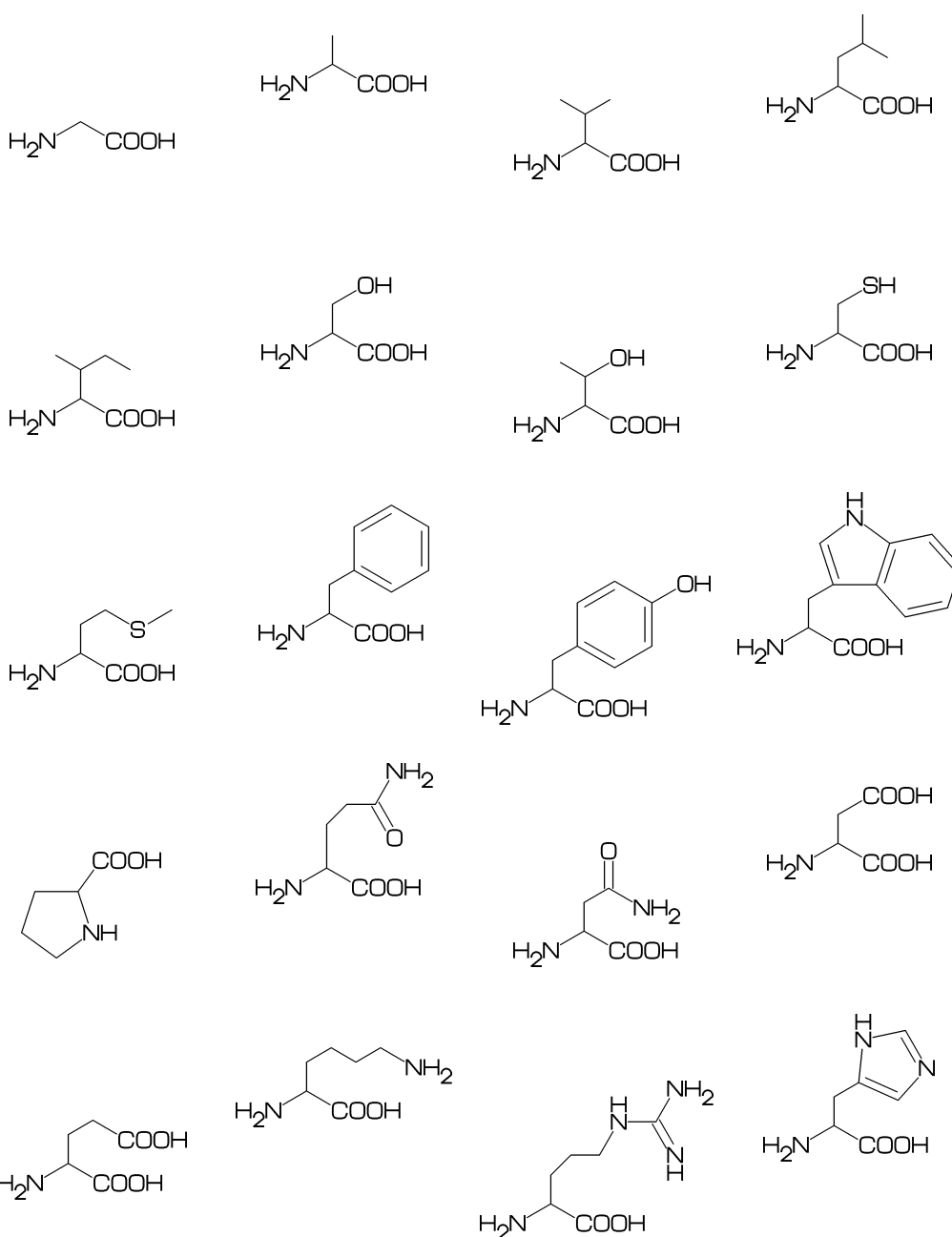


# Molecular Coding Format manual

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February 13, 2017

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



# Contents

<b>1</b>	<b>Introduction</b>	<b>1</b>
<b>2</b>	<b>MCF syntax</b>	<b>1</b>
2.1	Make bond	1
2.1.1	Chain	1
2.1.2	Jump and branch bond	1
2.1.3	Branch bond	1
2.1.4	Connect atom	1
2.1.5	Ring	1
2.1.6	Rotate current angle	1
2.2	Change bond type	2
2.2.1	Double,triple	2
2.2.2	Wedge	2
2.2.3	Vector	2
2.2.4	Dotted,wave	2
2.2.5	Broad	2
2.2.6	Change multi bond type	2
2.2.7	Over line	2
2.3	Change bond length	2
2.3.1	Chain length	2
2.3.2	Ring length	2
2.4	Change atom	3
2.4.1	Insert atom	3
2.4.2	Addressed atom	3
2.4.3	Brock address	3
2.4.4	Absolute address	3
2.4.5	Relative address	3
2.5	Fuse ring	3
2.5.1	Attached 1 bond	3
2.5.2	Attached 2 bond	3
2.5.3	Attached 3 bond	4
2.5.4	Attached 4 bond	4
2.5.5	Spiro ring	4
2.6	Substituent	4
2.6.1	Insert substituent	4
2.6.2	Insert modified substituent	4
2.6.3	Add substituent	4
2.6.4	Add modified substituent	4
2.7	Chain environment	5
2.7.1	Horizontal,vertical	5
2.7.2	Left-right,right-left	5
2.7.3	Fixed angle,multi angle	5
2.8	Miscellaneous	5
2.8.1	Change atom and Substituent	5
2.8.2	Change color	5
2.8.3	Make block	5
2.8.4	Chain start multiple characters	5
2.8.5	User definition	5
2.8.6	Inline definition	5
<b>3</b>	<b>Option parameter</b>	<b>6</b>
3.1	Size parameter	6
3.1.1	Font size	6
3.1.2	Margin left and right	6
3.1.3	Margin top and bottom	6
3.1.4	Offset thickness of bond	6
3.1.5	Offset of doublebond gap	6
3.1.6	Offset of atom width	6
3.1.7	Offset of wedge width	6
3.1.8	Max bond length	6
3.2	Ratio parameter	6
3.2.1	Thickness/bond length	6
3.2.2	Char/bond thickness	6
3.2.3	Bondgap/bond length	6
3.2.4	Atom/bond length	6
3.2.5	Wedge/bond length	7
3.2.6	Font atom gap/atom length	7
3.2.7	Chain/ring length	7
3.2.8	Zebra gap/bond length	7
3.3	Drawing mode	7
3.3.1	Numbering atom	7
3.3.2	Numbering bond	7
3.3.3	Clipping mode	7
3.3.4	Solid mode	7
3.3.5	Expand mode	8
3.3.6	Substituent off mode	8
3.3.7	Single bond mode	8
3.4	Frame	8
3.4.1	Font frame	8
3.4.2	Molecular frame	8
3.4.3	Atom frame	8
<b>4</b>	<b>Function</b>	<b>8</b>
4.1	Function MCd()	8
4.2	Function MCf()	8
4.3	Function EXT()	9
4.4	Function ext()	9
4.5	Local parameter setting	9
4.6	Global parameter setting	9
<b>5</b>	<b>Output information</b>	<b>10</b>
5.1	Output molecular information	10
5.2	Output additional information	10
5.3	Change aux information delimiter	10
5.4	Fixed aux information	10
<b>6</b>	<b>MCF example</b>	<b>11</b>
<b>7</b>	<b>Example to use mcf2graph</b>	<b>13</b>
7.1	Molecular definition file	13
7.2	Information auxfile output	14
7.3	Report output	15
7.4	Molfile output	16
7.5	LuaTeX file example	17
7.6	LaTeX file example	18

# 1 Introduction

Molecular Coding Format(MCF) is new linear notation represent chemical structure diagrams. This 'Coding' is named from coding(programing) technique like addressing,grouping,macro,etc. There are no Meta language commands in MCF. mcf2graph.m convert MCF file to graphics file pk font,PNG,SVG,EPS or MDL MOL file(V2000).

