

# Molecular Coding Format manual

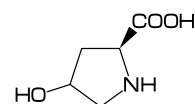
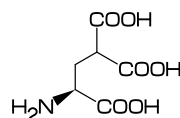
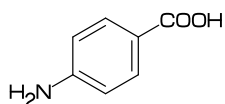
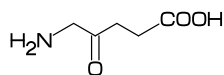
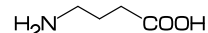
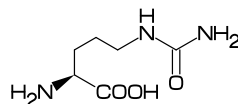
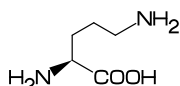
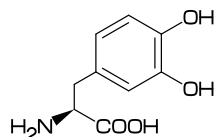
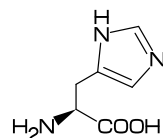
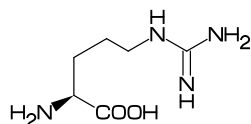
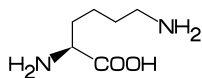
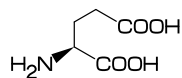
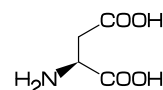
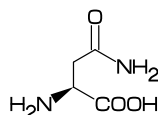
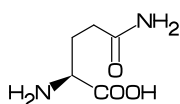
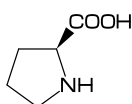
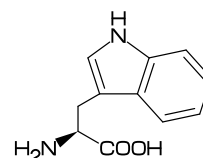
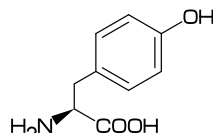
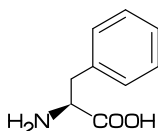
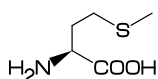
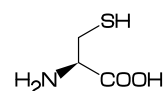
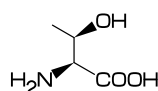
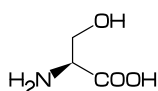
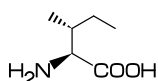
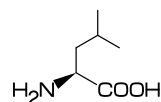
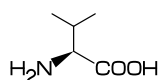
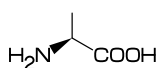
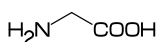
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June 6, 2026

mcf2graph version 5.30

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, MOL file. It is also able to calculate molecular weight, exact mass, molecular formula.

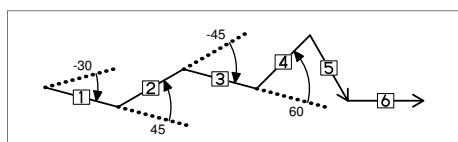
## 2 MCF syntax

### 2.1 Make bond

#### 2.1.1 Chain

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

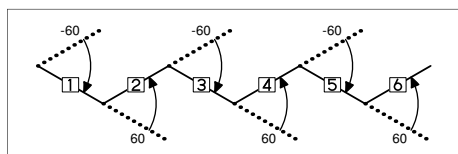
~10,-30,45,-45,60,\$300,\$0



#### 2.1.2 Chain with !,!n

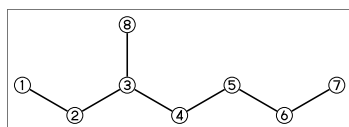
! : take value 60 or -60 depend on current angle  
!6 : !,!,!,!,!,!

~-30,!6



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

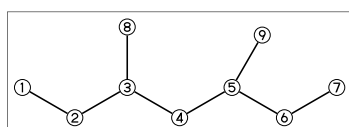
~-30,!5,3:,!



#### 2.1.3 Jump to atom

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

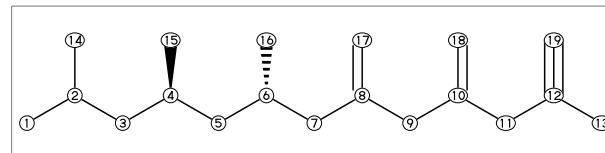
~-30,!6,3:,0,5:,-30



#### 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

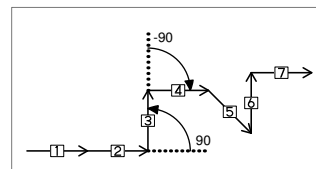
~30,!12,  
2:,!,4:,!w,6:,!z,8:,!d,10:,!dr,12:,!t



#### 2.1.5 Rotate current angle

^angle : rotate current angle

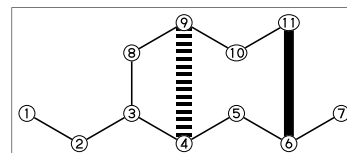
0,0,~90,0,~-90,0,~\$315,0,~\$90,0,~\$0,0



