

# Molecular Coding Format manual

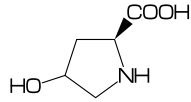
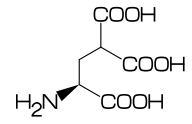
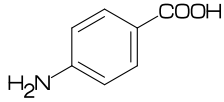
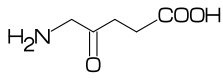
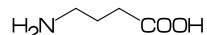
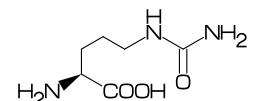
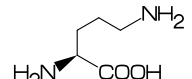
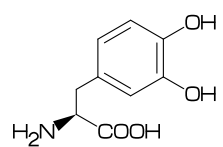
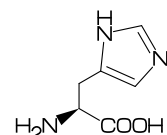
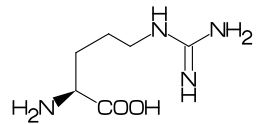
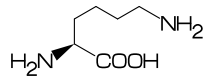
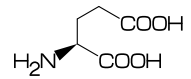
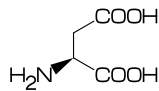
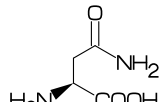
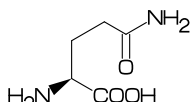
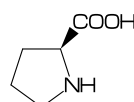
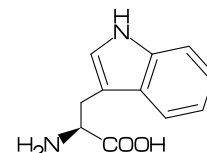
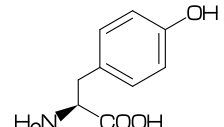
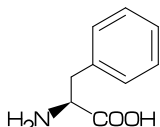
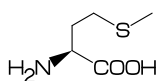
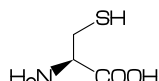
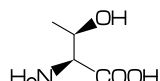
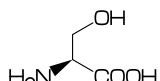
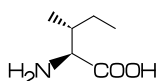
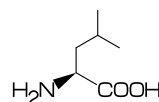
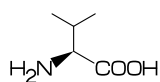
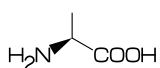
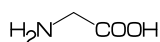
Akira Yamaji

May 28, 2023

mcf2graph version 5.02

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

Suggestion or request mail to: [mcf2graph@gmail.com](mailto: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.

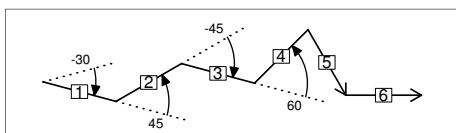
## 2 MCF syntax

### 2.1 Make bond

#### 2.1.1 Chain

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

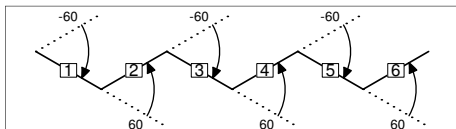
<10,-30,45,-45,60,\$300,\$0



#### 2.1.2 Chain with !,!n

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

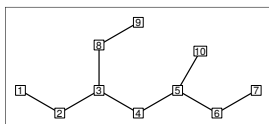
<-30,!6



#### 2.1.3 Jump to atom

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

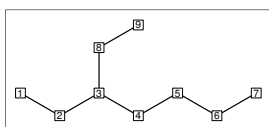
<-30,!6,@3,0,!,@5,-30



#### 2.1.4 Branch bond

\ : 0

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

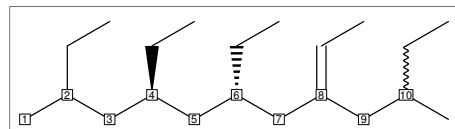


#### 2.1.5 Branch modified bond

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

<30,!8,

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

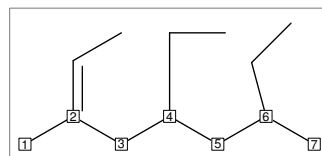


<30,!6,

\~dr,! : 0~dr,!

\^1.5,-90 : 0^1.5,-90

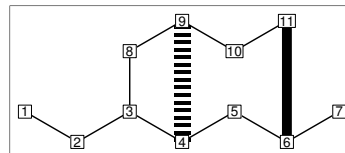
\^15,-60 : 0^15,-60



#### 2.1.6 Connect atom

&n : Connect to An

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

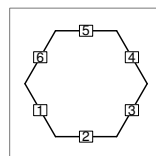


#### 2.1.7 Ring

?n : n membered ring(3<=n<=20)

?6 : <-120,60,60,60,60,60,&1

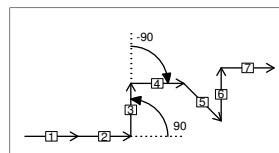
?6



#### 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

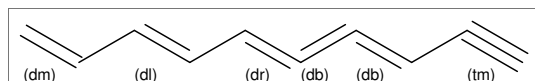
db : double left or right side

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

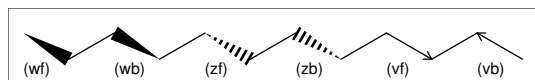
zb: hashed(zebra stripe) wedge backward

vf: vector forward

vb: vector backward

<-30,

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



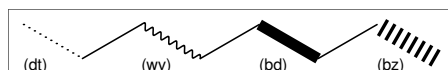
(Dotted, wave)

