

Molecular Coding Format manual

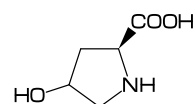
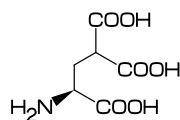
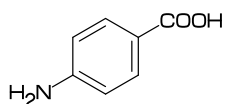
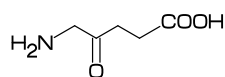
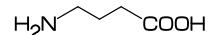
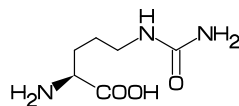
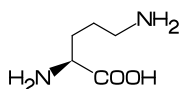
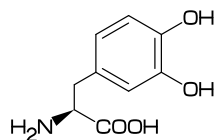
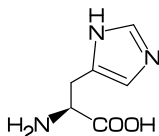
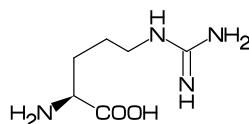
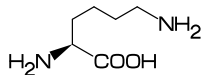
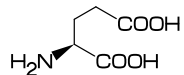
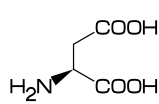
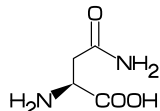
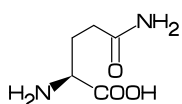
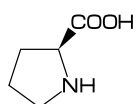
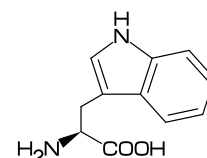
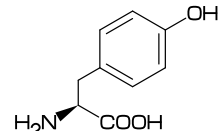
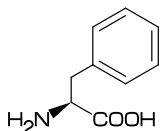
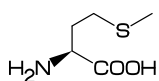
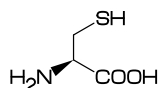
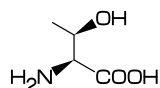
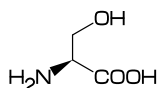
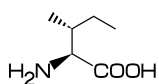
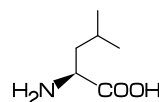
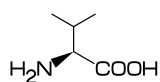
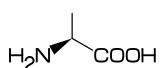
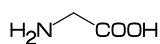
Akira Yamaji

July 27, 2025

mcf2graph version 5.25

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

Suggestion or request mail to: mcf2graph@gmail.com



Contents

1	Introduction	3
2	MCF syntax	3
2.1	Make bond	3
2.1.1	Chain	3
2.1.2	Chain with !,ln	3
2.1.3	Jump to atom	3
2.1.4	Branch bond	3
2.1.5	Rotate current angle	3
2.1.6	Connect atom	3
2.1.7	Ring	3
2.1.8	Ring length	3
2.2	Change bond type	4
2.2.1	Double,triple,wedge,vector	4
2.2.2	Over line	4
2.2.3	Steric ring	4
2.2.4	Change multiple bond type	4
2.3	Change bond length	4
2.3.1	Change chain length	4
2.3.2	Change multiple bond length	4
2.4	Change atom	4
2.4.1	Insert atom	4
2.4.2	Change atom	4
2.4.3	Brook address	5
2.4.4	Reset brook address	5
2.4.5	Absolute address	5
2.4.6	Relative address	5
2.4.7	Charged atom	5
2.5	Fuse ring	5
2.6	Spiro ring	6
2.7	Group	6
2.7.1	Insert group	6
2.7.2	Insert modified group	6
2.7.3	Add group	6
2.7.4	Add modified group	6
2.8	Chain environment	7
2.8.1	Horizontal,vertical	7
2.8.2	Left-right,right-left	7
2.8.3	Rotate fixed angle	7
2.8.4	Rotate multiple angle	7
2.9	Miscellaneous	7
2.9.1	Abbreviated parts	7
2.9.2	Define group,parts	7
2.9.3	Concatenate group,parts	7
2.9.4	Move position [@]	7
2.9.5	Serial number	8
2.9.6	Change color	8
2.9.7	Change font	8
3	Option parameter	8
3.1	Angle parameter	8
3.2	Size/Ratio parameter	8
3.2.1	Bond length [=]	8
3.2.2	Molecular size	8
3.2.3	Molecular position	8
3.3	Size parameter	9
3.3.1	Figure size [#]	9
3.3.2	Figure margin [#@]	9
3.3.3	Offset thickness of bond	9
3.3.4	Offset of double bond gap	9
3.3.5	Offset of atom width	9
3.3.6	Offset of wedge width	9
3.3.7	Max bond length [<]	9
3.4	Ratio parameter	9
3.4.1	Thickness/bond length	9
3.4.2	Atom/bond length	9
3.4.3	Char thickness/Atom width	9
3.4.4	Bond gap/bond length	9
3.4.5	Wedge/bond length	9
3.4.6	Figure atom gap/atom length	9
3.4.7	Chain/ring length	9
3.4.8	Hash gap/bond length	9
3.5	Drawing mode	10
3.5.1	Numbering atom,bond	10
3.5.2	Trimming mode	10
3.5.3	Omit group	10
3.5.4	Omit bond type	10
3.6	Frame	10
3.6.1	Figure frame	10
3.6.2	Molecular frame	10
3.6.3	Atom frame	10
3.7	Parameter setting	10
3.7.1	Local parameter setting	10
3.7.2	Global parameter setting	11
4	Command of mcf2graph	11
4.1	drawm	11
4.2	readm	11
4.3	getm	11
4.4	putm	11
4.5	allm	11
4.6	add [++]	12
4.7	ext [**]	13
4.7.1	Local ext setting	13
4.7.2	Global ext setting	13
5	Example	14
5.1	drawm example	14
5.2	readm example	14
5.3	loadm example	16
5.4	getm example	17
5.5	User define parts example	19
6	Example to use mcf2graph	20
6.1	MetaPost source file	20
6.2	Molecular library file	21
6.3	MCF aux file output	22
6.4	Report output	23
6.5	MOL file output	24
6.6	LuaTeX file example	25

1 Introduction

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

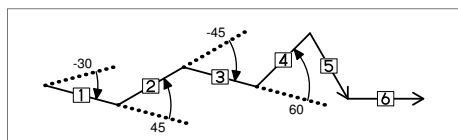
2 MCF syntax

2.1 Make bond

2.1.1 Chain

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

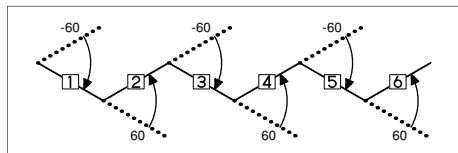
<10,-30,45,-45,60,\$300,\$0



2.1.2 Chain with !,n

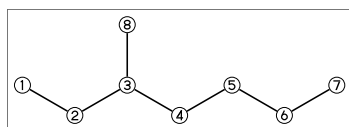
! : take value 60 or -60 depend on current angle
!6 : !,!,!,!,!,!

<-30,!6



take value 0 just after jump to atom @n,! : !=0

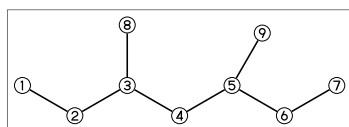
<-30,!5,@3,!