#### 2.1.6 Connect atom

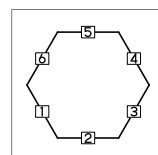
:n : Connect to An

~-30,!6,3:,!,!3,:6~bd,9:,:4~bz



#### 2.1.7 Ring

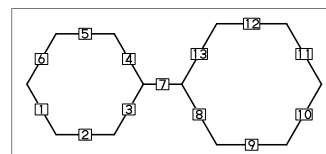
?n : n membered ring(3<=n<=20)  
?6



#### 2.1.8 Ring length

?n`length : change ring length

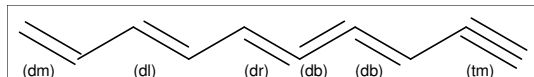
?6,4:,!,?6`1.2



## 2.2 Change bond type

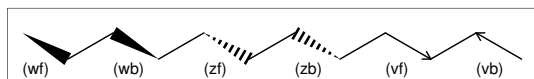
### 2.2.1 Double, triple, wedge, vector

(Double, triple)  
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

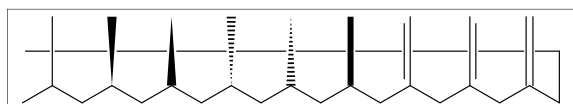
^~30, !7, 1=dt, 3=wv, 5=bd, 7=bz



### 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

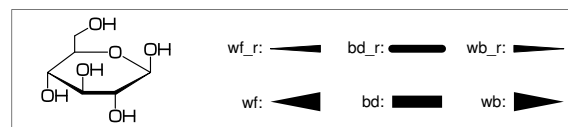
^30, !8, !, 60, 90^18,  
2~si\_'4~wf\_'6~wb\_'8~zf\_'10~zb\_'  
12~bd\_'14~dl\_'16~dr\_'18~dm\_:'?^2



### 2.2.3 Steric ring

wf\_r : wedge forward (half width)  
bd\_r : broad (half width, rounded)  
wb\_r : wedge backward (half width)

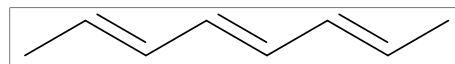
^1.25, -30~wf\_r, 30~bd\_r^1, 30~wb\_r,  
120, 0, 30, :1, ^, ^5, 6^90:/!OH,  
1^\$270'2^\$90'3^\$270'4^\$90:/OH



### 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

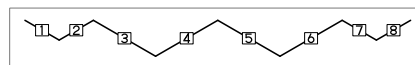


## 2.3 Change bond length

### 2.3.1 Change chain length

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

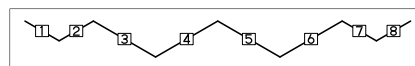
^~30, !2, !4^1.2, !2



### 2.3.2 Change multiple bond length

^n : bond length=n  
^ : reset bond length

^~30, !2, ^1.2, !4, ^, !2

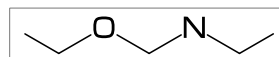


## 2.4 Change atom

### 2.4.1 Insert atom

Insert hetero atom

^~30, !2, 0, !2, N, !2

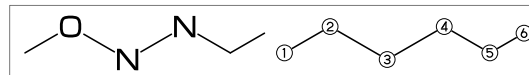


### 2.4.2 Change atom

2:0 : change A2 C to O

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

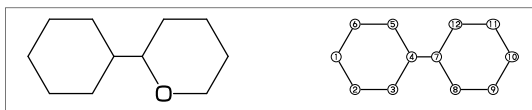
^30, !4, 2:0, 3'4:N



### 2.4.3 Begin local address

< : begin local address

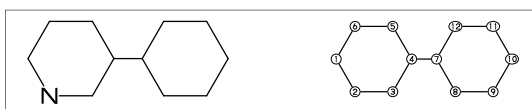
?6,4:,,!,<?6,2:0 or  
?6,4:,,!,<?6,2:0



### 2.4.4 End local address

> : end local address

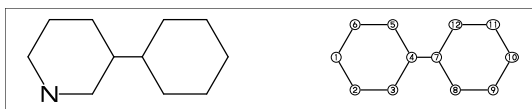
?6,4:,,!,<?6,>,2:N or  
?6,4:,,!,<?6,>,2:N



### 2.4.5 Absolute address

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

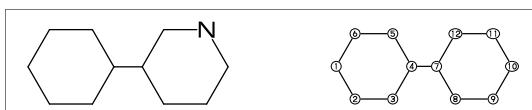
?6,4:,,!,<?6,\$2:N



### 2.4.6 Relative address

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

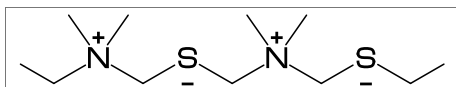
?6,4:,,!,<?6,-2:N



### 2.4.7 Charged atom

p : positive  
n : negative

^-30,!2,N,??,p,!2,S,n^180,  
!6,7:N,7:??,9:S,7:n,9:n^180

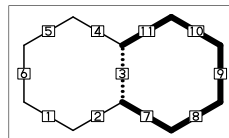


## 2.5 Fuse ring

(Attached 1 bond)

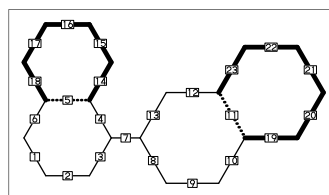
?6,3=?6 : fuse ?6 at B3  
\*\* Bn(n:-999<=n<=4095): bond number

?6,3=?6



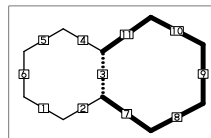
\*\* fused ring size depend on  
attached bond length

?6,4:,,!,<?6^1.2,5=?6,11=?6

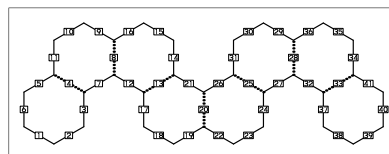


?6,3=?6^1.3'?6 : fuse #1.3'?6 at B3  
^1.3'?6 : 6 membered ring scaled 1.3  
\*\* ^n'?m (5<=m<=6,1.1<=n<=1.5)