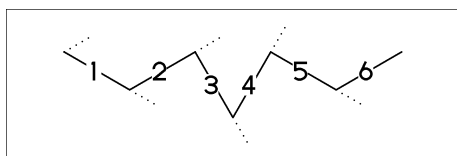
## 2 MCF syntax

### 2.1 Make bond

#### 2.1.1 Chain

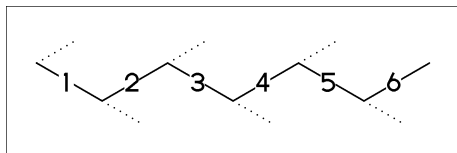
real number plus (+): anticlockwise  
real number minus(-): clockwise

<30,-60,60,-90,120,-90,60



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

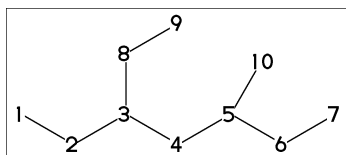
<30,! ,! ,! ,! ,! ,!  
<30,!6



#### 2.1.2 Jump and branch bond

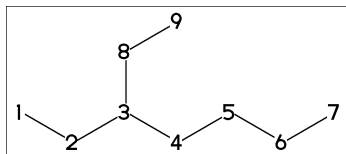
n\* : Jump to An  
\*\* An: atom number(-999<=n<=4095)

<30,!6,3\*,0,! ,5\*,-30



3\ : 3\*,0

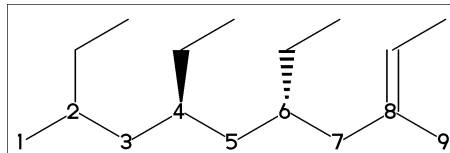
<30,!6,3\,! ,



#### 2.1.3 Branch bond

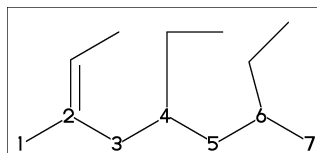
2\ : 2\*,0  
4\*\ : 4\*,0~wf  
6\\* : 6\*,0~zf  
8\\ : 8\*,0~dm

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



2\~dr : 2\*,0~dr  
4\'1.5 : 4\*,0\'1.5  
6\^15 : 6\*,0^15

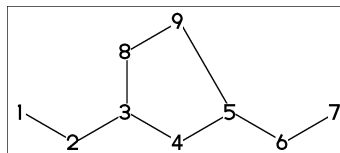
<-30,!6,  
2\~dr,! ,  
4\'1.5,-90,  
6\^15,-60



#### 2.1.4 Connect atom

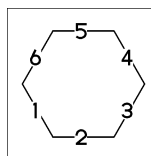
&n : Connect to An

<30,!6,3\,! ,&5



#### 2.1.5 Ring

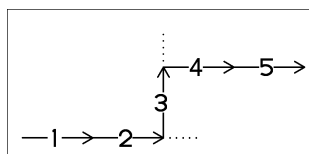
?n : n membered ring(3<=n<=20)  
?6 : <-120,60,60,60,60,60,&1  
?6



#### 2.1.6 Rotate current angle

<angle : rotate current angle

0,0,<90,0,<-90,0,0,\$(1,2,3,4,5)vf

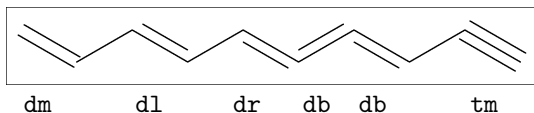


## 2.2 Change bond type

### 2.2.1 Double, triple

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

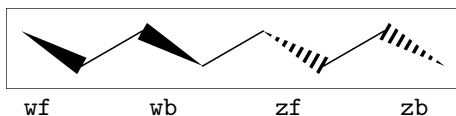
<30,!~dm,!~dl,!~dr,!~db,!~db,!~tm  
<30,!~dm,!~dl,!~dr,!! ,!! ,!!



### 2.2.2 Wedge

wf : wedge forward / wb : wedge backward  
zf : wedge dotted  
zb : wedge dotted backward

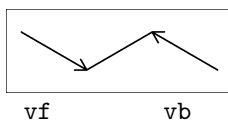
<30,!~wf,!~wb,!~zf,!~zb



### 2.2.3 Vector

vf:vector forward / vb:vector backward

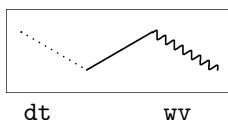
<30,!~vf,!~vb



### 2.2.4 Dotted, wave

Bn=bond type : change bond type at Bn  
dt : dotted / ww : wave

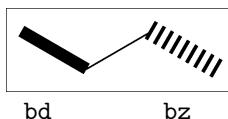
<30,!3,1=dt,3=ww



### 2.2.5 Broad

bd : broad / bz : broad dotted

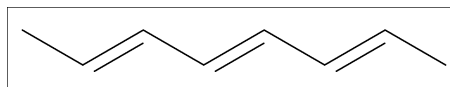
<30,!3,1=bd,3=bz



### 2.2.6 Change multi bond type

\$(2,4,6)dr : 2=dr,4=dr,6=dr

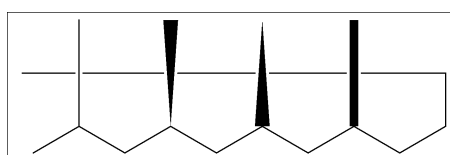
<30,!7,\$(2,4,6)dr



### 2.2.7 Over line

si\_ : single over line  
wf\_ : wedge forward over line  
wb\_ : wedge backward over line  
bd\_ : broad over line