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

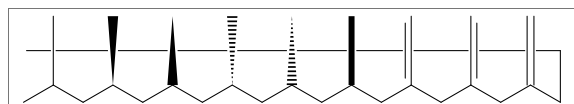
dr\_ : double right over line

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)

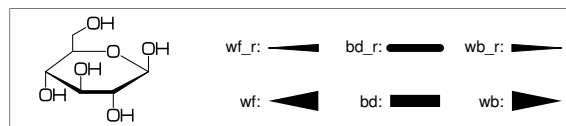
bd\_r : broad (half width, rounded)

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,

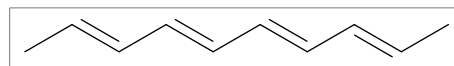
{1~\$-90, 2~\$90, 3~\$-90, 4~\$90}:/OH,



### 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

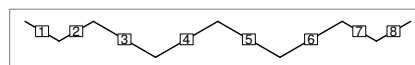


## 2.3 Change bond length

### 2.3.1 Chain length

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

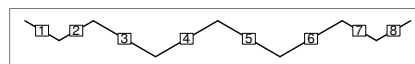
<-30, !2, !4`1.2, !2



#n : bond length=n

## : reset bond length

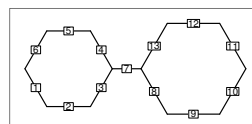
<-30, !2, #1.2, !4, ##, !2



### 2.3.2 Ring length

?n`length : change ring length

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

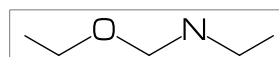


## 2.4 Change atom

### 2.4.1 Insert atom

Insert hetero atom

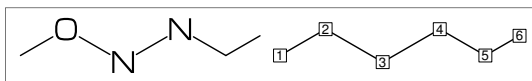
<-30, !2, 0, !2, N, !2



## 2.4.2 Addressed atom

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

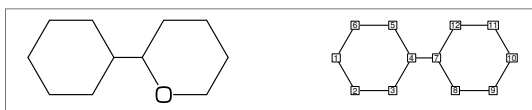
<30,14,2:0,{3,4}:N



## 2.4.3 Brock address

| : divide brock

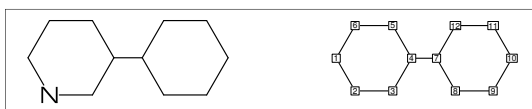
?6,@4,\,|,?6,2:0



## 2.4.4 Reset brock address

|| : reset brock address

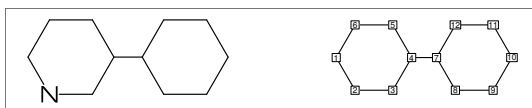
?6,@4,\,|,?6,||,2:N



## 2.4.5 Absolute address

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

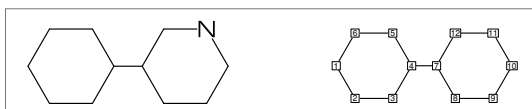
?6,@4,\,|,?6,\$2:N



## 2.4.6 Relative address

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

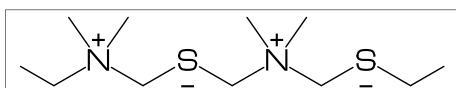
?6,@4,\,?6,-2:N



## 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



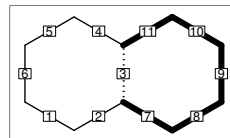
## 2.5 Fuse ring

(Attached 1 bond)

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

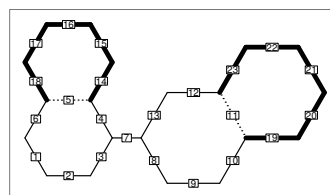
\*\* Bn(n:-999<=n<=4095): bond number

?6,3=?6



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

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

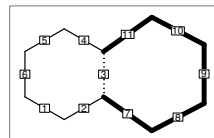


?6,3=?6[13] : fuse ?6[13] at B3

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

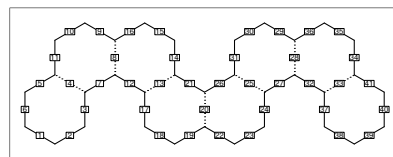
\*\* ?m[n] (5<=m<=8,11<=n<=15)

?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

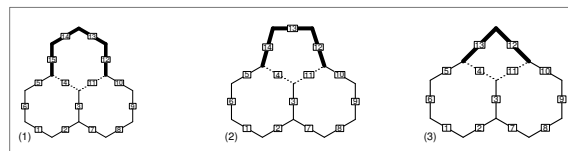
4--11=?5 : fuse 3/5 ring to B11..B4

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



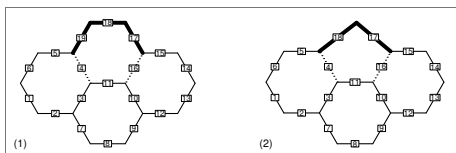
(Attached 3 bond)

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

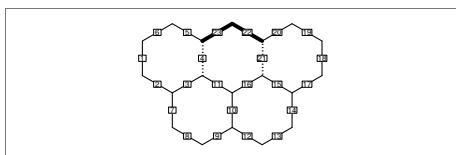
2:?6,{3,10}=?6,16---4=?5



(Attached 4 bond)