2.1.3 Jump to atom

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

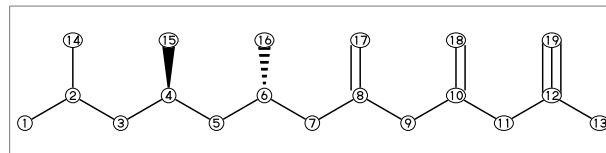
<-30,!6,@3,0,@5,-30



2.1.4 Branch bond

@n,! : @n,!
@n,!w : @n,!~wf
@n,!z : @n,!~zf
@n,!d : @n,!~db
@n,!dr : @n,!~dr
@n,!t : @n,!~tm

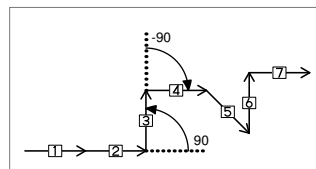
<30,!12,
@2,!,@4,!w,@6,!z,@8,!d,@10,!dr,@12,!t



2.1.5 Rotate current angle

<angle : rotate current angle

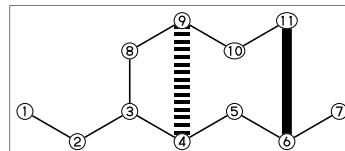
0,0,<90,0,<-90,0,<\$315,0,<\$90,0,<\$0,0



2.1.6 Connect atom

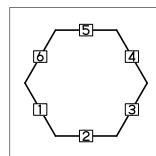
&n : Connect to An

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



2.1.7 Ring

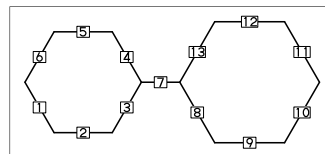
?n : n membered ring(3<=n<=20)
?6



2.1.8 Ring length

?n`length : change ring length

?6,@4,! ,?6`1.2



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

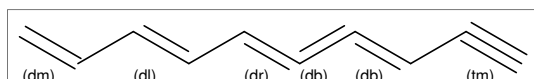
db : double left or right side

tm : triple

!db, !d : !~db / !tm, !t : !~tm

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

<-30, !dm, !, !dl, !, !dr, !d, !d, !, !t



(Wedge, Vector)

wf: wedge forward

wb: wedge backward

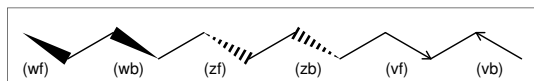
zf: hashed(zebra stripe) wedge forward

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

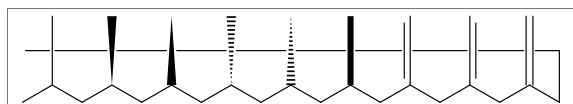
dr_ : double right over line

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)

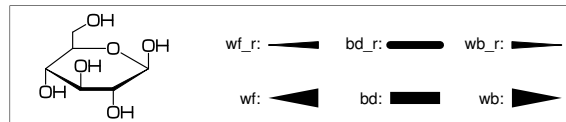
bd_r : broad (half width, rounded)

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,

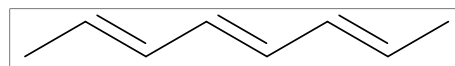
1~\$270'2~\$90'3~\$270'4~\$90: / OH,



2.2.4 Change multiple bond type

2'4'6=d1 or 2'4'6=d1 : 2=d1, 4=d1, 6=d1

<30, !7, 2'4'6=d1 or <30, !7, 2'4'6=d1

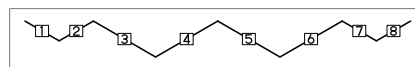


2.3 Change bond length

2.3.1 Change chain length

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

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

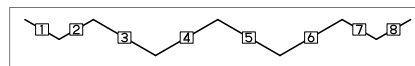


2.3.2 Change multiple bond length

#n : bond length=n

: reset bond length

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

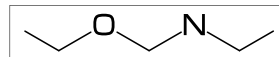


2.4 Change atom

2.4.1 Insert atom

Insert hetero atom

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

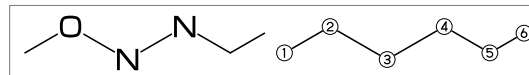


2.4.2 Change atom

2:0 : change A2 C to O

3'4:N : change A3, A4 C to N

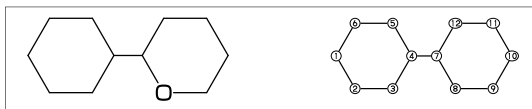
<30, !4, 2:0, 3'4:N



2.4.3 Brock address

| : divide brock

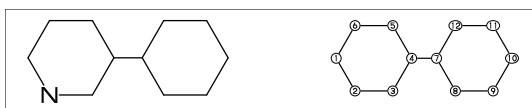
?6,@4,! ,| ,?6,2:0



2.4.4 Reset brock address

|| : reset brock address

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

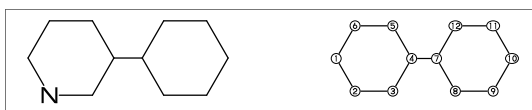


2.4.5 Absolute address

\$2:n : change A\$2 C to N

**1<=n<=3095

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

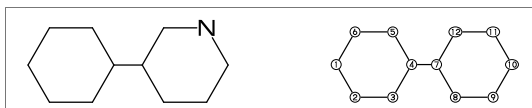


2.4.6 Relative address

-2:n : change A(-2) C to N

** -999<=n<=-1

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



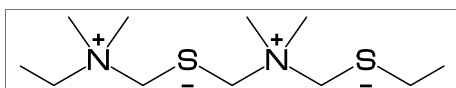
2.4.7 Charged atom

p_ : positive

n_ : negative

<-30,!2,N,??,p_ ,!2,S,n_ ^180,

!6,7:N,7:??,9:S,7:n_ ,9:n_ ^180



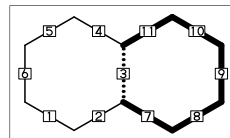
2.5 Fuse ring

(Attached 1 bond)

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

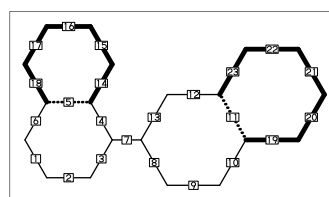
** Bn(n:-999<=n<=4095): bond number

?6,3=?6



** fused ring size depend on attached bond length

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

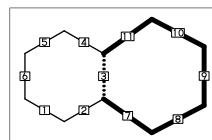


?6,3=#1.3'?6 : fuse #1.3'?6 at B3

#1.3'?6 : 6 membered ring scaled 1.3

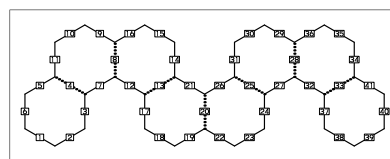
** #n'?m (5<=m<=6,1.1<=n<=1.5)

?6,3=#1.3'?6



?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

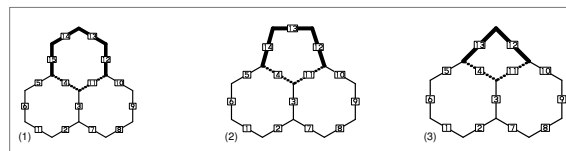
4--11=?5 : fuse 3/5 ring to B11..B4

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

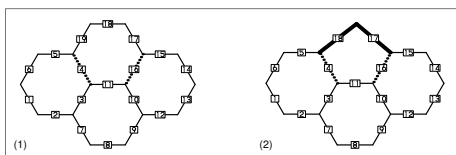
3:<30,?6,3=?6,11--4=?4



(Attached 3 bond)