?6,3=?6^1.3'?6



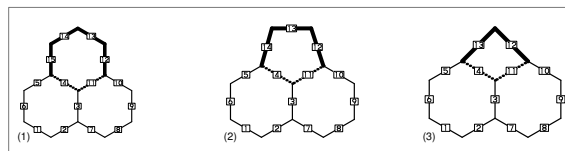
?6,-3'-4'-4'-2'-2'-4'-4=?6  
?6,4'8'13'20'25'28'33=?6



(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

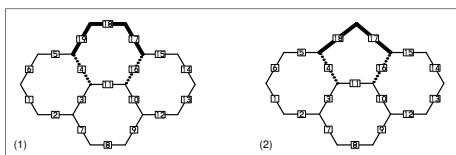
1:~30,!2,N,??,p,!2,S,n^180,  
!6,7:N,7:??,9:S,7:n,9:n^180  
1:~30,!2,N,??,p,!2,S,n^180,  
!6,7:N,7:??,9:S,7:n,9:n^180  
1:~30,!2,N,??,p,!2,S,n^180,  
!6,7:N,7:??,9:S,7:n,9:n^180



(Attached 3 bond)

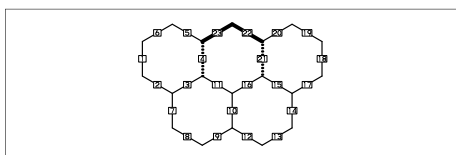
16---4=?6 : fuse 3/6 ring to B16..B4  
16---4=?5 : fuse 2/5 ring to B16..B4

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



(Attached 4 bond)

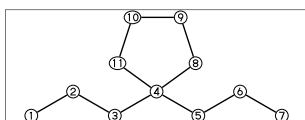
21----4=?6 : fuse 2/6 ring to B21..B4  
~30,?6,3'10'15' (21----4)=?6



## 2.6 Spiro ring

:4,?5 : add ?5 at A4

~30,!6,4:,?5

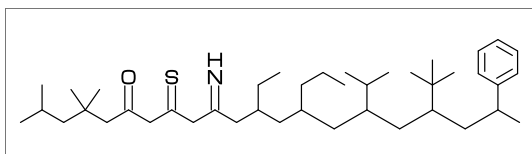


## 2.7 Group

### 2.7.1 Insert group

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

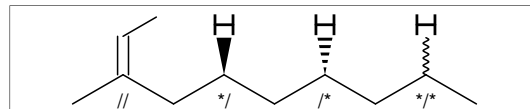
~30,!?,!2,??,!2,?O,!2,?S,!2,  
?NH,!2,/!,!2,/!2,!2^1,/?!,!2^1,  
/???,!2^1,/^.6'Ph,!



### 2.7.2 Insert modified group

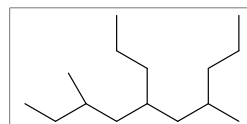
// : double (double middle)  
\*/ : wedge forward  
/\* : hashed wedge forward  
\*\* : wave

~30,! ,//!,!2,\* /H,!2,\* /H,!2,\* /H,!



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

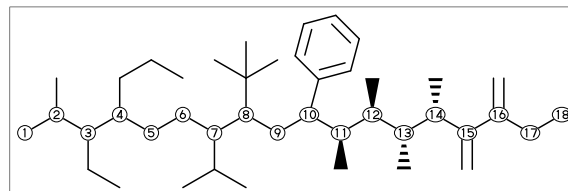
~30,`1,! ,  
?`2^30,!2,/!2^lr,!2,/!2^rl,!



### 2.7.3 Add group

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

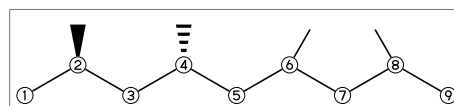
~30,!17,2:?,3:/!,4:/!2,7:/?!,  
8:/??!,10~15:/^.6'Ph,  
11'12':?w,13'14'?z,15'16'?d



### 2.7.4 Add modified group

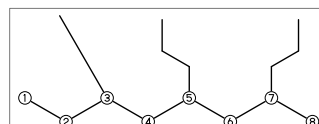
~,^,` : change type,angle,length

~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



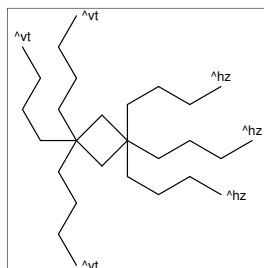
## 2.8 Chain environment

### 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
```

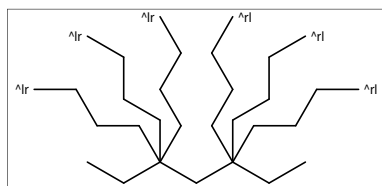


### 2.8.2 Left-right,right-left

`^lr` : left-right environment

`^rl` : right-left environment

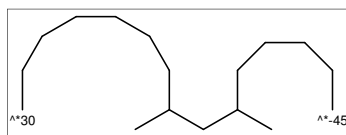
```
~-30,!6,  
3~-30'3'3^30:/!3^lr,
```



### 2.8.3 Rotate fixed angle

`^*n` : rotate n

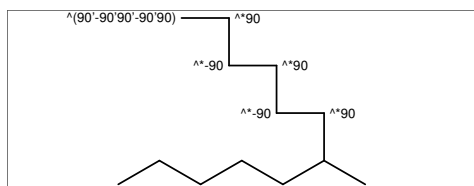
```
~30,!4,  
2:/!6^*30, % :2,! ,30,30,30,30,30,30  
4:/!4^*-45 % :4,! ,-45,-45,-45,-45
```



### 2.8.4 Rotate multiple angle

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