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

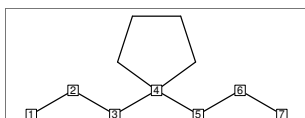
<-30,?6,{3,10,15,21----4}=?6



## 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

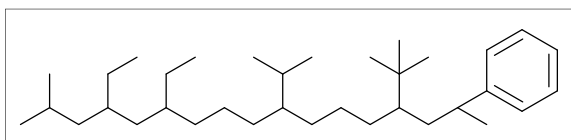
/?! : isopropyl

/??! : tert-butyl

/Ph : phenyl

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

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



### 2.7.2 Insert modified group

// : double (double middle)

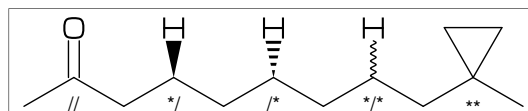
\*/ : wedge forward

/\* : hashed wedge forward

\*/\* : wave

\*\* : direct

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



~ : change type

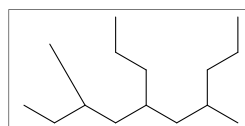
^ : change angle

` : change length

> : change environment

<-30,`^1,!,

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

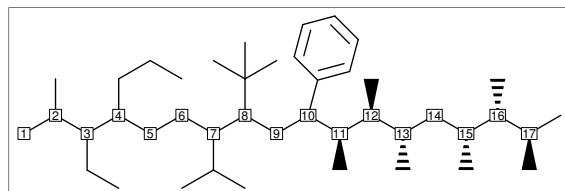


### 2.7.3 Add group

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

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

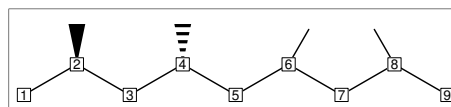
{11,12,13'}:\*/\_,{15,16,17'}:/\*\_



### 2.7.4 Add modified group

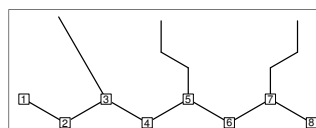
~,^,` : change type,angle,length

<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

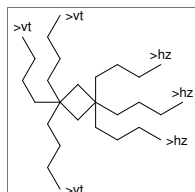


## 2.8 Chain environment

### 2.8.1 Horizontal,vertical

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

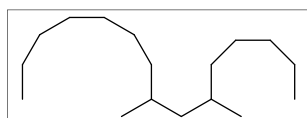
```
?4,  
{3^-90,3^-30,3^90}:/!3>hz,  
{1^-60,1,1^60}:/!3>vt
```



### 2.8.2 Left-right,right-left

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

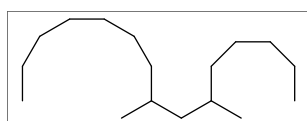
```
<-30,!6,  
{3^-30,3,3^30}:/!3>lr,  
{5^-30,5,5^30}:/!3>rl
```



### 2.8.3 Fixed rotate angle

>n : rotate n

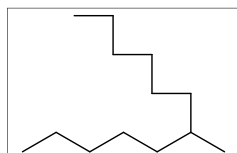
```
<30,!4,  
2:/!6>30 % 2:\,30,30,30,30,30,30  
4:/!4>-45 % 4:\,-45,-45,-45,-45
```



### 2.8.4 Multiple rotate angle

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

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

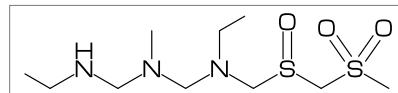


## 2.9 Miscellaneous

### 2.9.1 Abbreviated parts

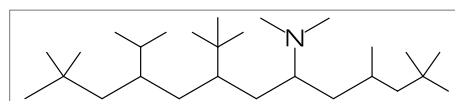
```
NH : N,/H~n1 N! : N,/_ N!2 : N,/!  
SO : S,//0 S00 : S,//0^35,/^-35
```

```
<-30,!2,NH,!2,N!,!2,N!2,S0,!2,S00,!
```



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

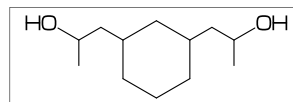
```
<30,!9^1,?!,! ,?!,! ,2:??,4:/??,6:/?! ,8:/N?!
```



### 2.9.2 Parts definition

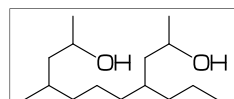
'(..) : user defined parts

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



### 2.9.3 Parts inline definition

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



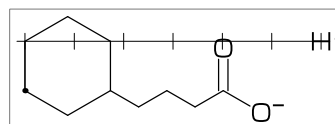
### 2.9.4 Move position

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

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

\*\* l=bond length of ring

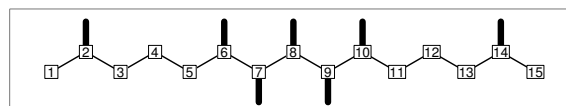
```
<30,?6,@3,!4,//0,! ,0,n_^60,@$(6,1),H,p_^15
```