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

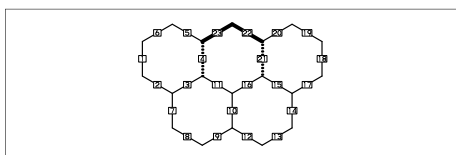
1:?6,3'10'16---4=?6
2:?6,3'10=?6,16---4=?5



(Attached 4 bond)

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

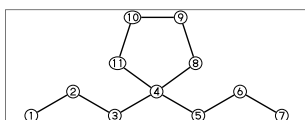
<-30,?6,3'10'15'(21----4)=?6



2.6 Spiro ring

@4,?5 : add ?5 at A4

<30,!6,@4,?5

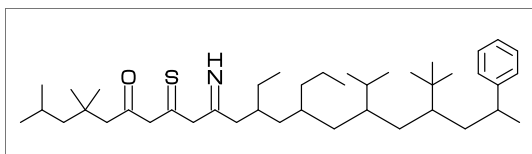


2.7 Group

2.7.1 Insert group

? : methyl
?? : dimethyl
?0 : carbonyl
?S : thioketone
?NH : imino
/! : ethyl
/!2 : propyl
/?! : isopropyl
/??! : tert-butyl
/Ph : phenyl

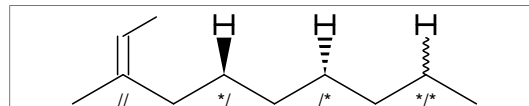
<30,!?,!2,??,!2,?0,!2,?S,!2,
?NH,!2,/!,!2,/!2,!2`1,/?!,!2`1,
/??!,!2`1,/#.6'Ph,!



2.7.2 Insert modified group

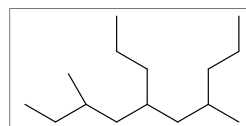
// : double (double middle)
*/ : wedge forward
/* : hashed wedge forward
** : wave

<30,!//!,!2,*H,!2,*H,!2,*H,!



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

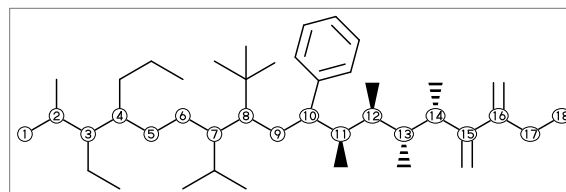
<-30,#1,!,
?`2^30,!2,/!2>lr,!2,/!2>rl,!



2.7.3 Add group

?w : ?~wf
?z : ?~zf
?d : ?~dm

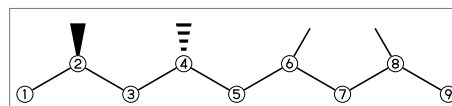
<30,!17,2:?,3:/!,4:/!2,7:/?!,
8:/??!,10^-15:/#.6'Ph,
11'12':?w,13'14':?z,15'16':?d



2.7.4 Add modified group

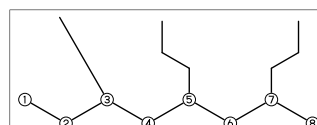
~,^,` : change type,angle,length

<30,!6,2~wf'4~zf'6^-30'8^\$120:?



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

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

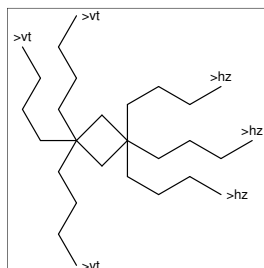


2.8 Chain environment

2.8.1 Horizontal,vertical

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

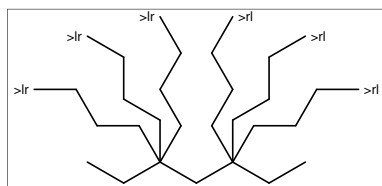
```
?4,  
3^-90'3^-30'3^90:/!3>hz,  
1^-60'1'1^60:/!3>vt
```



2.8.2 Left-right,right-left

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

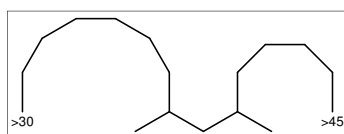
```
<-30,!6,  
3^-30'3'3^30:/!3>lr,
```



2.8.3 Rotate fixed angle

>n : rotate n

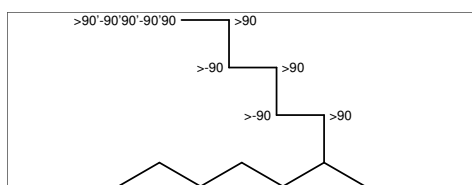
```
<30,!4,  
2:/!6>30, % 2:\,30,30,30,30,30,30  
4:/!4>-45 % 4:\,-45,-45,-45,-45
```



2.8.4 Rotate multiple angle

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

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

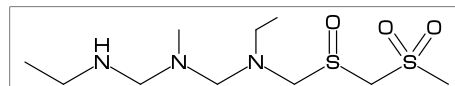


2.9 Miscellaneous

2.9.1 Abbreviated parts

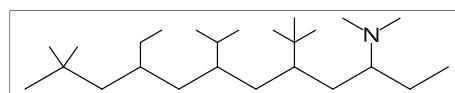
```
NH : N,/H~n1 N? : N,  
N?2 : N,/! S?0 : S,?  
S?0?0 : S,?0^35,/^~35
```

```
<-30,!2,NH,!2,N?,!2,N?2,S?0,!2,S?0?0,!
```



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

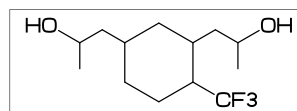
```
<30,!11^1,2:??,4:/!,6:/?!,8:/??!,10:/N?!
```



2.9.2 Define group,parts

```
^(..) : define group  
^(..)(..) : define group with atoms  
'^(..) : define parts
```

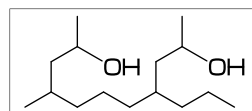
```
CF3:=`("{CF3}") ; % ** group weight =0  
CF3:=`^("{CF3}") (C,F,F,F) ;  
** group weight =12(C)+19(F)*3=69  
iBuOH:=`'(!?! ,OH) ;  
drawm("<30,?6,4'6:/iBuOH,3:/CF3")
```



2.9.3 Concatenate group,parts

a'b : '(a,b)

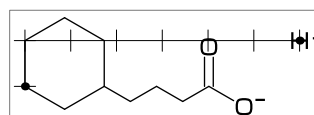
```
<30,!8,2'6:/!?!'OH
```



2.9.4 Move position [@]

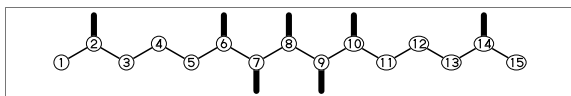
```
@(x'y) : Move l*(x,y) from current position  
@$(x'y) : Move l*(x,y) from origin(@1)  
** l=bond length of ring
```

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

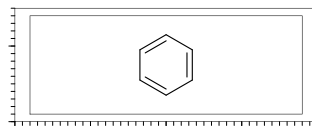


2.9.5 Serial number

```
6_10 : 6,7,8,9,10  
<30,!14,2'6_10'14:~bd_r`0.5
```

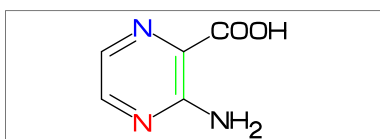


```
(ratio bond/figure width)  
blength=0.1 ** (0<blength<=1)  
blength=60mm(width)*0.1=6mm
```