```
~30,!6,6:/!5^(90'-90'90'-90'90)
```



## 2.9 Miscellaneous

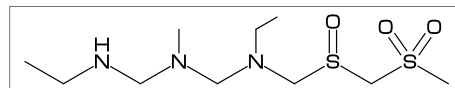
### 2.9.1 Abbreviated parts

`NH` : N,/H~n1    `N?` : N,?

`N?2` : N,/!    `S?0` : S,?0

`S?0?0` : S,?0^35,/^~35

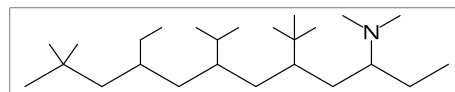
```
~-30,!2,NH,!2,N?,!2,N?2,S?0,!2,S?0?0,!
```



`??` : ?^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

`'('...')` : define parts with string

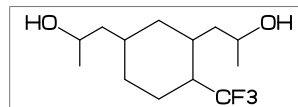
```
CF3:=^("{CF3}"); % ** group weight =0
```

```
CF3:=^("{CF3}")(C,F,F,F);
```

```
    ** group weight =12(C)+19(F)*3=69
```

```
iBuOH='(!?! ,OH);
```

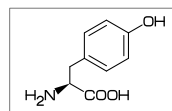
```
drawm("~30,?6,4'6:/iBuOH,3:/CF3")
```



### 2.9.3 Concatenate group,parts

`a'b` : concat a,b

```
~30,NH2,!wb,/!Ph'5:/OH,!COOH
```



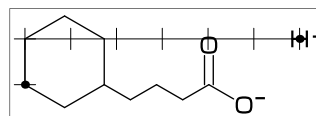
### 2.9.4 Move position [ ( ): ]

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

`$(x'y):` : Move l\*(x,y) from origin(01)

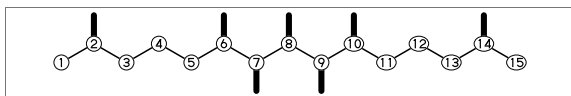
    \*\* l=bond length of ring