### 2.9.5 Serial number

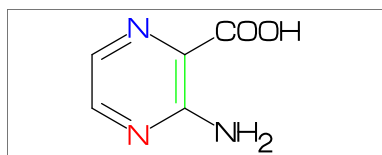
```
6:10 : 6,7,8,9,10
```

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



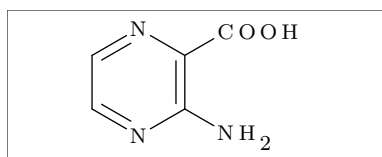
## 2.9.6 Change color

```
beginfigm
\(  
  <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
```

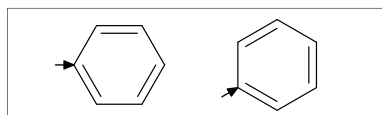


# 3 Option parameter

## 3.1 Angle parameter

mangle=0 \*\* default

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

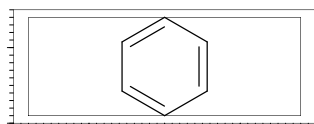


## 3.2 Size/Ratio parameter

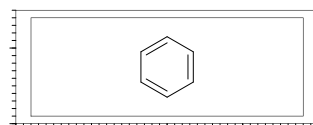
### 3.2.1 Bond length [ |(=) ]

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

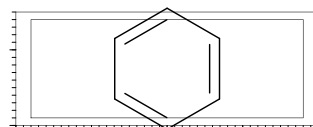
(fit to figure size)  
blength=0 \*\* default



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

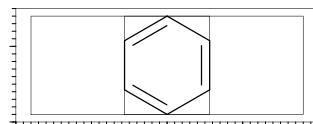


(bond length)  
blength=9mm  
\*\* (blength>1) ignore msize(w,h)

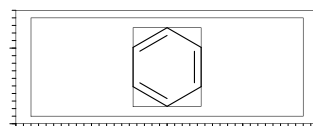


### 3.2.2 Molecular size

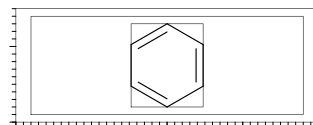
##(1,1) : msize=(1,1) \*\* default  
## p : abbreviated form of msize:=p;



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

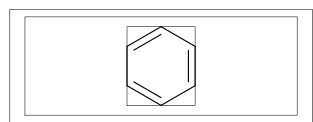


##(11mm,11mm) : msize=(11mm,11mm)

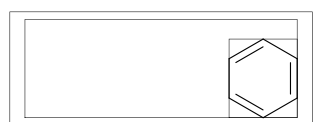


### 3.2.3 Molecular position

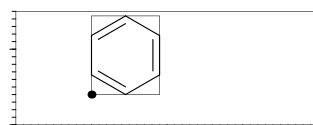
@(0.5,0.5) : mposition=(0.5,0.5) \*\*default



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



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



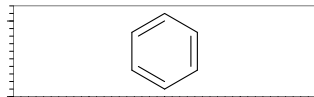


### 3.3 Size parameter

#### 3.3.1 Figure size [ #() ]

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

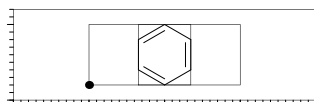
#(40mm,15mm) : fsize=(40mm,15mm)



#### 3.3.2 Figure margin [ #@() ]

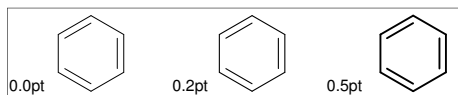
fmargin=(margin left right,top bottom)  
\*\* default: (0.4mm,0.4mm)  
#@ p : abbreviated form of fmargin:=p;

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



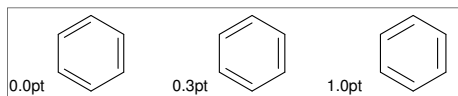
#### 3.3.3 Offset thickness of bond

default: offset\_thickness=0.2pt



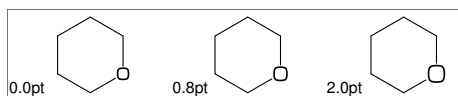
#### 3.3.4 Offset of double bond gap

default: offset\_bond\_gap=0.3pt



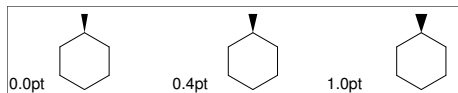
#### 3.3.5 Offset of atom width

default: offset\_atom=0.8pt



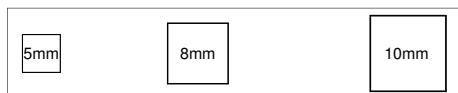
#### 3.3.6 Offset of wedge width

default: offset\_wedge=0.4pt



#### 3.3.7 Max bond length [ |<=() ]

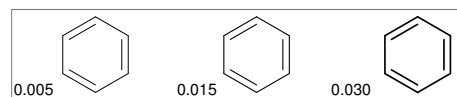
|<(n): abbreviated form of max\_blength:=n;  
default: max\_blength=10mm