<-30,!8,!60,90'8,  
@(2~si\_,4~wf\_,6~wb\_,8~bd\_)/\_'2



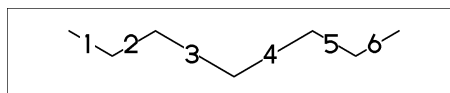
## 2.3 Change bond length

### 2.3.1 Chain length

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

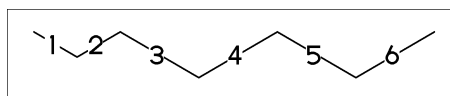
<30,!2,!2'1.2,!2

\*\* !2'1.2 : ''1.2,!2



''length : change all bond length after

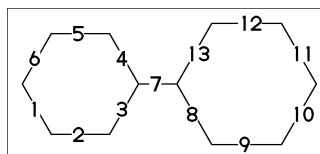
<30,!2, ''1.2,!4



### 2.3.2 Ring length

?n'length : change ring length

?6,4\,?6'1.2

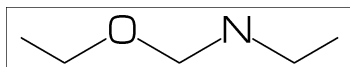


## 2.4 Change atom

### 2.4.1 Insert atom

Insert hetero atom

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

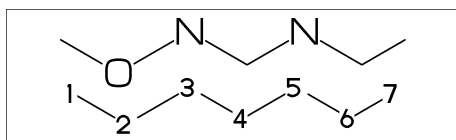


### 2.4.2 Addressed atom

2:0 : change A2 C to O

@(3,5)N : change A3,A5 C to N

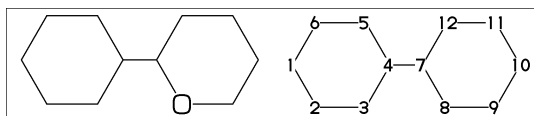
<30,!6,2:0,@(3,5)N



### 2.4.3 Brock address

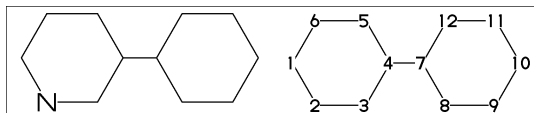
| : divide brock

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



|| : reset brock address

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

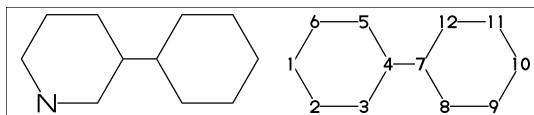


### 2.4.4 Absolute address

#2:N : change A#2 C to N

\*\* #n : (1<=n<=3095)

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

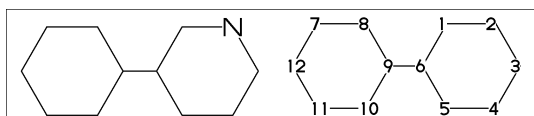


### 2.4.5 Relative address

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

\*\* -n : (1<=n<=999)

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



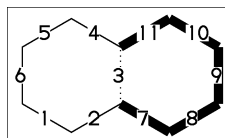
## 2.5 Fuse ring

### 2.5.1 Attached 1 bond

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

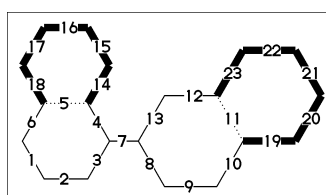
\*\* Bn(n:-999<=n<=4095): bond number

?6,3=?6



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

?6,4\,?6'1.2,5=?6,11=?6

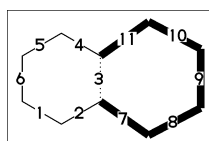


?6,3=?6[13] : fuse ?6[13] at B3

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

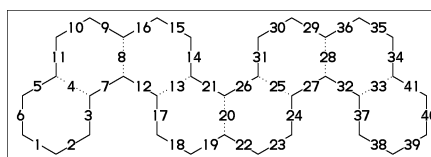
\*\* ?m[n] (5<=m<=8,11<=n<=15)

?6,3=?6[13]



?6,\$(-3,-4,-4,-2,-2,-4,-4)?6

?6,\$(4,8,13,20,25,28,33)?6



### 2.5.2 Attached 2 bond

(4,11)=?6[4] : fuse 4/6 ring to B11..B4

(4,11)=?5[3] : fuse 3/5 ring to B11..B4

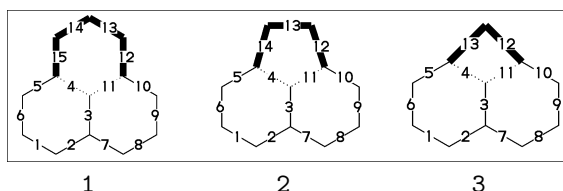
(4,11)=?4[2] : fuse 2/4 ring to B11..B4

\*\* ?m[n] (4<=m<=6,n=m-2)

1:MCd(1,.7)( 0,0)<30,?6,3=?6,(11,4)=?6[4])

2:MCd(1,.6)(.54,1)<30,?6,3=?6,(11,4)=?5[3])

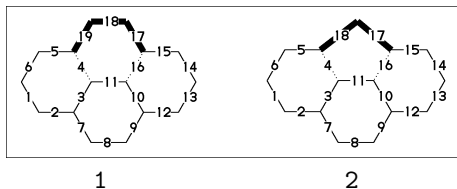
3:MCd(1,.6)( 1,0)<30,?6,3=?6,(11,4)=?4[2])



### 2.5.3 Attached 3 bond

(16,4)=?6[3] : fuse 3/6 ring to B16..B4  
 (16,4)=?5[2] : fuse 2/5 ring to B16..B4  
 \*\* ?m[n] (5<=m<=6,n=m-3)

1:MCd(1,.55)(0,0)(?6,\$(3,10)?6,(16,4)=?6[3])  
 2:MCd(1,.55)(1,0)(?6,\$(3,10)?6,(16,4)=?5[2])

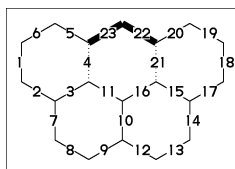


### 2.5.4 Attached 4 bond

(21,4)=?6[2] : fuse 2/6 ring to B21..B4

MCf(<-30,?6,\$(3,10,15)?6,(21,4)=?6[2])

\*\* ?m[n] (m=6,n=2)

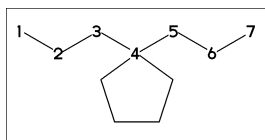


### 2.5.5 Spiro ring

4\*,?5 : add ?5(5 membered ring) at A4

<30,!6,4\*,?5

An\* : jump to An



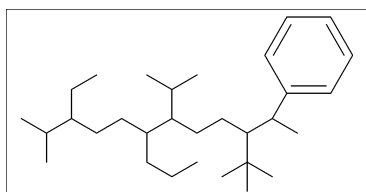
## 2.6 Substituent

### 2.6.1 Insert substituent

/ : single

<30,!/,Me,!,/Et,!3,/Pr,!,/iPr,  
 !3,/tBu,!,/Ph^-30,!)

\*\* Me:methyl(/\_) Et:ethyl(!)  
 Pr:propyl(!2) iPr:isopropyl  
 tBu:tertial buthyl Ph:phenyl



### 2.6.2 Insert modified substituent

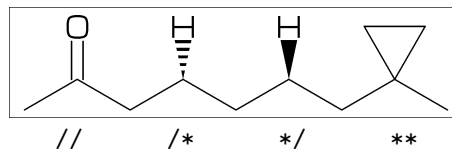
// : double (double middle)

\*/ : wedge forward

/\* : wedge dotted forward

\*\* : direct

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



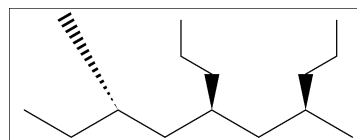
~ : change type

^ : change angle

' : change length

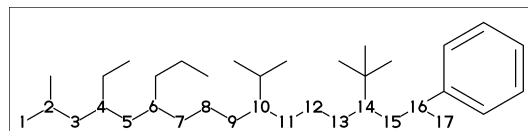
> : change enviroment

<30,'^1,!/,~zf'^2^30,  
 !2,\*/!2>lr,!2,\*/!2>r1,!)