```
~30,?6,3:,!4,?0,! ,0,n_~60,$(6'1): ,H,p^15
```



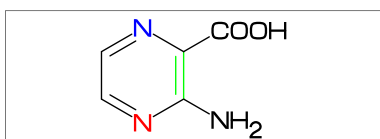
### 2.9.5 Serial number

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



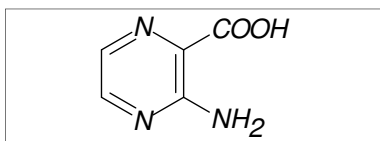
### 2.9.6 Change color

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



### 2.9.7 Change font

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

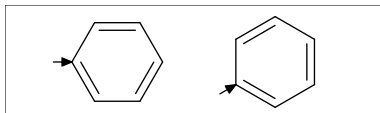


## 3 Option parameter

### 3.1 Angle parameter

mangle=0 \*\* default

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

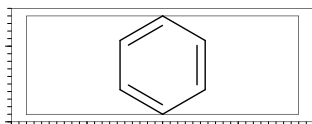


### 3.2 Size/Ratio parameter

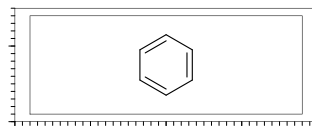
#### 3.2.1 Bond length [ |= ]

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

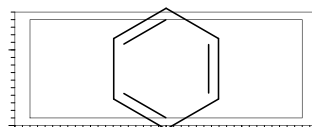
(fit to figure size)  
blength=0 \*\* default



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

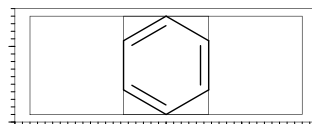


(bond length)  
blength=9mm  
\*\* (blength>1) ignore msize(w,h)

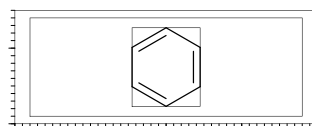


#### 3.2.2 Molecular size

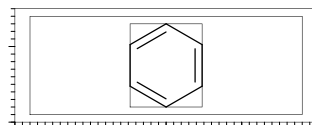
##(1,1) : msize=(1,1) \*\* default  
## p : abbreviated form of msize:=p;



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

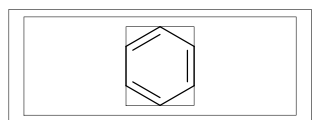


##(11mm,11mm) : msize=(11mm,11mm)



#### 3.2.3 Molecular position

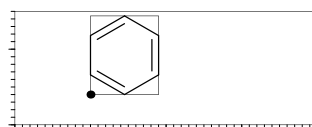
@(0.5,0.5) : mposition=(0.5,0.5) \*\*default



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



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



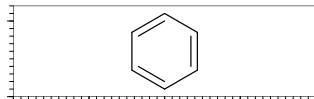


### 3.3 Size parameter

#### 3.3.1 Figure size [ # ]

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

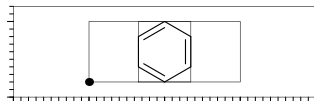
#(40mm,15mm) : fsize=(40mm,15mm)



#### 3.3.2 Figure margin [ #@ ]

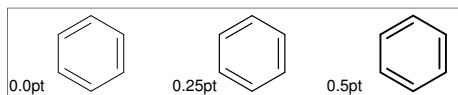
fmargin=(margin left right,top bottom)  
\*\* default: (0.4mm,0.4mm)  
#@ p : abbreviated form of fmargin:=p;

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



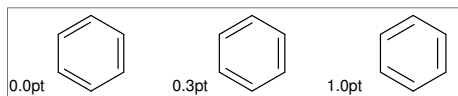
#### 3.3.3 Offset thickness of bond

default: offset\_thickness=0.25pt



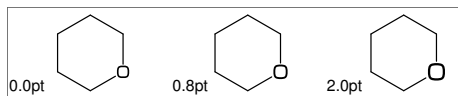
#### 3.3.4 Offset of double bond gap

default: offset\_bond\_gap=0.3pt



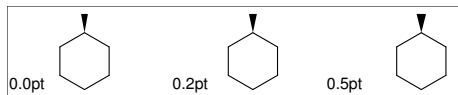
#### 3.3.5 Offset of atom width

default: offset\_atom=0.8pt



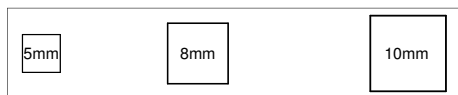
#### 3.3.6 Offset of wedge width

default: offset\_wedge=0.2pt



#### 3.3.7 Max bond length [ |< ]

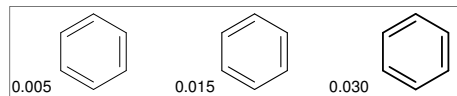
|<(n): abbreviated form of max\_blength:=n;  
default: max\_blength=10mm



### 3.4 Ratio parameter

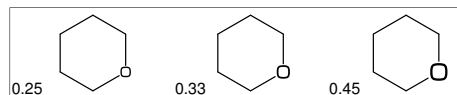
#### 3.4.1 Thickness/bond length

default: ratio\_thickness\_bond=0.012



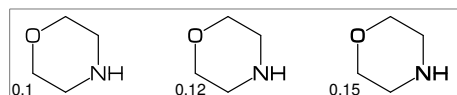
#### 3.4.2 Atom/bond length

default: ratio\_atom\_bond= 0.36



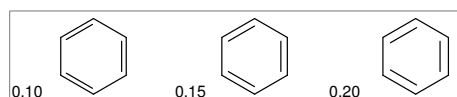
#### 3.4.3 Char thickness/Atom width

default: ratio\_char\_atom=0.12



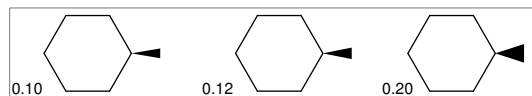
#### 3.4.4 Bond gap/bond length

default: ratio\_bondgap\_bond= 0.15



#### 3.4.5 Wedge/bond length

default: ratio\_wedge\_bond=0.12



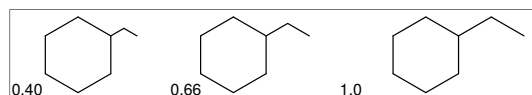
#### 3.4.6 Figure atom gap/atom length

default: ratio\_atomgap\_atom= 0.050



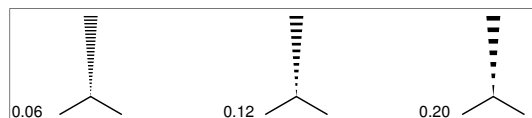
#### 3.4.7 Chain/ring length

default: ratio\_chain\_ring= 0.66



#### 3.4.8 Hash gap/bond length

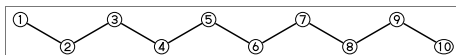
default: ratio\_hashgap\_bond=0.12



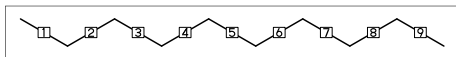
## 3.5 Drawing mode

### 3.5.1 Numbering atom,bond

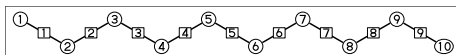
sw\_numbering:=Atom;



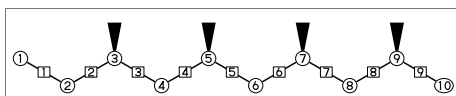
sw\_numbering:=Bond;



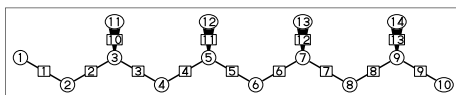
sw\_numbering:=Atom+Bond;



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

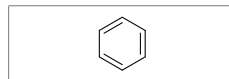
\*\* default: sw\_omit=Bond



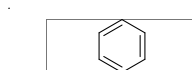
## 3.6 Frame

### 3.6.1 Figure frame

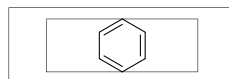
```
** default:sw_frame=0
(Draw figure frame)
fmargin:=(5mm,2mm);
sw_frame=Outside
```



(Frame inside margin)  
sw\_frame=Inside

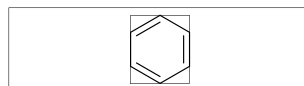


(Draw both frame)  
sw\_frame=Bothside=Inside+Outside



### 3.6.2 Molecular frame

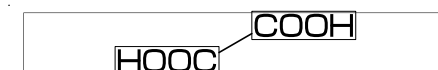
```
sw_frame=Mol
** default:sw_frame=0
```



### 3.6.3 Atom frame

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

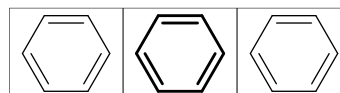
drawm("^30,COOH,! ,COOH")



## 3.7 Parameter setting

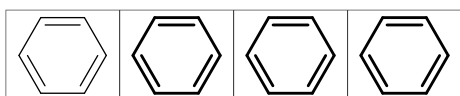
### 3.7.1 Local parameter setting