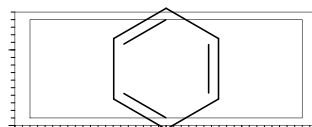


2.9.6 Change color

```
beginfigm  
  drawm("<30,Ph,2'5:N,3:/NH2,4:/COOH,"&  
        "2:red,5:blue,3=green");  
endfigm
```

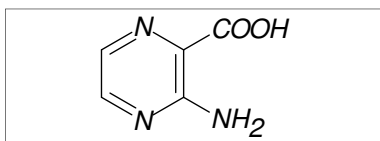


```
(bond length)  
blength=9mm  
** (blength>1) ignore msize(w,h)
```



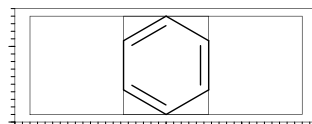
2.9.7 Change font

```
beginfigm  
  %-----  
  atomfont:="phvro8g";  
  %-----  
  drawm("<30,Ph,2'5:N,3:/NH2,4:/COOH");  
endfigm
```

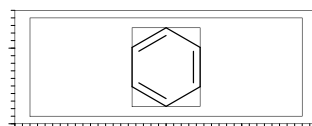


3.2.2 Molecular size

```
##(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
```

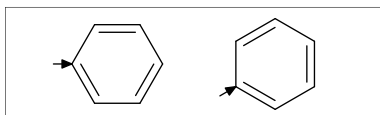


3 Option parameter

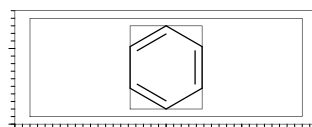
3.1 Angle parameter

```
mangle=0 ** default
```

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



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

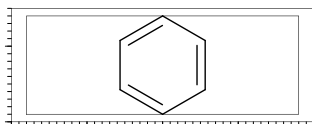


3.2 Size/Ratio parameter

3.2.1 Bond length [|=]

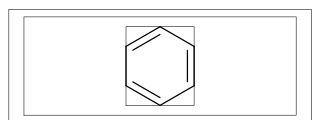
```
|=(n) : abbreviated form of blength:=n;
```

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

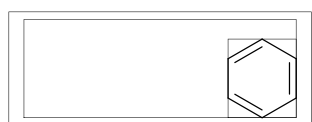


3.2.3 Molecular position

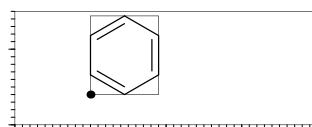
```
@(0.5,0.5) : mposition=(0.5,0.5) **default
```



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



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

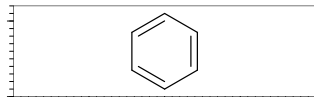


3.3 Size parameter

3.3.1 Figure size [#]

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

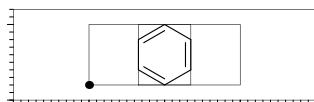
#(40mm,15mm) : fsize=(40mm,15mm)



3.3.2 Figure margin [#@]

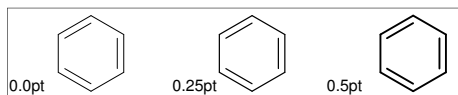
fmargin=(margin left right,top bottom)
** default: (0.4mm,0.4mm)
#@ p : abbreviated form of fmargin:=p;

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



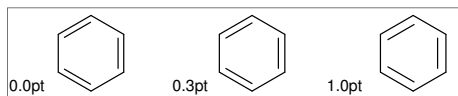
3.3.3 Offset thickness of bond

default: offset_thickness=0.25pt



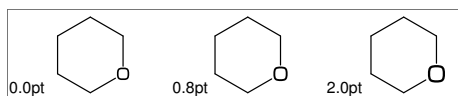
3.3.4 Offset of double bond gap

default: offset_bond_gap=0.3pt



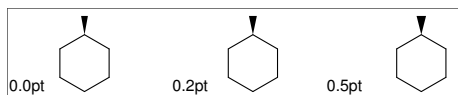
3.3.5 Offset of atom width

default: offset_atom=0.8pt



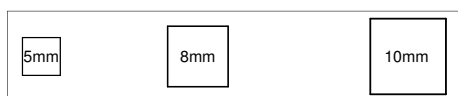
3.3.6 Offset of wedge width

default: offset_wedge=0.2pt



3.3.7 Max bond length [|<]

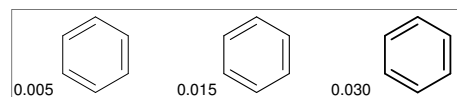
|<(n): abbreviated form of max_blength:=n;
default: max_blength=10mm



3.4 Ratio parameter

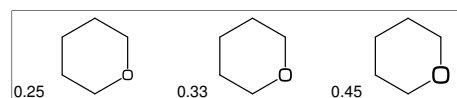
3.4.1 Thickness/bond length

default: ratio_thickness_bond=0.012



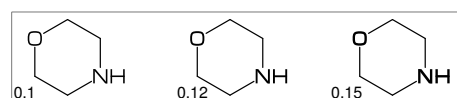
3.4.2 Atom/bond length

default: ratio_atom_bond= 0.36



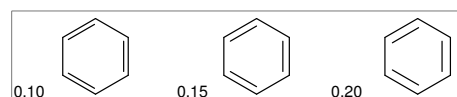
3.4.3 Char thickness/Atom width

default: ratio_char_atom=0.12



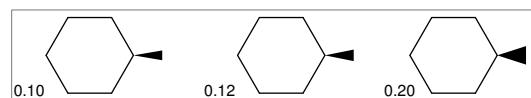
3.4.4 Bond gap/bond length

default: ratio_bondgap_bond= 0.15



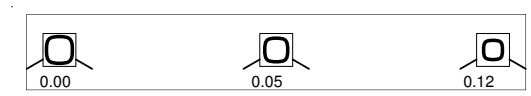
3.4.5 Wedge/bond length

default: ratio_wedge_bond=0.12



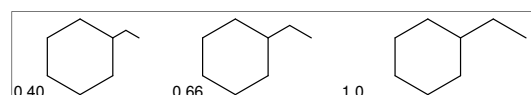
3.4.6 Figure atom gap/atom length

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

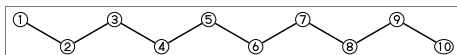
default: ratio_hashgap_bond=0.12



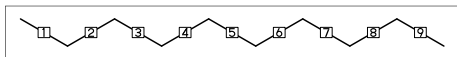
3.5 Drawing mode

3.5.1 Numbering atom,bond

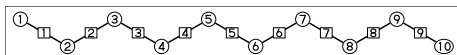
```
sw_numbering:=Atom;
```



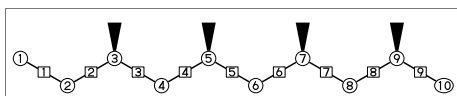
```
sw_numbering:=Bond;
```



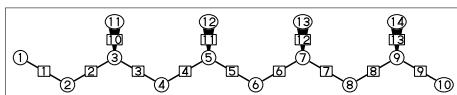
```
sw_numbering:=Atom+Bond;
```



```
sw_numbering:=Atom+Bond;
```