### 2.6.3 Add substituent

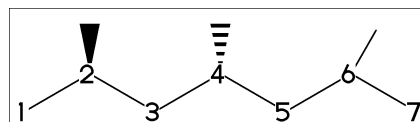
<-30,!17,2:/\_,4:/!,6:/!2,  
 10:/iPr,14:/tBu,16:/Ph^-60



### 2.6.4 Add modified substituent

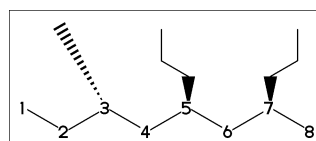
~,^,' : change type,angle,length

<-30,!6,  
 @ (2~wf,4~zf,6^-30)/\_



~,^,'> : change angle,length,environment

<30,!7'^1,  
 3:/\*'^2^30,5:\*/!2>lr,7:\*/!2>r1

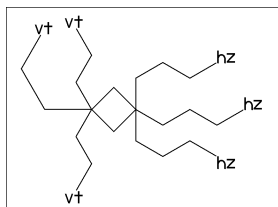


## 2.7 Chain environment

### 2.7.1 Horizontal,vertical

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

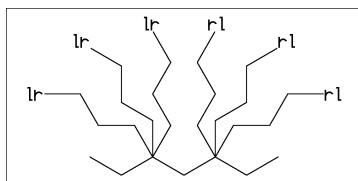
```
?4,@(3^-90,3^-30,3^90)/'(!3,"{hz}")>hz,  
  @(1^-60,1^2,1^60)/'(!2,"{vt}")>vt
```



### 2.7.2 Left-right,right-left

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

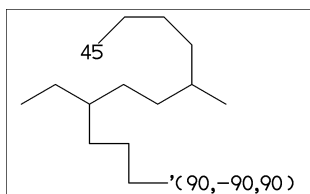
```
<30,!6,  
  @(3^-30,3,3^30)/'(!3,"{lr}")>lr,  
  @(5^-30,5,5^30)/'(!3,"{rl}")>rl
```



### 2.7.3 Fixed angle,multi angle

>45 : fixed angle environment  
>'(-90,90,-90) : multi angle environment

```
<-30,!6,@(2>45)/'(!3,"{45}")  
  @(6>'(-90,90,-90))/'(!3,"{(-90,90,-90)}")
```

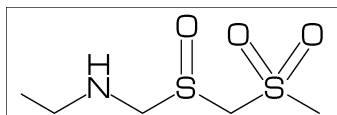


## 2.8 Miscellaneous

### 2.8.1 Change atom and Substituent

NH,S0,S00 :  
 inset hetero atom and substituent  
 simultaneously

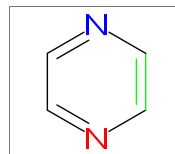
```
<30,!2,NH,! ,S0,! ,S00,!3
```



### 2.8.2 Change color

@(5)green : change color of A5 green  
\$(3)red : change color of B3 red  
\*\* METAFONT ignore color command

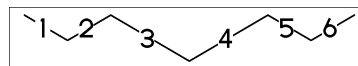
```
<30,Ph,@(2,5)N,2:red,5:blue,3:green
```



### 2.8.3 Make block

{ : start block  
} : end block

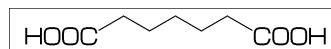
```
<30,!2,{,'1.2,!2,!2
```



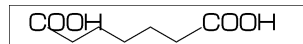
### 2.8.4 Chain start multiple characters

if chain start multi character string,  
use !0 instead of !

```
MCf(<30,COOH,!0,!3,COOH)
```



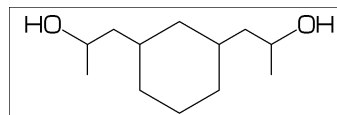
```
MCf(<30,COOH,!4,COOH)
```



### 2.8.5 User definition

iBuOH : user defined substructure

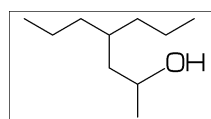
```
iBuOH:= '(!,/_,!,OH)  
MCf(<30,!6,@(4,6)/iBuOH)
```



### 2.8.6 Inline definition

Insert user defined substructure

```
<30,!3,/ '(!,/_,!,OH),!3
```

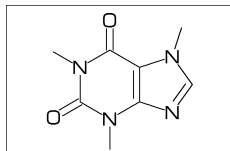


## 3 Option parameter

### 3.1 Size parameter

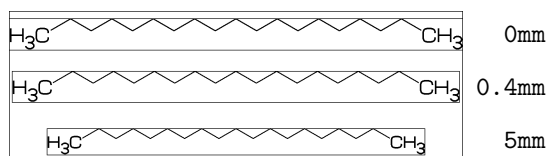
#### 3.1.1 Font size

```
beginfont("EN:Caffeine")
font_wd#:=30mm#; %<=font width
font_ht#:=20mm#; %<=font height
MCf(<30,?6,-4=?5,$(3,8)d1,@(2,6,7,9)N,
    @(2,6,9)/_,@(1,5)//0) endfont
```