### 3.4 Ratio parameter

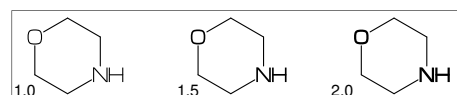
#### 3.4.1 Thickness/bond length

default: ratio\_thickness\_bond=0.015



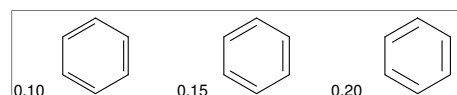
#### 3.4.2 Char/bond thickness

default: ratio\_char\_bond=1.5



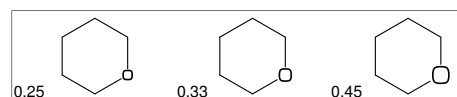
#### 3.4.3 Bond gap/bond length

default: ratio\_bondgap\_bond= 0.15



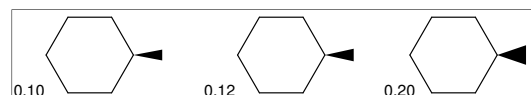
#### 3.4.4 Atom/bond length

default: ratio\_atom\_bond= 0.36



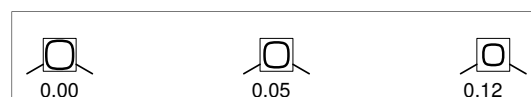
#### 3.4.5 Wedge/bond length

default: ratio\_wedge\_bond=0.12



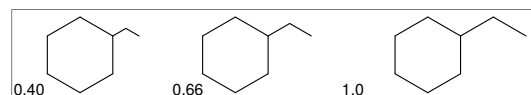
#### 3.4.6 Figure atom gap/atom length

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

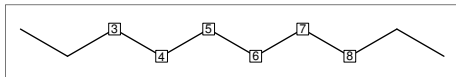


## 3.5 Drawing mode

### 3.5.1 Numbering atom

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

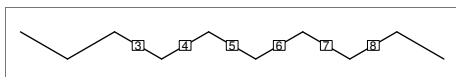
```
sw_numbering:=Atom;
\(<-30,!9)
```



### 3.5.2 Numbering bond

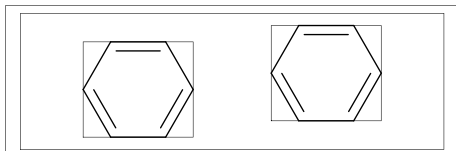
```
sw_numbering=Bond
numbering_start:=3;
numbering_end:=8;
default: sw_numbering=0
```

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

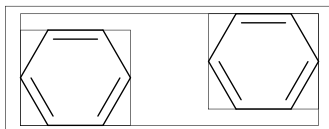


### 3.5.3 Trimming mode

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

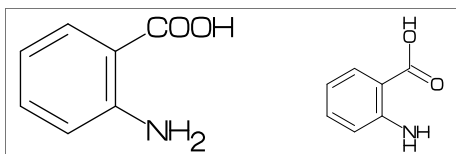


```
sw_trimming:=1;
@(0.2,0.3)\(Ph)
@(0.8,0.7)\(Ph)
```



### 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

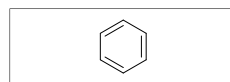
```
** default: sw_abbreviate=Bond
```



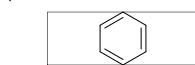
## 3.6 Frame

### 3.6.1 Figure frame

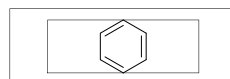
```
** default:sw_frame=0
(Draw figure frame)
fmargin:=(5mm,2mm);
sw_frame=0outside
```



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

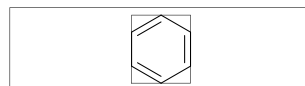


```
(Draw both frame)
sw_frame=Bothside=Inside+Outside
```



### 3.6.2 Molecular frame

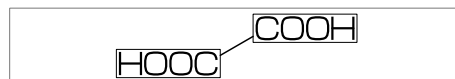
```
sw_frame=Mol
** default:sw_frame=0
```



### 3.6.3 Atom frame

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

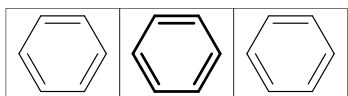
```
\(<30,COOH,! ,COOH)
```



## 3.7 Parameter setting

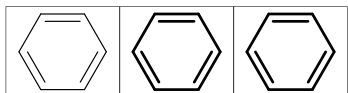
### 3.7.1 Local parameter setting

```
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

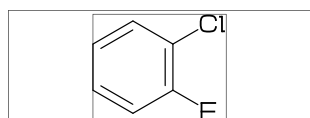
### 4.1 drawm [ \() ]

(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 height/figure height  
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)

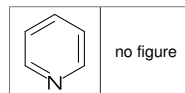
```
'("<30,Ph,{1,2,6}:/O!,{-4,-5}=?7,"
  "{-1,-4,-6}=d1,-2://0,-3:/O!, "
  "@9,\,NH,!,//0,!")
```

### 4.3 checkm() [ \\*() ]

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

(check mcf and compile)

```
beginfigm
  '("<30,Ph,}2:N") % ** extra '}'
  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)