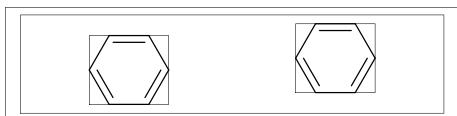


```
sw_numbering:=Atom+Bond+All;
```



3.5.2 Trimming mode

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



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



3.5.3 Omit group

```
** default: sw_omit=Group
```



3.5.4 Omit bond type

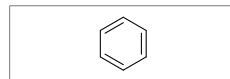
```
** default: sw_omit=Bond
```



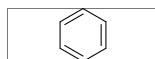
3.6 Frame

3.6.1 Figure frame

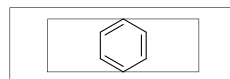
```
** default:sw_frame=0  
(Draw figure frame)  
fmargin:=(5mm,2mm);  
sw_frame=Outside
```



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

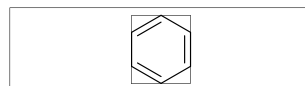


```
(Draw both frame)  
sw_frame=Bothside=Inside+Outside
```



3.6.2 Molecular frame

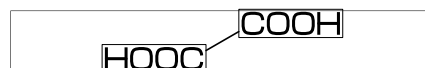
```
sw_frame=Mol  
** default:sw_frame=0
```



3.6.3 Atom frame

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

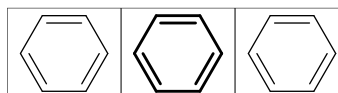
```
drawm("<30,COOH,!,COOH");
```



3.7 Parameter setting

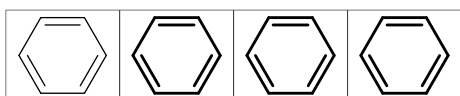
3.7.1 Local parameter setting

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



3.7.2 Global parameter setting

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



4 Command of mcf2graph

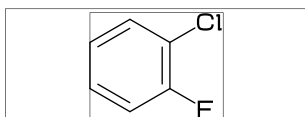
4.1 drawm

(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

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

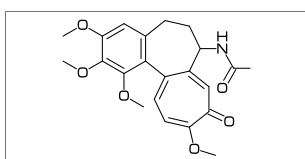


4.2 readm

```
readm(string1,string2, ...);
** string = mcf code
```

(example)

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



4.3 getm

```
getm(number)
** number = numeric
** ucount = molecular data unit count

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

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

(example)

```
beginfigm
  getm("Adenine");
  putm;
endfigm
```

4.4 putm

putm : put figure

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

4.5 allm

allm : put all loaded molecule

```
for i=1 upto ucount:
  beginfigm getm(i); putm; endfigm
endfor
```

4.6 add [++]

(Add label to molecule)

++(): add()

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

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

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

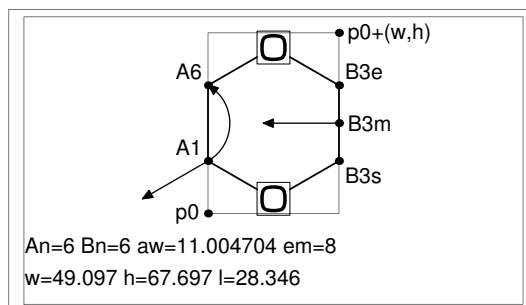
plus : '+' circled
minus : '-' circled
circlediam = 0.6aw (default)
circlepen = 0.2bp (default)

lonelapair r: ':' rotated r
lonelapairdiam = 0.3aw (default)
lonelapairspace = 0.7aw (default)

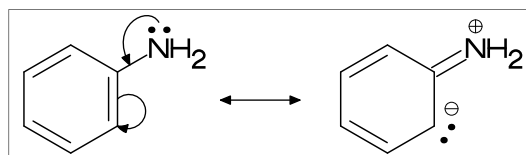
: scaled
<< : rotated
a /* b : point b of a

```
beginfigm
#(70mm,40mm) ##(.91,.9) |<(10mm)
sw_frame:=sw_frame+Atom+Mol;
@(.5,.85) drawm("<30,?6,2'5:0");
++(
defaultscale:=.8;
labeloffset:=.3aw;
dotlabel.lft("p0",p0);
dotlabel.rtl("p0+(w,h)",p0+(w,h));
dotlabel.ulft("A1",A1);
drawarrow A1..A1+__*l<<A1ang;
dotlabel.lrt("B3s",B3s);
dotlabel.rtl("B3m",B3m);
drawarrow B3m..B3m+__*l<<(B3ang+90);
dotlabel.ulft("A6",A6);
drawarrow A1{A1down}..A6;
```

```
dotlabel.rtl("B3e",B3e);
label.rtl("An"&decimal(An)&
" Bn"&decimal(Bn)&
" aw"&decimal(aw)&
" em"&decimal(em),
p0+(-9em,-1.5em));
label.rtl("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) drawm("<30,Ph,3=d1,4://NH2");
%-----
++(
labeloffset:=.7aw;
label.top(lonelapair 90,A7);
drawarrow
(A7+up#1.2aw){A7left}
..{B7right}B7/*0.3;
drawarrow
B3m..A3+B2up#1.5aw..{A3down}A3;
)
%-----
@ (1,0) drawm("<30,?6,1'5=d1,4://NH2");
%-----
++(
labeloffset:=.7aw;
label.top(plus,A7);
label.rtl(minus,A3);
label(lonelapair A3ang,A3+A3up#.7aw);
)
%-----
** (drawdblarrow (.4w,.4h)..(.55w,.4h));
%-----
endfigm
```



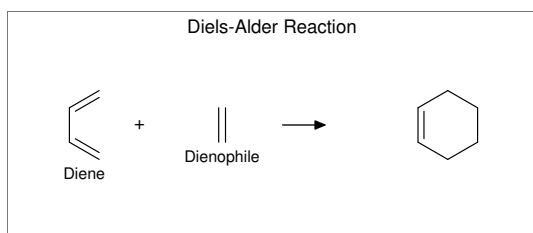
4.7 ext [**]

(Extra label to figure)

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

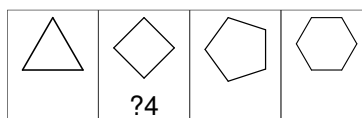
n:   molecular number
p[m]: molecular origin position
w[m]: molecular width
h[m]: molecular height

ratio_thickness_char:
pen thickness / char width
%-----
beginfigm
#(70mm,30mm)
|= (0.065)
%-----
@(0.1,0.5)
drawm("<-210,60`1,60`1,60`1,1'3=d1")
++(
  defaultscale:=0.6;
  label.bot("Diene",p0+(0.5w,0));
)
@(0.4,0.5)
drawm("<-30,-60`1,1=dm");
++(
  defaultscale:=0.6;
  label.bot("Dienophile",p0+(.5w,0));
)
@(0.9,0.5) drawm("<30,?6,6=d1");
%-----
**(
  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

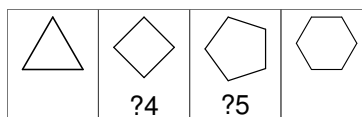
```
beginfigm
EN:="?3";@(0.5,1) drawm("<30,?3");
endfigm
beginfigm
EN:="?4";@(0.5,1) drawm("<?4");
%-----
**(label.top(EN,(0.5w,0));)
%-----
endfigm
beginfigm
EN:="?5";@(0.5,1) drawm("<?5");
endfigm
beginfigm
EN:="?6";@(0.5,1) drawm("<?6");
endfigm
```



4.7.2 Global ext setting

```
ext_clear: reset global ext()

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

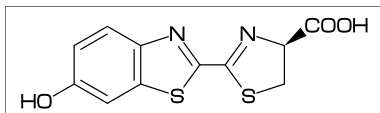


5 Example

5.1 drawm example

(Luciferin)