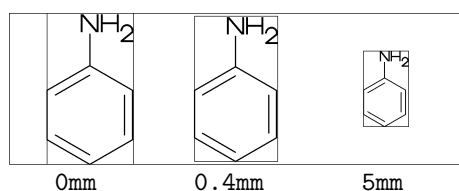
#### 3.1.2 Margin left and right

default: margin\_left\_right=0.4mm



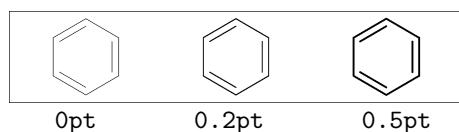
#### 3.1.3 Margin top and bottom

default: margin\_top\_bottom=0.4mm



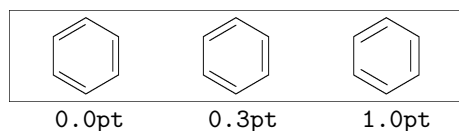
#### 3.1.4 Offset thickness of bond

default: offset\_thickness#=0.2pt#



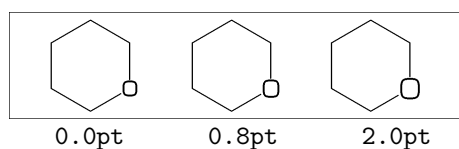
#### 3.1.5 Offset of doublebond gap

default: offset\_bond\_gap#=0.3pt#



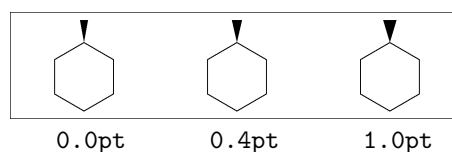
#### 3.1.6 Offset of atom width

default: offset\_atom#=0.8pt#



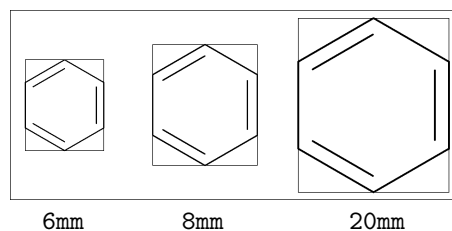
#### 3.1.7 Offset of wedge width

default: offset\_wedge#=0.4pt#



#### 3.1.8 Max bond length

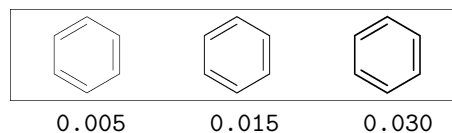
default: max\_bond\_length#=10mm#



## 3.2 Ratio parameter

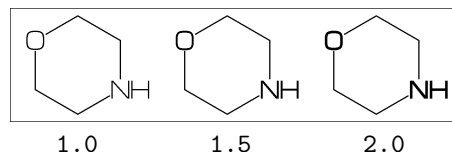
#### 3.2.1 Thickness/bond length

default: ratio\_thickness\_bond=0.015



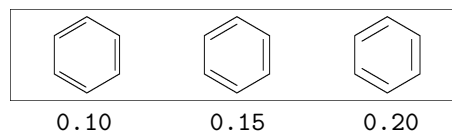
#### 3.2.2 Char/bond thickness

default: ratio\_char\_bond=1.5



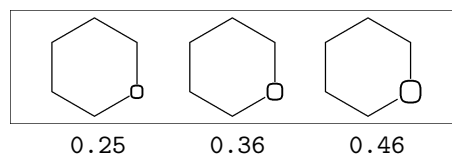
#### 3.2.3 Bondgap/bond length

default: ratio\_bondgap\_bond= 0.15



#### 3.2.4 Atom/bond length

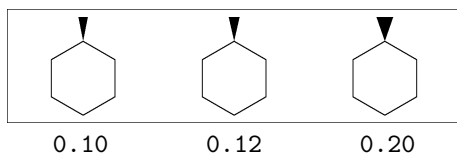
default: ratio\_atom\_bond= 0.36





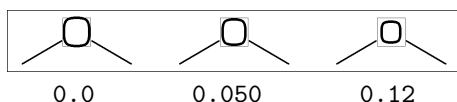
### 3.2.5 Wedge/bond length

default: ratio\_wedge\_bond=0.12



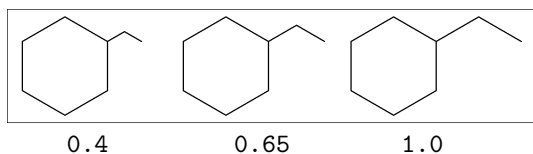
### 3.2.6 Font atom gap/atom length

default: ratio\_atomgap\_atom= 0.050



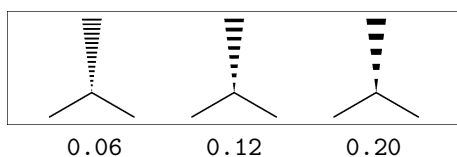
### 3.2.7 Chain/ring length

default: ratio\_chain\_ring= 0.66



### 3.2.8 Zebra gap/bond length

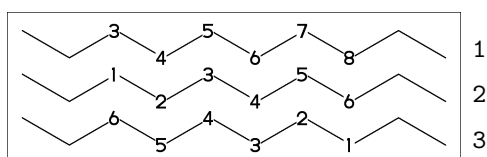
default: ratio\_zebragap\_bond=0.12



## 3.3 Drawing mode

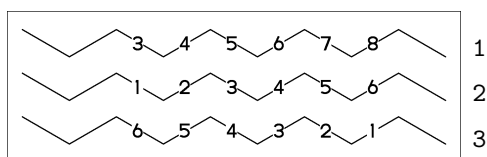
### 3.3.1 Numbering atom

```
numberA_start:=3; numberA_end:=8;  
default: sw_numberA=0 :  
    numberA_start=1 numberA_end=4095
```



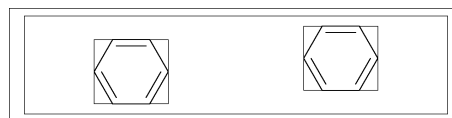
### 3.3.2 Numbering bond

```
numberB_start:=3; numberB_end:=8;  
default: sw_numberB=0 :  
    numberB_start=1 numberB_end=4095
```



### 3.3.3 Clipping mode

```
sw_clip:=0;  
MCd(1,0.7)(0.2,0.3)(Ph)  
MCd(1,0.7)(0.8,0.7)(Ph)  
** default: sw_clip=0
```

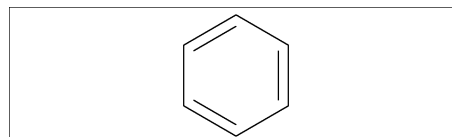


```
sw_clip:=1;  
MCd(1,0.7)(0.2,0.3)(Ph)  
MCd(1,0.7)(0.8,0.7)(Ph)
```

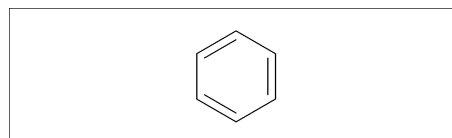


### 3.3.4 Solid mode

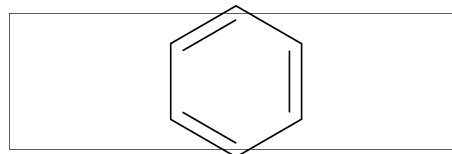
```
(fit to font size)  
sw_solid=0    ** default
```



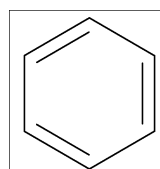
```
(solid ratio bond/font width)  
sw_solid:=1;  
ratio_bond_width=0.1  
font_width=60mm  
(bond_len#=60mm#*0.1=6mm#)  
** ignore bond_len#
```



```
(solid bond length)  
sw_solid:=2;  
bond_len#=10mm#  
** ignore ratio_bond_width
```

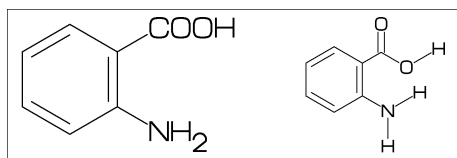


```
(solid bond length and clip)  
sw_solid:=2;  
sw_clip:=1;  
bond_len#=10mm#
```