```
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

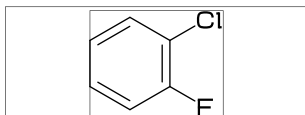
### 4.1 drawm

(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")
```

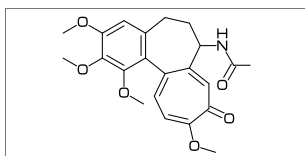


### 4.2 readm

```
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

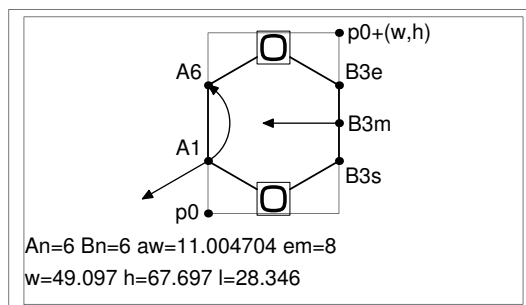
plus : '+' circled  
minus : '-' circled  
circlediam = 0.6aw (default)  
circlepen = 0.2bp (default)

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

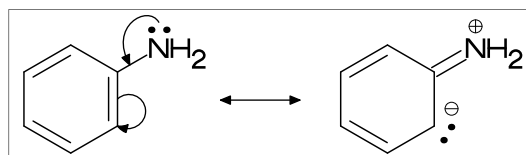
# : scaled  
<< : rotated  
a /\* b : point b of a

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

```
dotlabel.rft("B3e",B3e);
label.rft("An"&decimal(An)&
" Bn"&decimal(Bn)&
" aw"&decimal(aw)&
" em"&decimal(em),
p0+(-9em,-1.5em));
label.rft("w"&decimal(w)&
" h"&decimal(h)&
" l"&decimal(l),
p0+(-9em,-3em));
)
endfigm
```



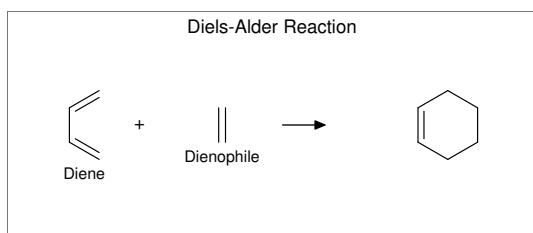
```
beginfigm
#(60mm,20mm) ##(1,0.85)
%-----
@(.0,0) drawm("~30,Ph,3=d1,4:/NH2")
%-----
++(
labeloffset:=.7aw;
label.top(lone_pair 90,A7);
drawarrow
(A7+up#1.2aw){A7left}
..{B7right}B7/*0.3;
drawarrow
B3m..A3+B2up#1.5aw..{A3down}A3;
)
%-----
@(.1,0) drawm("~30,?6,1'5=d1,4:/NH2")
%-----
++(
labeloffset:=.7aw;
label.top(plus,A7);
label.rft(minus,A3);
label(lonepair A3ang,A3+A3up#.7aw);
)
%-----
** (drawdblarrow (.4w,.4h)..(.55w,.4h);)
%-----
endfigm
```



## 4.7 ext [ \*\* ]

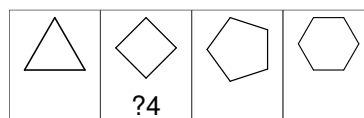
(Extra label to figure)

```
**(): ext()  
w: figure width  
h: figure height  
w0: figure width-2xpart(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

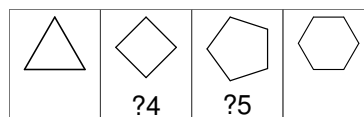
```
beginfigm  
  EN:="?3";@(0.5,1) drawm("^30,?3")  
endfigm  
beginfigm  
  EN:="?4";@(0.5,1) drawm("?4")  
  %-----  
  ** (label.top(EN, (0.5w,0)));  
  %-----  
endfigm  
beginfigm  
  EN:="?5";@(0.5,1) drawm("?5")  
endfigm  
beginfigm  
  EN:="?6";@(0.5,1) drawm("?6")  
endfigm
```



### 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
```

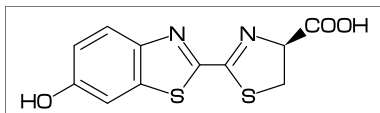


## 5 Example

### 5.1 drawm example

(Luciferin)

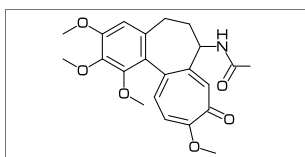
```
beginfigm
  #(50mm,15mm)
  drawm("^30,Ph,3=?5,8:!,?5,9'16=d1,"&
    "9'14:N,7'11:S,1:/OH,-2:*/COOH")
endfigm
```