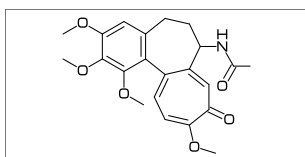
```
beginfigm
  #(50mm,15mm)
  drawm("<30,Ph,3=?5,@8,! ,?5,9'16=d1,"&
        "9'14:N,7'11:S,1:/OH,-2:*/COOH")
endfigm
```



5.2 readm example

(Colchicine)

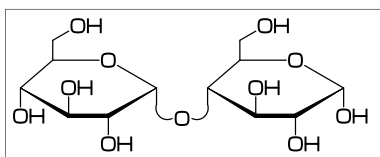
```
beginfigm
  readm(
    "<30,Ph,1'2'6:/O!, -4'-5=?7,      ",
    " -1'-4'-6=d1, -2:?0, -3:/O!,    ",
    " 9:/NH!'?0!                       ")
  #(40mm,20mm) putm;
endfigm
```



(Maltose)

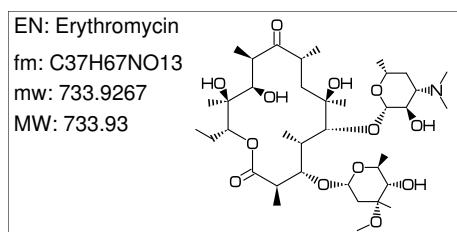
(bond type for glycan)
arc_lb : arc left > bottom
arc_br : arc bottom right

```
beginfigm
  %"EN:Maltose", "MW:342.3",
  readm(
    %-----
    "hexose_hp, #.5, 1~$270'2~$90'3~$270:/OH, 6~$90:/!OH, ##, ",
    "@4, $310~arc_lb`1, 0, $50~arc_br`1, <$0, ",
    "|, hexose_hp, #.5, 2~$90'3~$270'4~$270:/OH, 6~$90:/!OH  ")
    %-----
  #(50mm,20mm) putm
endfigm
```



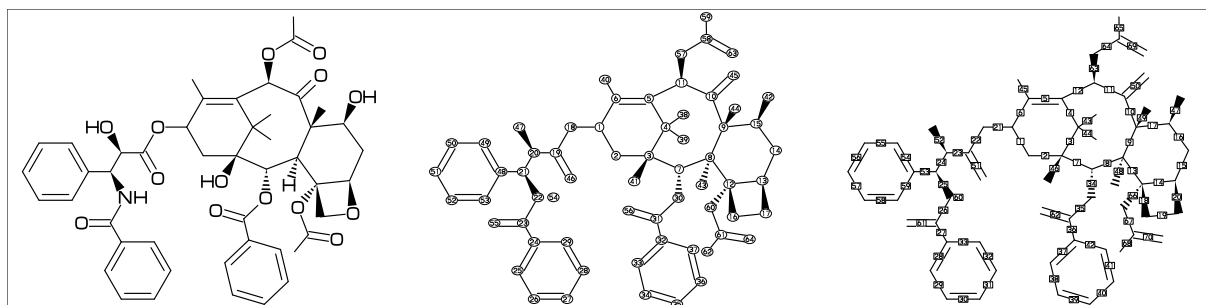
(Erythromycin)

```
beginfigm
EN:=Erythromycin"; MW="733.93";
#(60mm,30mm) @(1,0.5)
readm(
%-----
"<30,#1,<-120,60,60,60,-60,60,60,-60,60,60,60,-60,60,60,##,&1,      ",
" 14:0,13:/*!,1'9:?0,                                                ",
" *2'4'6^-35'8'*10'12^35:?z,                                          ",
" 6^35'11'12^-35:*/OH,                                                ",
" @$3,!z,0,30~zb,|,?6`.7,6:0,#.5,5~wf'3^35:?,4:/*OH,3^-35:/*0!,##,  ",
" @$5,!z^30`1.7,0,!~zb,|,?6`.7,6:0,#.5,5:?z,2:*/OH,3:/*N?!      ")
%-----
putm;
**(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:?w^60,10:?0,                    ",
" @1,! ,0,! ,?0,! ,*/OH,! ,/Ph,60~wf,NH,-60,?0,60,Ph,                ",
" @7,!z,0,-45,?0,60,Ph,11>r1'*12^-15>lr:*/O!'?0!                    ")
%-----
#(140mm,30mm)
@(0,0.5) putm;
sw_numbering:=Atom+All;
@(0.6,0.5) putm;
sw_numbering:=Bond+All;
@(1,0.5) putm;
endfigm
```



5.3 loadm example

(Example)

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

(output)

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

row[1][1]="CAT:biological;EN:Luteolin;MW:286.24;EXA:-"
row[1][2]=":"
row[1][3]="<30,Ph,3=?6,9=dl,10:0,7:?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=dl,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=dl,6:/OH,8^180:*/H,12:/*OH"
row[3][5]=";"
row[4][1]="CAT:biological;EN:Piperine;MW:285.343;EXA:1"
row[4][2]=":"
row[4][3]="<30,Ph,-1=?5,-1'-3:0,@4,!,!d,!,!d,!,?0,!,?6,-6:N"
row[4][4]=";"
%-----
```

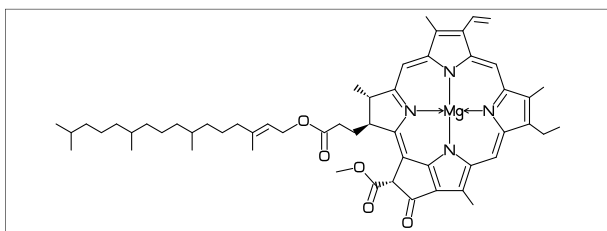
(Tag)

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

5.4 getm example

(Chlorophyll a)

```
beginfigm
  getm("Chlorophyll a")
  sw_output:=Fig+Mcode;
  #(80mm,30mm)
  putm
  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}%
```

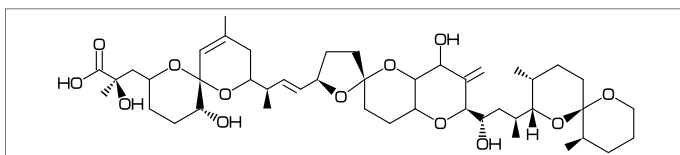


```
<-36,?5,@3,!`1,54`1,?5,@-2,!`1,54`1,?5,
@-2,!`1,54`1,?5,@-2,!`1,&5,@6,22`1,70`1,&8,
4'6'8'10'14'16'18'21'23'27=d1,@4,!`1.48~vf,Mg,&17~vb,@11,&27,@27,&23,
4'11'17'23:N,1~zf'9'15'21:?,14:/!,20:/!d,25:/*?0!'0!,26:?0,
@2,-6~wf,!2,?0!,0!2,!d,|,!13,1'5'9'13:?
```

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

(Dinophysistoxin-1)

