,{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}=d1,{2,6,9}:N,5:/NH2,7:NH
;
%-----
CAT:biological;EN:Guanine;MW:151.13;EXA:1
:
<30,?6,3=?5,{1,3,9}=d1,{2,9}:N,{6,7}:NH,5://0,1:/NH2
;
%-----
CAT:biological;EN:Cytosine;MW:111.10;EXA:1
:
<30,?6,{4,6}=d1,4:N,3://0,2:NH,5:/NH2
;
%-----
CAT:biological;EN:Thymine;MW:126.11;EXA:1
:
<30,?6,3=d1,{2,6}:NH,{1,5}://0,4:/_
;
%-----
CAT:biological;EN:Uracil;MW:112.09;EXA:1
:
<30,?6,6=d1,{3,5}://0,{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 ahlenght=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}=d1,{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}=d1,{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,!//0,!1,OH,  
3=wb,11=d1,15=dr,17=wf,19=wf,38=wb,{5,7,16,24,25,33,42}:0,  
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[3],Name<Cytosine>,Category<biological>,File<main_lib.mcf>
-----
<30,?6,{4,6}=dl,4:N,3://0,2: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
=====
```

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 D  0 0 0 0
  0.86603    2.36383    0 D  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;
  %-----
  fsize:=(50mm,50mm);
  EN:="Limonin";
  MW="470.51";
  beginfigm
    readm(
      %-----
      "<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}=d1,3:0          ")
      %-----
    putm;
  endfigm
\end{mplibcode}\\
%-----
\begin{mplibcode}
  fsize:=(80mm,50mm);
  EN:="beta-carotene";
  MW="536.87";
  beginfigm
    readm(
      %-----
      "<30,?6,3=d1,{3,5^35,5^-35}:/_,      ",
      " @4,\,|,!18,{1,3,5,7,9,11,13,15,17}=dr, ",
      " {3,7,12,16}:/_,                      ",
      " |,?6,6=d1,{6,2^35,2^-35}:/_         ")
      %-----
    putm;
  endfigm
\end{mplibcode}\\
%-----
\end{document}
```

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