### 3.3.5 Expand mode

default: sw\_expand=0

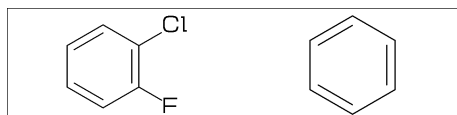


0 :default

1

### 3.3.6 Substituent off mode

default: sw\_subst\_off=0

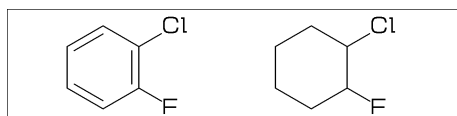


0 :default

1

### 3.3.7 Single bond mode

default: sw\_bond\_single=0



0 :default

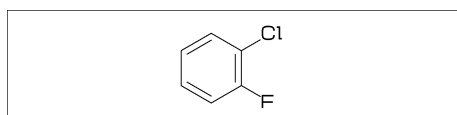
1

## 3.4 Frame

### 3.4.1 Font frame

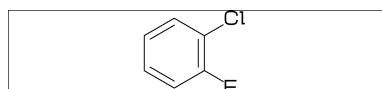
(Draw font frame)

```
margin_left_right:=5mm;  
margin_top_bottom:=2mm;  
sw_font_frame:=1;  
MCf(<30,Ph,4:/Cl,3:/F)
```



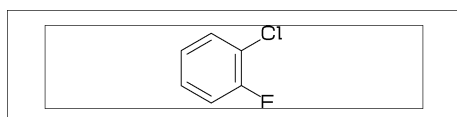
(Draw frame inside margin)

sw\_font\_frame=2



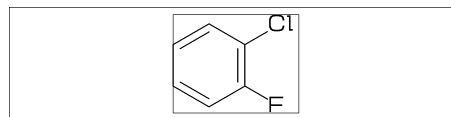
(Draw both frame)

sw\_font\_frame=3



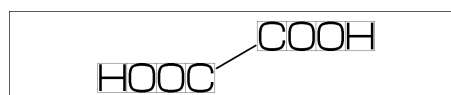
### 3.4.2 Molecular frame

```
sw_mol_frame:=1;  
MCd(1,.5)(1,0.5)(<30,Ph,4:/Cl,3:/F)  
** default: sw_mol_frame=0
```



### 3.4.3 Atom frame

```
sw_atom_frame:=1;  
MCf(<30,COOH,!0,COOH)  
** default: sw_atom_frame=0
```



## 4 Function

### 4.1 Function MCd()

(Draw molecular structure)

MCd(a,b)(c,d)(...)

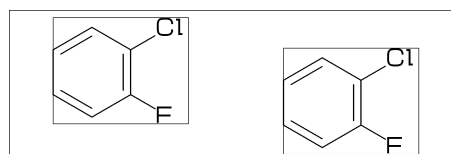
a: ratio molecular width/font width  
b: ratio molecular height/font height  
c: x axis position  
d: y axis position

beginfont()

MCd(1,0.8)(0.2,0.9)(<30,Ph,3:/F,4:/Cl)

MCd(1,0.8)(0.8,0.1)(<30,Ph,3:/F,4:/Cl)

endfont



### 4.2 Function MCf()

(Draw molecular fit to font size)

MCf(...) : MCd(1,1)(0.5,0.5)(...)

beginfont()

font\_wd#:=25mm#;

font\_ht#:=15mm#;

MCf(<30,Ph)

endfont

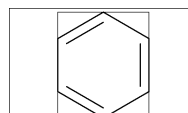
beginfont()

font\_wd#:=13mm#;

font\_ht#:=25mm#;

MCf(<30,Ph)

endfont



### 4.3 Function EXT()

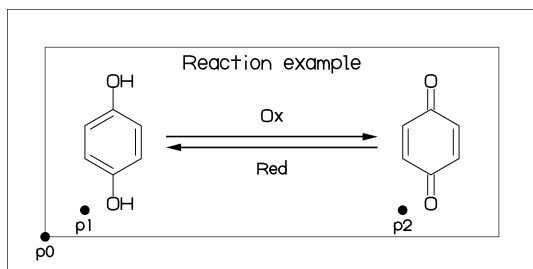
(Add extra graphic to font)

```
w: font width
h: font height
wd: font width-margin_left_right*2
ht: font height-margin_top_bottom*2
em: embedded font size
p0: x=margin_left_right
    y=margin_top_bottom
n: molecular number
p[m]: molecular origin position
```

(Function for EXT(), ext())

```
draw_vector(pos,angle,thickness,length):
    draw vector at pos
use_font(wd#):
    make font for 'label'
label:
    sw_label_mp=0: ** default
        use embedded font
    sw_label_mp=1:
        use original metapost 'label'
```

```
beginfont()
sw_font_frame:=3;
%-----
MCd(1,0.8)(0.1,0.5)
(<30,Ph,2:/OH,5:/OH)
MCd(1,0.8)(0.9,0.5)
(<30,?6,$(3,6)d1,@(2,5)//0)
%-----
EXT(
    draw_vector((0.7w,0.48h), 0,0.2mm,0.4w):
    draw_vector((0.3w,0.52h),180,0.2mm,0.4w):
    drawdot p0 withpen pencircle scaled 3pt;
    drawdot p1 withpen pencircle scaled 3pt;
    drawdot p2 withpen pencircle scaled 3pt;
    %-----
    label.bot("p0",p0);
    label.bot("p1",p1);
    label.bot("p2",p2);
    label("Ox", (0.5w,0.6h));
    label("Red", (0.5w,0.4h));
    use_font(6pt#); % **default 5pt#
    label("Reaction example", (0.5w,0.8h));
)
%-----
endfont
```



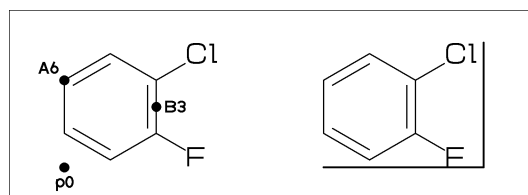
### 4.4 Function ext()

(Add extra graphic to molecule)

```
wd: molecular width
ht: molecular height
p0: origin of molecular structure
l: bond length
An: atom number
A[m]: atom position
A[m]bra: branch angle of A[m]
Bn: bond number
B[m]: bond position
B[m]ang: bond angle
```

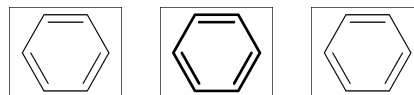
beginfont()

```
%-----
MCd(1,0.9)(0.1,0.5)(<30,Ph,3:/F,4:/Cl)
ext(
    drawdot p0 withpen pencircle scaled 3pt;
    drawdot A6 withpen pencircle scaled 3pt;
    drawdot B3 withpen pencircle scaled 3pt;
    label.bot("p0",p0);
    label.ulft("A6",A6);
    label.rt("B3",B3);
)
%-----
MCd(1,0.9)(0.9,0.5)(<30,Ph,3:/F,4:/Cl)
ext(draw p0--(p0+(wd,0))--(p0+(wd,ht));)
%-----
endfont
```



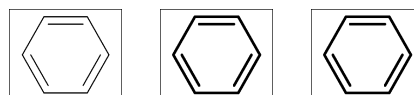
### 4.5 Local parameter setting

```
beginfont() MCf(Ph) endfont
beginfont()
    ratio_thickness_bond:=0.05;
    MCf(Ph)
endfont
beginfont() MCf(Ph) endfont
```



### 4.6 Global parameter setting

```
beginfont() MCf(Ph) endfont
ratio_thickness_bond:=0.05;
beginfont() MCf(Ph) endfont
beginfont() MCf(Ph) endfont
```