```
beginfigm
  getm("Okadaic acid")
  readm(",38:?w,65=red")          %%% add methyl group (color red) %%%
  sw_output:=Fig+Mcode;          %%% output temp-mc.aux %%%
  EN:="Dinophysistoxin-1"; #(90mm,20mm)
  MW:="819";
  putm;
  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}%
```

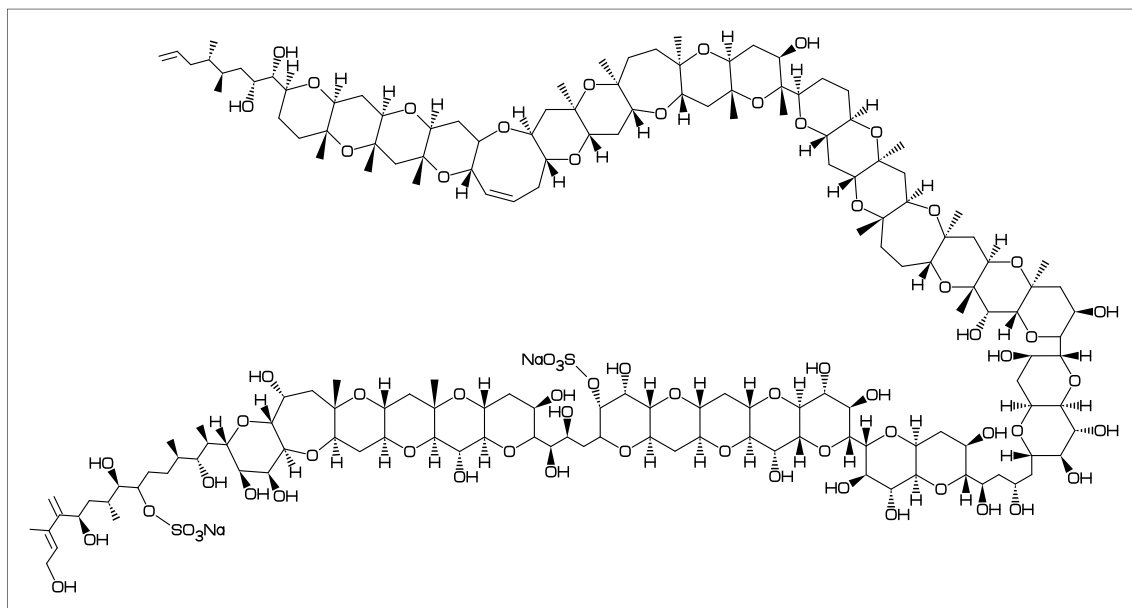


```
<30,?6,@4,?6,@-4,!4,<-12,?5,@-3,<-12,?6,-3=?6,@-3,!w,!3,
?6,@-4,?6,@6,!2,?z^-40,*/OH^20,!?0!,OH,
3'38=wb,11=d1,15=dr,17'19=wf,5'7'16'24'25'33'42:0,
32:*/H^60,10:?,12'31'*37:?w,27:?d,28:/OH,3'29:/*OH,
38:?w,65=red
```

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

(Maitotoxin)

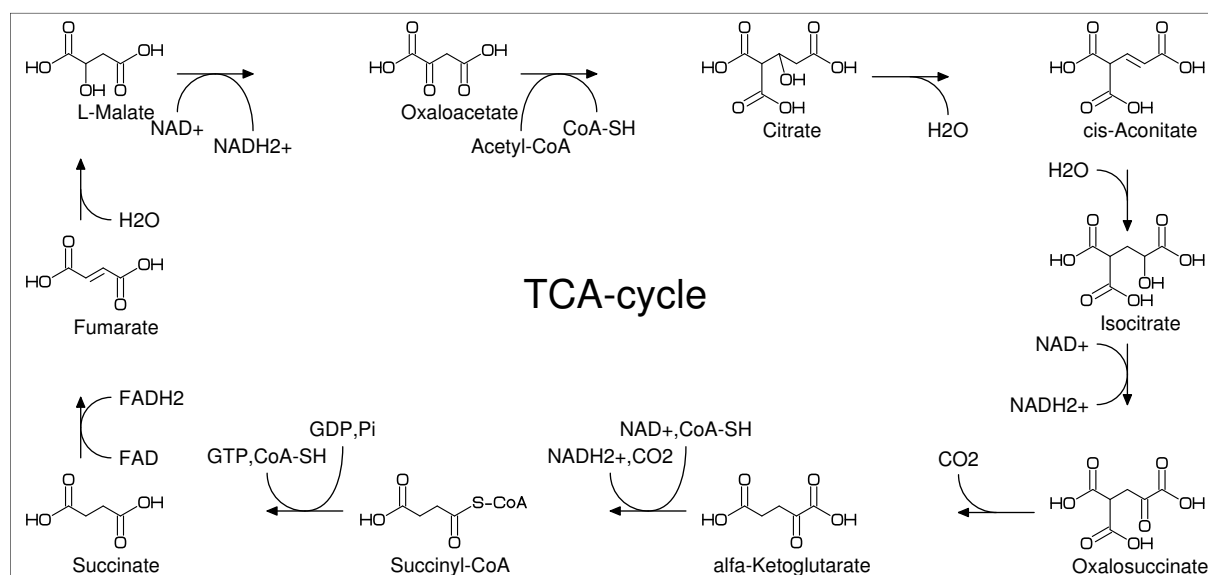
```
%-----  
\begin{mplibcode}  
  beginfigm  
    getm("Maitotoxin") #(150mm,80mm) #@ (3mm,3mm)  
    sw_output:=Fig+Mcode;          %%% output temp-mc.aux %%%  
    sw_frame:=Outside;  
    putm;  
    VerbatimTeX("\gdef\EN{"&EN&"}\gdef\MW{"&MW&"}");  
    VerbatimTeX("\gdef\mw{"&mw&"}\gdef\fm{"&fm&"}");  
  endfigm  
\end{mplibcode}  
\verbatiminput{temp-mc.aux}          %%% input temp-mc.aux %%%  
{\tt ** EN:\EN \quad mw:\MW \quad MW:\mw \quad fm:\fm}%  
%-----
```



```
<55.8,?6,-4=?7,-4'-3'-3'-3=?6,@-3,!4,?6,-4'-3'-3'-3=?6,@-3,! ,?6,-3=?6,  
@-3,!4,60,<-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:?w^60^1,80'88'97'*108'115'120'124:?z^-60^1,  
@$6,! ,| ,!11,60~dr,-60,60,OH,*2'7'10:*/OH,1'3'*8:?w,11:?d,12:?,@6,!0,30,S03Na,  
@$36,-45~zf,0,30,S03Na,  
@$150,! ,| ,!7,1'2:*/OH,4:?w,5:?z,7=d1
```

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

5.5 User define parts example