### 5.2 readm example

(Colchicine)

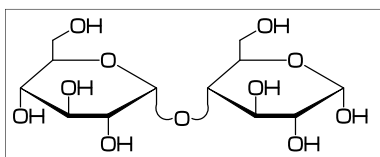
```
beginfigm
  readm(
    "^30,Ph,1'2'6:/O!,-4'-5=?7,      ",
    " -1'-4'-6=d1,-2:?0,-3:/O!,      ",
    " 9:/NH!'?0!                        ")
  #(40mm,20mm) putm
endfigm
```



(Maltose)

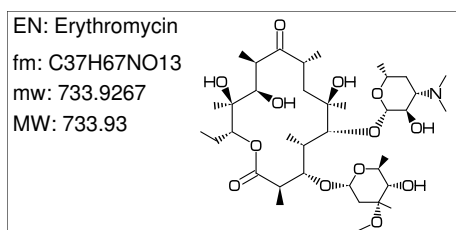
(bond type for glycan)  
arc\_lb : arc left > bottom  
arc\_br : arc bottom right

```
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
```



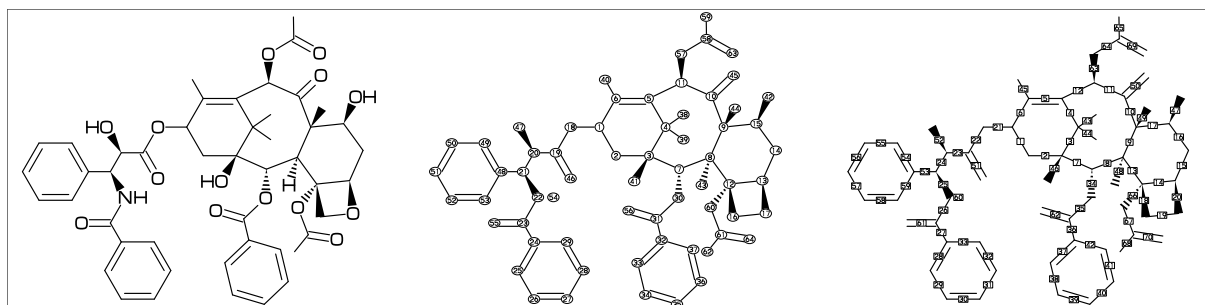
## (Erythromycin)

```
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
  ** (defaultsacle:=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;LV:-"
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;LV: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;LV: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;LV: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
LV : level	LN : long name



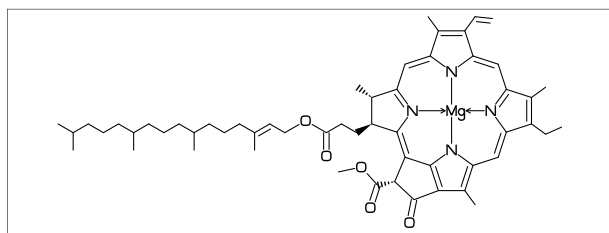
## 5.4 getm example

### (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=dl,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:?

```

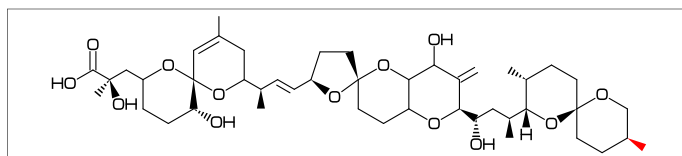
```
** EN:Chlorophyll a mw:893.509 MW:893.4889 fm:C55H72MgN4O5
```

### (Dinophysistoxin-1)

```

beginfigm
  sw_output:=Fig+Mcode;          %%% output temp-mc.aux %%%
  getm("Okadaic acid")           %%% select Okadaic acid %%%
  readm(",40:?w,65=red")         %%% add methyl group %%%
  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}%

```



```

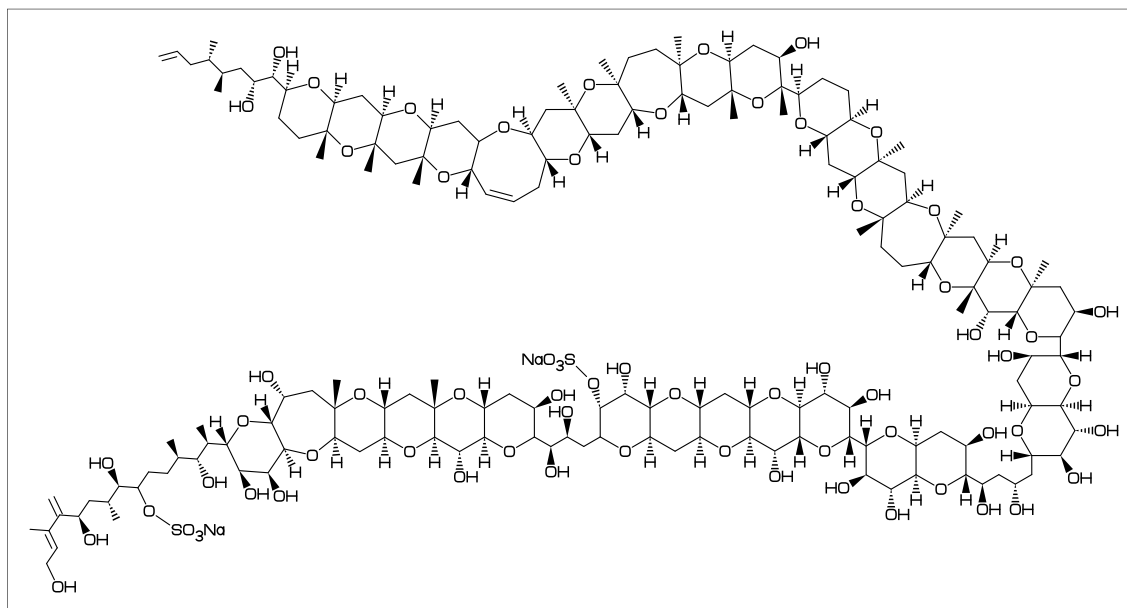
~30,?6,4:,?6,-4:,!4,~12,?5,-3:,~12,?6,-3=?6,-3:,!w,!3,
?6,-4:,?6,6:,!2,?z~40,*/OH^20,!?0!,OH,
3'38=wb,11=dl,15=dr,17'19=wf,5'7'16'24'25'33'42:0,
32:*/H^60,10:?,12'31'*37:?w,27:?d,28:/OH,3'29:/*OH
,40:?w,65=red