## 5 Output information

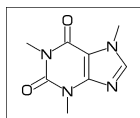
### 5.1 Output molecular information

```
tag3="cMW"; var3="calc_weight";
tag4="cFM"; var4="calc_formula";
%-----
beginfont()
  MCf(<30,?6,3=d,
      @ (2,6)N,@ (2,6)/_,@ (1,5)//0,
      |,-4=?5,2=d1,@ (1,3)N,3:/_)
endfont
beginfont(.....)
.....
endfont
.....

%% Output to mcf_man_soc-info.aux %%
..... ;C:85;cMW:194.19174;cFM:C8H10N4O2
.....
```

```
** default value
tag1="F"; var1="jobname";
tag2="C"; var2="char_num";
```

cMW:calculated molecular weight  
cFM:calculated molecular formula



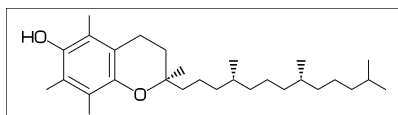
### 5.2 Output additional information

```
beginfont("EN:Tocopherol","CAS:59-02-9")
  MCf(<30,Ph,3=?6,
      7:0,@ (1,2,5)/_,8:/*_^60,6:/OH,
      8\,|,!12,@ (4,8)/*_ ,12:/_)
endfont
beginfont(.....)
.....
endfont
.....

%% Output to mcf_man_soc-info.aux %%
F:mcf_man_soc;C:86;EN:Tocopherol;CAS:59-02-9
.....

1* F:filename
2* C:char number
3 EN:molecular name
4 CAS:CAS number

*:default output
```

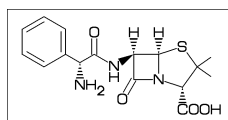


### 5.3 Change aux information delimiter

```
aux_delimiter="/";
beginfont("EN:Ampicillin","CAS:69-53-4")
  MCf(<45,?4,2:N,2=?5,-1:S,
      @ (3^45,4^-45)/*H,1:/O^15,
      5:/*COOH^-18,@ (6^35,6^-35)/_,
      4*\^75,NH,! ,/O,! ,/*NH2,! ,Ph)
endfont
beginfont(.....)
.....
endfont
.....

%% Output to mcf_man_soc-info.aux %%
F:mcf_man_soc/C:90/EN:Ampicillin/CAS:69-53-4
.....

**default aux_delimiter=","
```

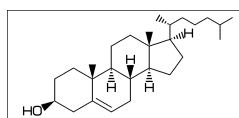


### 5.4 Fixed aux information

```
tag3="NO"; var3="inf_NO";
tag4="EN"; var4="inf_EN";
sw_auxfix=1;
auxtag_out; % output tag list
%-----
beginfont("EN:Cholesterol","NO:1")
  MCf(
    <30,?6,$(-4,-2)?6,-4=?5,7=d1,
    1:/OH,@ (4,12)/*_^60,9:/H^60,
    10:/H^180,11:/H^60,17:/H^54,
    -1\^18,/*_,-60,!3,/_,!
  )
endfont
%-----
beginfont(.....)
.....
endfont
%-----
.....

%% Output to mcf_man_soc-info.aux %%
F;C;NO;EN
mcf_man_soc;91;1;Ampicillin
.....
.....

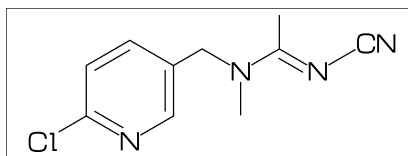
** default sw_auxfix=0
```



## 6 MCF example

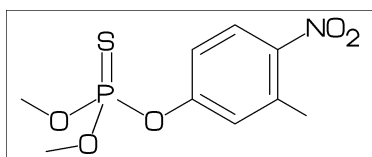
### Acetamiprid

<30,Ph,2:N,1:/Cl,  
4\,!,N,/\_,!/\_,!N,!,CN



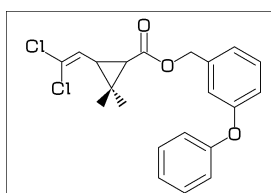
### Fenitrothion

<30,!,0,!,P,//S,/O!^160,!,0,!,  
|,Ph,3:/\_,4:/NO2



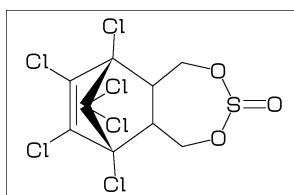
### Permethrin

<-30,?3,2^-35:\*/\_-,2^35:/\*\_,  
1\,!!,/Cl,!,Cl,  
3\,//0,!,0,!,2,|,Ph,  
3\,0,-60,Ph



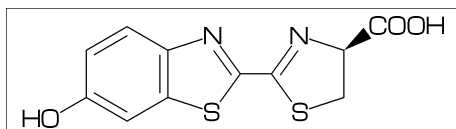
### Endosulfan

<26,?7,7=?6[13],11\*,208~wf'1.45,&8~wb,  
10=d,@(3,5)0,4:S,4://0,  
@(8,9,10,11,12^-210,12^-150)/Cl



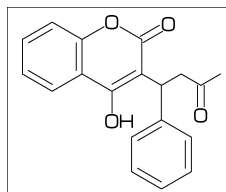
### Luciferin

<30,Ph,3=?5,8\,?5,\$(9,16)d,  
@(9,14)N,@(7,11)S,  
1:/OH,-2:\*/COOH



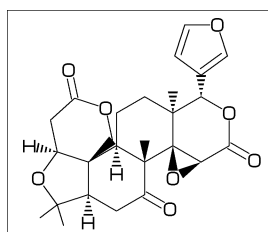
### Warfarin

<30,Ph,3=?6,8=d1,  
10:0,7:/OH,9://0,  
8\,/Ph'1,60,!//0,!



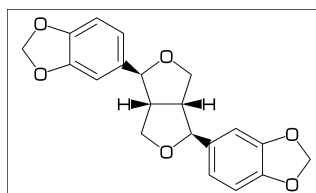
### Limonin

<30,?6,\$(-3,-4)?6,-5=?3,  
-2=wf,-1=wb,6=?5,-4=?6,-5=wf,  
@(13,15,17,20)0,@(3,12,21)//0,  
@(4~wf^60,8~zf^60,18^35,18^-35)/\_,  
@(1^60,5^180,16^60)/\*H,  
14\\*,|,?5,\$(1,4)d1,3:0



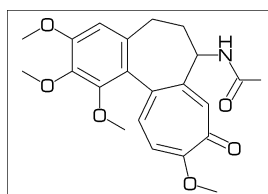
### Sesamine

<54,?5,1=?5,  
@(4,7)0,@(1^-54,2^54)\*H,  
#5\*\^-12,Ph,|,-3=?5,@(-1,-3)0,  
#8\*\^-12,Ph,|,-3=?5,@(-1,-3)0