```

beginfigm
#(160mm,75mm) |<(4mm)
COOH:=''(?0,! ,OH); % define COOH
HOCO:=''(OH,! ,?0,); % define HOCO
S_CoA:=''({S-CoA}); % define S_CoA
@(0.33, 1) drawm("<30,HOCO,! ,?0,!2,COOH") % Oxaloacetate
@(0.66, 1) drawm("<30,HOCO,!4,COOH,@-4`1,! ,COOH,4:/OH^-165") % Citrate
@(1, 1) drawm("<30,HOCO,!2,!~dr,! ,COOH,@-4`1,! ,COOH") % cis-Aconitate
@(1, 0.58) drawm("<30,HOCO,!4,COOH,@-4,!`1,COOH,5:/OH") % Isocitrate
@(1, 0.05) drawm("<30,HOCO,!3,?0,! ,COOH,@-4,!`1,COOH") % Oxalosuccinate
@(0.66,0.05) drawm("<30,HOCO,!3,?0,! ,COOH") % alfa-Ketoglutarate
@(0.33,0.05) drawm("<30,HOCO,!3,?0,! ,S_CoA") % Succinyl-CoA
@(0, 0.05) drawm("<30,HOCO,!3,COOH") % Succinate
@(0, 0.55) drawm("<30,HOCO,! ,!~dr,! ,COOH") % Fumarate
@(0, 1) drawm("<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,-0.6h3))("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:=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  
  drawm("<45,?4,-3=?5,2:N,7:S,"&  
    "3^45:/*H,1:?0^15,5:/*COOH^-18,6:??,"&  
    "@4,!w^15,NH,! ,?0,! ,/*NH2,! ,Ph") > immediately compile  
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:?w^60, ", > mc3  
    "@-1,18,?z,-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=dl,2'6'9:N,5:/NH2,7:NH
*
  defaultscale:=.5;
  label.bot(decimal(fig_num)&" "&EN,(.5w,0));
+
  defaultscale:=.3;
  label.bot("A2",A2) withcolor red;
  label.top("A6",A6) withcolor red;
  label.top("A9",A9) withcolor red;
;
%=====
CAT:biological;EN:Adenine;MW:135.13;EXA:1
:
<30,?6,3=?5,1'3'5'9=dl,2'6'9:N,5:/NH2,7:NH
;
%-----
CAT:biological;EN:Guanine;MW:151.13;EXA:1
:
<30,?6,3=?5,1'3'9=dl,2'9:N,6'7:NH,5:?0,1:/NH2
;
%-----
CAT:biological;EN:Cytosine;MW:111.10;EXA:1
:
<30,?6,4'6=dl,4:N,3:?0,2:NH,5:/NH2
;
%-----
CAT:biological;EN:Thymine;MW:126.11;EXA:1
:
<30,?6,3=dl,2'6:NH,1'5:?0,4:?
;
%-----
CAT:biological;EN:Uracil;MW:112.09;EXA:1
:
<30,?6,6=dl,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 ahlengh=3 FILENAME (sw_output=Fig Expand mode)
```

(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
```

(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,!w,!3,  
?6,@-4,?6,@6,!,!,?z^-40,*OH^20,!,?0,!1,OH,  
3=wb,11=d1,15=dr,17'19=wf,38=wb,5'7'16'24'25'33'42:0,  
32:*/H^60,10:?,12'31:?w,27:?d,37:?z,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[148],Name<Phenol>,Category<synthetic>,File<main_lib.mcf>
-----
Row[1],Length[12],Block[3],BackboneA[6],BackboneB[6],Group[1]
-----
<30,Ph,3:/OH
-----
[1 ] <30
[2 ] Ph
[3 ] 3:/OH
-----
Width[35.80607],Height[24.55503], Shift x[-1.77635],Shift y[-7.54719]
Bond length[11.33855],Atom size[4.881881]
-----
Atom[7],Bond[7],Ring[1],Hide H[5]
< NO. ><atom(s) >( x axis , y axis )<bond><hideH><chg>
A1 C ( 0 , 0 ) 3 1
A2 C ( 1 , -1 ) 3 1
A3 C ( 2 , 0 ) 4
A4 C ( 2 , 1 ) 3 1
A5 C ( 1 , 1 ) 3 1
A6 C ( 0 , 1 ) 3 1
A7 OH ( 3 , 0 ) 1
-----
< NO. >< bond (sdt)><angle +( +- )><length ( pt )>
B1 1 -> 2 ( 2) 330 ( -30) 1 ( 11)
B2 2 -> 3 ( 1) 30 ( 30) 1 ( 11)
B3 3 -> 4 ( 2) 90 ( 90) 1 ( 11)
B4 4 -> 5 ( 1) 150 ( 150) 1 ( 11)
B5 5 -> 6 ( 2) 210 ( -150) 1 ( 11)
B6 6 -> 1 ( 1) 270 ( -90) 1 ( 11)
B7 3 -> 7 ( 1) 330 ( -30)0.660000 ( 7)
-----
<atom>( atom wt ) [ mi wt ] < cnt > < sum wt > [ sum mi wt ]
C ( 12.0107) [ 12 ] * 6 72.0642 [ 72 ]
H ( 1.0079400) [ 1.0078250 ] * 6 6.04764 [ 6.0469501933 ]
O ( 15.9994) [ 15.994914 ] * 1 15.9994 [ 15.994914619 ]
Molecular Weight [Mono Isotopic] = 94.11123 [ 94.0418648 ]
-----
Weight Calc: 94.11123 - Input: 94.11 = 0.0012399
Fomula Calc: C6H6O
=====
```

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)
    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,!z,|,?5,1'4=d1,3:0        ")
      %-----
    putm
  endfigm
\end{mplibcode}\\
%-----
\begin{mplibcode}
  EN:="beta-carotene";
  MW:="536.87";
  beginfigm
    #(80mm,50mm)
    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}
```

Index

!, 3
!d, 3, 4
!db, 4
!dl, 4
!dm, 4
!dr, 4
!t, 4
!tm, 4
!w, 3
!z, 3
' , 7
**, 12, 13
*/ , 6
*/ * , 6
++ , 12
-- , 5
--- , 5
---- , 6
/ , 6
/* , 6, 12
// , 6
: , 4
? , 6
?! , 7
?? , 6, 7

dt, 4
 em, 12, 13
 endfigm, 10
 ethyl, 6
 ext, 13
 ext_clear, 13
 Fig, 25
 fmargin, 9
 fsize, 9
 getm, 11
 getm(), 20
 green, 8
 Group, 10
 h, 12
 h0, 13
 hashed wedge, 6
 hz, 7
 imino, 6
 Inside, 10
 isopropyl, 6
 l, 12
 labeloffset, 12
 loadm(), 16
 lonepair, 12
 lonepairdiam, 12
 lonepairspace, 12
 lr, 7
 mangle, 8
 max_blength, 9
 mcf2graph.mp, 20
 Mcode, 22
 methyl, 6
 minus, 12
 Mol, 10
 MOL2000, 24
 MOL3000, 24
 mposition, 8
 msize, 8
 n, 13
 N!, 7
 N!2, 7
 N?!, 7
 NH, 7
 offset_atom, 9
 offset_bond_gap, 9
 offset_thickness, 9
 offset_wedge, 9
 Outside, 10
 p0, 12
 Ph, 6
 phenyl, 6
 plus, 12, 20
 propyl, 6
 putm, 11, 20
 ratio_atom_bond, 9
 ratio_atomgap_atom, 9
 ratio_bondgap_bond, 9
 ratio_chain_ring, 9
 ratio_char_atom, 9
 ratio_hashgap_bond, 9
 ratio_thickness_bond, 9
 ratio_thickness_char, 13
 ratio_wedge_bond, 9
 readm, 9
 readm(), 11
 red, 8
 Report, 23
 rl, 7
 S?O, 7
 S?O?O, 7
 si_, 4
 sw_comment, 16
 sw_frame, 10
 sw_numbering, 10
 sw_output, 20, 23, 24
 sw_trimming, 10
 tert-butyl, 6
 thioetone, 6
 tm, 4
 ucount, 11, 20
 vb, 4
 vf, 4
 vt, 7
 w, 12
 w0, 13
 wave, 6
 wb, 4
 wb_, 4
 wb_r, 4
 wedge forward, 6
 wf, 4
 wf_, 4
 wf_r, 4
 wv, 4
 zb, 4
 zb_, 4
 zf, 4
 zf_, 4