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

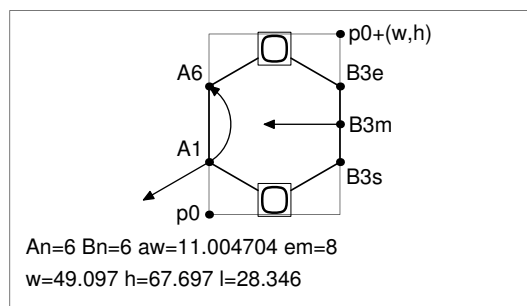
plus : '+' circled  
minus : '-' circled  
circlediam = 0.6aw (default)  
circlepen = 0.2bp (default)

lonpair r: ':' rotated r  
lonpairdiam = 0.3aw (default)  
lonpairspace = 0.7aw (default)

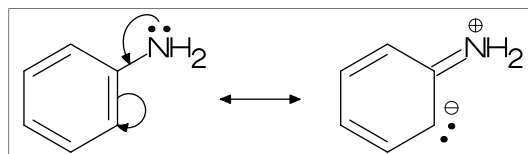
\*\* : scaled  
<< : rotated  
a /\* b : point b of a

```
beginfigm
#(70mm,40mm) ##(.91,.9) |<(10mm)
sw_frame:=sw_frame+Atom+Mol;
@(.5,.85)\(<30,?6,{2,5}: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+__*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=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;
)
%-----
@(1,0)\(<30,?6,{1,5}=d1,4://NH2)
%-----
add(
labeloffset:=.7aw;
label.top(plus,A7);
label.urt(minus,A3);
label(lonpair A3ang,A3+A3up**0.7aw);
)
%-----
ext(drawdblarrow (.4w,.4h)..(.55w,.4h));
%-----
endfigm
```



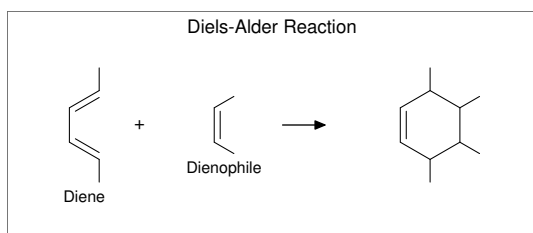
## 4.7 ext()

(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

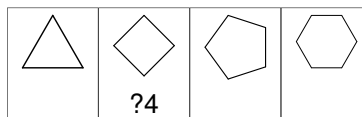
ratio_thickness_char:
pen thickness / char width
%-----
beginfig
#(70mm,30mm) |(0.065)
%-----
@(0.1,0.5)\(
  <-210,60`1,60`1,60`1,{1,3}=d1,
  1:/R1,4:/R2~-60
)
add(
  defaultscale:=0.6;
  label.bot("Diene",p0+(0.5w,0));
)
@(0.4,0.5)\(
  <-30,-60`1,1=d1,1:/R3,2:/R4^60
  add(defaultscale:=0.6;
  label.bot("Dienophile",p0+(.5w,0));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



### 4.7.1 Local ext() setting

\_s : abbreviated form of EN:=s;

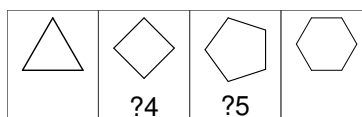
```
beginfig
_"?3"@(.5,1)\(<30,?3)
endfig
beginfig
_"?4"@(.5,1)\(?4)
%-----
ext(label.top(EN,(0.5w,0));)
%-----
endfig
beginfig
_"?5"@(.5,1)\(?5)
endfig
beginfig
_"?6"@(.5,1)\(?6)
endfig
```



### 4.7.2 Global ext() setting

ext\_clear: reset global ext()

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

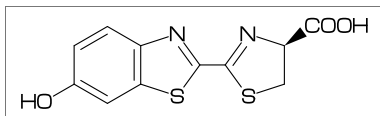


## 5 Example

### 5.1 drawm() example

(Luciferin)

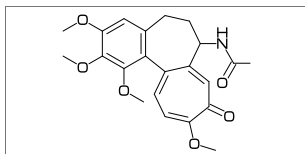
```
beginfigm
  #(50mm,15mm)
  \(<30,Ph,3=?5,@8,\,?5,{9,16}=d1,{9,14}:N,{7,11}:S,1:/OH,-2:*/COOH)
endfigm
```



### 5.2 readm() example

(Colchicine)

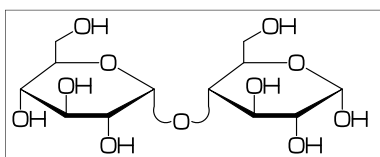
```
beginfigm
  '(
    "<30,Ph,{1,2,6}:/O!,{-4,-5}=?7, ",
    " {-1,-4,-6}=d1,-2://0,-3:/O!, ",
    " @9,\,NH,!,//0,! )"
  #(40mm,20mm) \\
endfigm
```



(Maltose)

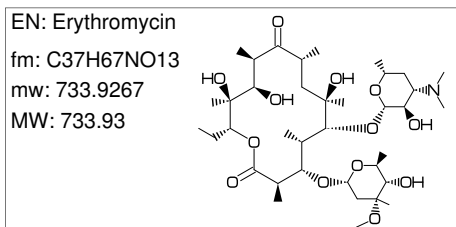
(bond type for glycan)  
arc\_lb : arc left > bottom  
arc\_br : arc bottom right

```
beginfigm
  %"EN:Maltose","MW:342.3",
  '(
    %-----
    "#1.25,-30~wf_r,30~bd_r`1,30~wb_r,120,0,30,&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 )"
    %-----
  #(50mm,20mm) \\
endfigm
```