```

```
** 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

## 6 Example to use mcf2graph

### 6.1 MetaPost source file

```
input mcf2graph;                                % input main macro
#(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,"&                % immediately write
    "3^45:/*H,1:?0^15,5:/*COOH^18,6:??,"&
    "4:,!w^15,NH,! ,?0,! ,/*NH2,! ,Ph")
endfigm
%-----
beginfigm
  % EN:Cholesterol MW:386.65
  readm("^30,?6,-4'-2=?6,-4=?5,7=d1," ,          % mc1
    "10:/*H^180,11:/*H^60,17:/*H^54,4'12:?w^60, ", % mc2
    "-1:,18,?z,-60,!3,?!")                       % mc3
  putm                                           % put figure
endfigm
%-----
loadm()                                         % load all unit
beginfigm getm("Adenine") putm endfigm         % get EN=Adenine
beginfigm getm(4) putm endfigm                 % select No.4
for i=1 upto ucount:                           % figure count
  beginfigm getm(i) putm endfigm                % select No.i
endfor
bye
```

### 6.2 Molecular library file

```
% first character of line
% "%":comment out / " ": start MCF / ";": stop MCF
% "=":start parameter setting / "*" : start ext(...) / "+" : start add(...)
% CAT : Category,EN : Name,MW : Molecular weight LV : Level
%-----
CAT:-;EN:-;MW:0;LV:-
=
  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;
;
%=====
CAT:biological;EN:Adenine;MW:135.13;LV: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;LV:1
:
^30,?6,3=?5,1'3'9=d1,2'9:N,6'7:NH,5:?0,1:/NH2
;
%-----
```

### 6.3 MCF aux file output

(Option parameter setting)

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

(Command line)

```
>mpost -s ahlenght=3 FILENAME (sw_output=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
Formula 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

\*\* file mcf2graph.mp must be in the same directory to typeset

```

\documentclass{article}
\usepackage{luamplib}%
\mplibcodeinherit{enable}%
\mplibverbatim{enable}%
\mplibnumbersystem{double}%
\begin{document}
\noindent%
%-----
\begin{mplibcode}
  input mcf2graph;
  max_blength:=4.5mm;
  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}

```

## 6.7 Batch file mcf\_to\_graph.cmd

Batch file for compile mcf or mp file

\*\* drag and drop mcf or mp file on this batch : >mcf\_to\_graph filename

\*\* file mcf2graph.mp , main\_lib.mcf must be in the same directory

```
::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::
:: Batch file for compile MCF 2025.09.15
:: <drag and drop library or metapost file on this batch>
::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::
@echo off
if %~x1 == .mp (
if %~n1 == mcf2graph goto end
mkdir %~n1-mp
mpost -output-directory=./%~n1-mp %~n1
goto end )
if not %~x1 == .mcf goto end
echo **** Select output format / Library file [%~n1] ****
echo [1:svg 2:png-600dpi 3:png-1200dpi 4:MOL-v2000 5:MOL-v3000 6:report 0:cancel]
choice /c 1234560
if %errorlevel% == 7 goto end
echo input mcf2graph; libm:="%~n1.mcf"; loadm() allm bye> temp_soc.mp
if %errorlevel% == 1 (mkdir %~n1-svg
mpost -output-directory=./%~n1-svg temp_soc)
if %errorlevel% == 2 (mkdir %~n1-pn0600
mpost -output-directory=./%~n1-pn0600 -s ahandle=1 temp_soc)
if %errorlevel% == 3 (mkdir %~n1-pn1200
mpost -output-directory=./%~n1-pn1200 -s ahandle=2 temp_soc)
if %errorlevel% == 4 (mkdir %~n1-molv2k
mpost -output-directory=./%~n1-molv2k -s ahlength=5 temp_soc)
if %errorlevel% == 5 (mkdir %~n1-molv3k
mpost -output-directory=./%~n1-molv3k -s ahlength=6 temp_soc)
if %errorlevel% == 6 (mkdir %~n1-report
mpost -output-directory=./%~n1-report -numbersystem=double -s ahlength=7 temp_soc)
del temp_soc.mp
:end
```



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