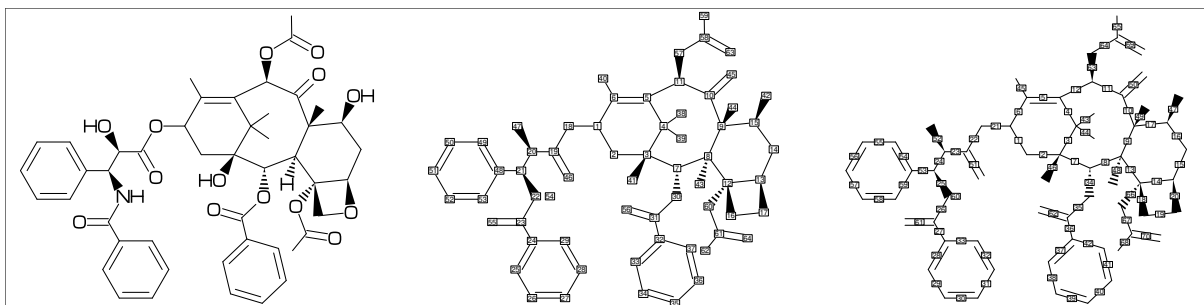
## (Erythromycin)

```
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,      ",
" 14:0,13:/*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?!      ")
%-----
\\
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",
' '(
%-----
"?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         ")
%-----
#(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=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)

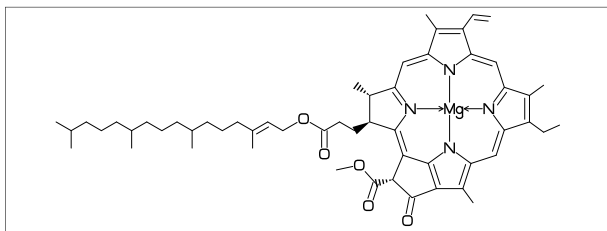
|    |                               |     |                              |
|----|-------------------------------|-----|------------------------------|
| J  | : jobname                     | CAT | : category                   |
| EN | : english name                | JN  | : japanese name            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



## 5.4 getm() example

### (Chlorophyll a)

```
beginfigm
  $("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}%
```

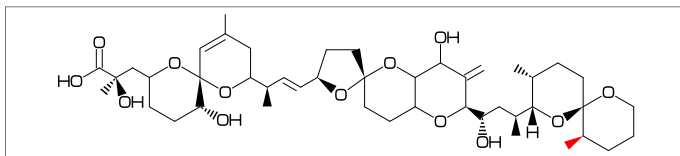


```
<-36,#1,?5,@3,\,54,?5,@-2,\,54,?5,@-2,\,54,?5,@-2,\,&5,@6,22,70,&8,##,
{4,6,8,10,14,16,18,21,23,27}=d1,@4,\`1.48~vf,Mg,&17~vb,@11,&27,@27,&23,
{4,11,17,23}:N,{1~zf,9,15,21}:/_ ,14:!/ ,20:!! ,25:/*COO! ,26://0,
@2,*\^-6,!2,//0,!0,!2,!! ,|,!13,{1,5,9,13}:/_
```

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

### (Dinophysistoxin-1)

```
beginfigm
  $("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}%
```

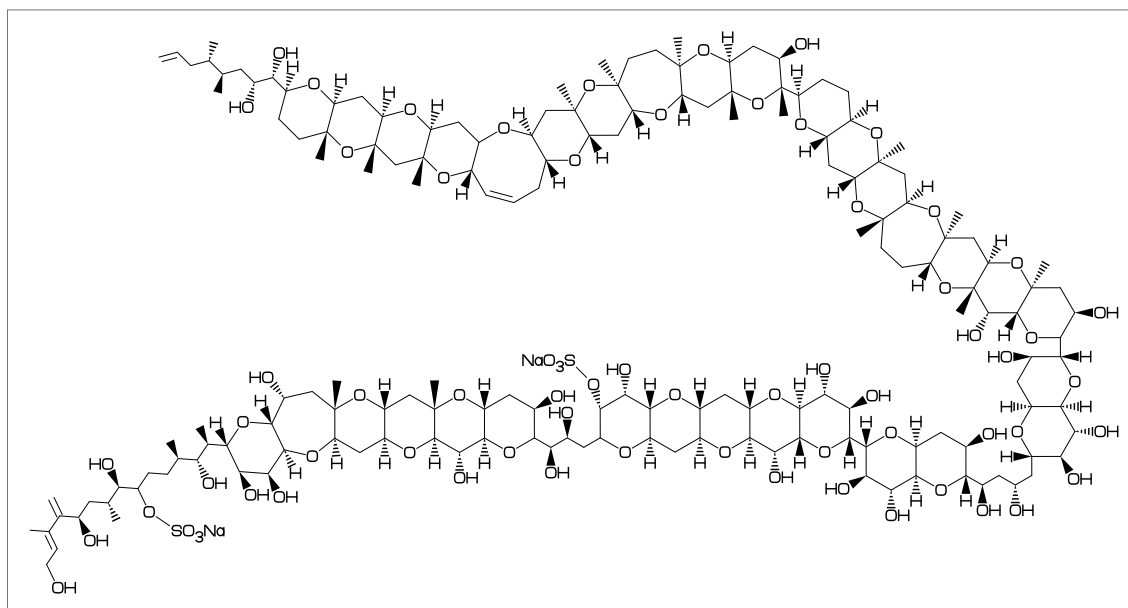


```
<30,?6,@4,?6,@-4,\,!3,<-12,?5,@-3,<-12,?6,-3=?6,@-3,*\,!3,
?6,@-4,?6,@6,\,!,/*\^-40,*OH^20,! ,//0,!1,OH,
3=wb,11=d1,15=dr,17=wf,19=wf,38=wb,{5,7,16,24,25,33,42}:0,
32:*/H^60,10:/_ ,{12,31,37'}:*/_ ,27://_ ,28:/OH,{3,29}:/*OH,
38:*/_ ,65=red
```

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

## (Maitotoxin)

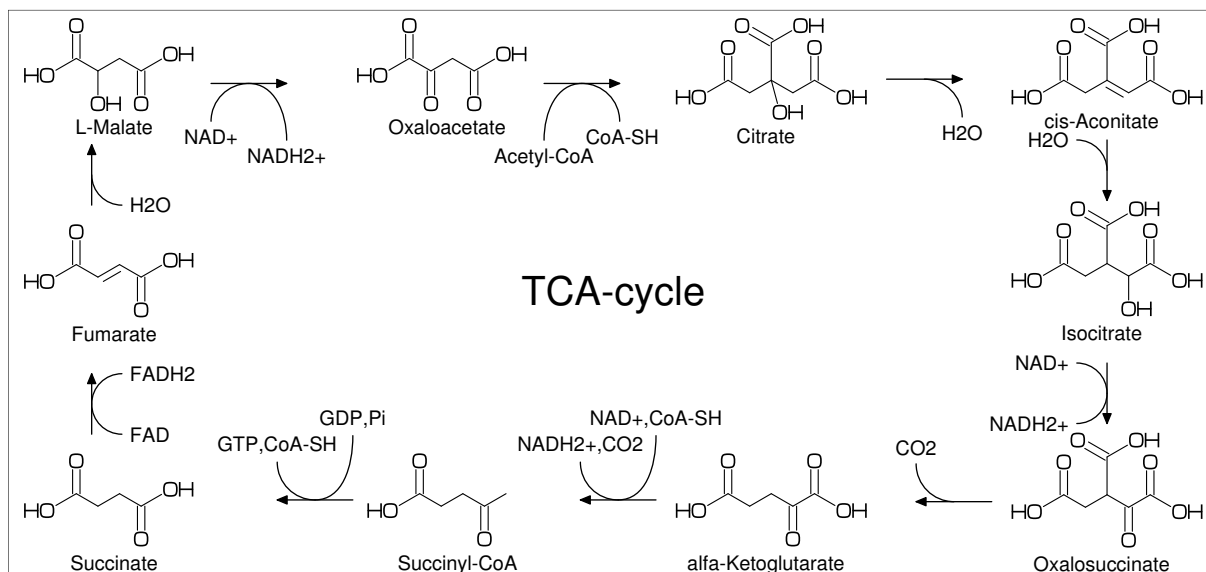
```
%-----  
\begin{mplibcode}  
  beginfigm  
    $("Maitotoxin") #(150mm,80mm) #@ (3mm,3mm)  
    sw_output:=Fig+Calc+Mcode;      %%% output temp-mc.aux %%%  
    sw_frame:=Outside;  
    if *(mc)=0: \ (scantokens(mc))  
      VerbatimTeX("\gdef\EN{"&EN&"}\gdef\MW{"&MW&"}");  
      VerbatimTeX("\gdef\mw{"&mw&"}\gdef\fm{"&fm&"}");  
    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=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:C164H256Na2O68S2
```

## 5.5 User define parts example



```

beginfigm
#(160mm,75mm) |<(5mm)
COOH:='(//0,! ,OH); % define COOH
HOCO:='(OH,! ,//0,); % define HOCO
@(0.33, 1)\(<30,HOCO,! ,//0,!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,//0,! ,COOH,@-4,\`1,COOH) % Oxalosuccinate
@(0.66,0.05)\(<30,HOCO,!3,//0,! ,COOH) % alfa-Ketoglutarate
@(0.33,0.05)\(<30,HOCO,!3,//0,! ,"{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=d1,          ",          > 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}=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 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}=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}=d1,4: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;
  %-----
  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}=d1,3:0          ")
    %-----
  \\\
  endfigm
\end{mplibcode}\\
%-----
\begin{mplibcode}
  EN:="beta-carotene";
  MW:="536.87";
  beginfigm
    #(80mm,50mm)
    '(
    %-----
    "<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}:/_        ")
    %-----
  \\\
  endfigm
\end{mplibcode}\\
%-----
\end{document}

```

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