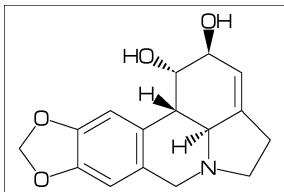
### Colchicine

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



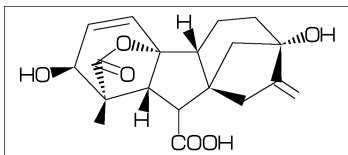
## Lycorine

<30,Ph,  
-4=?6,-2=?6,6=?5,(9,12)=?5[3],  
13=d1,  
8:N,@(15,17)O,  
9:/\*H^180,10:/\*H^60,  
13:\*/OH,14:/\*OMe



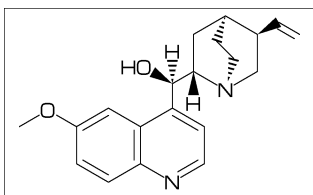
## Gibberellin

<18,?5,3=?7,5=?6[12],  
8\*,160'1.3,&3,  
13=d1,6=wf,8=wb,  
5\*,40~zf'1,0,60,//0^180,&14~zb,  
2:/COOH,7://\_,13:\*/OH,8:\*/OH,  
14:\*/\_,@(1^60,4^60)\*/H



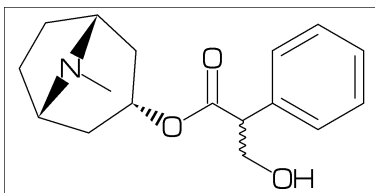
## Quinine

<30,Ph,3=Ph,7:N,6:/O!,  
10\,\*/OH,/H~zf^-60,!,  
|,?6,2:N,1:\*/H^60,  
4\*\,!!,  
2\*,165~zf,60,&5~zb



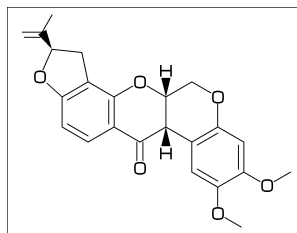
## Atoropin

<-30,0,!,//0,!,!,Ph,  
#1~zb^-120,  
|,?7,6\*\^190'1.02,N,/\_,&3~wb,  
#3~wv,!,OH



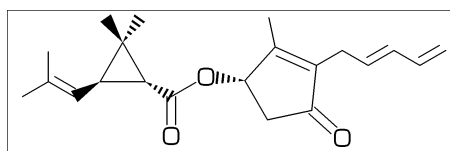
## Rotenone

<-60,?5,\$(-3,-2,-3,-4)?6,  
\$(7,9,-2,-4)d1,\$(3,17)dr,  
@(2,13,16)O,10:/O, @(11^-60,12^60)\*/H,  
@(-2,-3)/O!,1\*\,/\_,!!



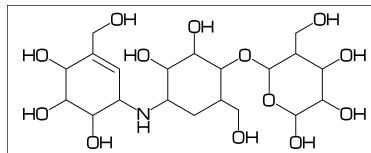
## Pyrethrin I

<30,?3,@(3^35~wf,3^-35~zf)/\_,  
1\*\,!!,iPr,2\\*,//0,!,0,-36~zb,|,  
?5,-2=d,-1:/\_,-3:/O,-2\,!4,\$(-1,-3)d1



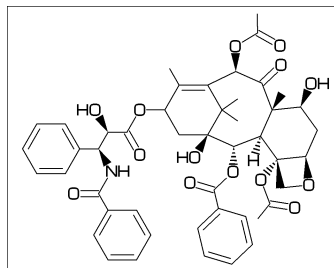
## Validamycin

<30,?6,@(5,6)/OH,3:/!OH>r1,  
#4\,0,-60,|,?6,2:O,@(3,4,5)/OH,6:/!OH,  
#1\,NH,!,|,?6,2=d1,@(4,5,6)/OH,3:/!OH



## Paclitaxel

?6,5=d,3\*{,' '1,36,45,45,45,45,}&#5,  
-4=?6,-4=?4,-1=wb,-3=wf,-1:O,||,  
@(4^35,4^-35,6)/\_,@(3^-60,15)\*/OH,  
8:/\*H^-60,9:\*/\_ ^60,10:/O,  
1\,0,!,//0,!,\*/OH,!,/Ph,  
60~wf,NH,-60,//0,60,Ph,  
7\\*,0,-45,//0,60,Ph,11\*\,0,-60,//0,60,  
12\\*^-15,0,60,//0,-60



## 7 Example to use mcf2graph

### 7.1 Molecular definition file

```
%-----
input mcf2graph.mf;                                     % input macro
%-----
sw_auxout:=1;      % aux(information) file output on > Gloval setting
font_wd#:=60mm#;   % font width                      >
font_ht#:=40mm#;   % font height                     >
var3:="cal_MW"; tag3:="cMW";                          > AUX file table
var4:="cal_FM"; tag4:="cFM";                          >
%%% sw_report:=1;  > Report output
%%% sw_MOLout:=1;  > MOL file output
outputformat:="png"; hppp:=vppp:=0.1;                  > PNG output
outputtemplate:="%j-%3c.png";                          >
%-----
beginfont("NO:1","EN:Ampicillin")                      > begin font(information)
  MCF(<45,?4,2:N,2=?5,-1:S,                             > begin MCF (1)
    @(3^45,4^~45)*H,1://0^15,5:/*COOH^~18,              >
    @(6^35,6^~35)/_,                                    >
    4\^75,NH,!,//0,!/*NH,! ,Ph)                        > end MCF
endfont                                                  > end font
%-----
beginfont("NO:2","EN:Cholesterol")                      > begin font(information)
  MCF(<30,?6,$(-4,-2)?6,-4=?5,7=d1,                     > begin MCF (2)
    1:*/OH,@(4,12)*/_^60,9:*/H^60,                      >
    10:/*H^180,@(11,-1)*H^~60,                         >
    -1\^17,/*_,!4,/_,!)                                > end MCF
endfont                                                  > end font
%-----
beginfont("NO:3","EN:Limonin")                          > begin font(information)
  MCF(<30,?6,$(-3,-4)?6,                                > begin MCF (3)
    -5=?3,-2=wf,-1=wb,6=?5,-4=?6,-5=wf,               >
    @(13,15,17,20)0,@(3,12,21)//0,                    >
    @(4~wf^60,8~zf^60,18^35,18^~35)/_,                >
    @(1^60,5^180,16^60)*H,                             >
    14\*,|,?5,$(1,4)d1,3:0)                            > end MCF
endfont                                                  > end font
%-----
beginfont("NO:4","EN:beta-carotene")                    > begin font(information)
  MCF(<30,?6,3=d1,@(3,5^35,5^~35)/_,                   > begin MCF (4)
    4\,|,!18,$(1,3,5,7,9,11,13,15,17)dr,               >
    @(3,7,12,16)/_,                                    >
    |,?6,6=d1,@(6,2^35,2^~35)/_)                       > end MCF
endfont                                                  > end font
%-----
beginfont("NO:5","EN:Gibberellin A3");                  > begin font(information)
  MCF(<18,?5,3=?7,5=?6[12],                             > begin MCF (5)
    8*,160'1.3,&3,13=d1,6=wf,8=wb,                    >
    5*,40~zf'1,0,60,//0^180,&14~zb,                   >
    2:/COOH,7://_,13:*/OH,8:/*OH,                     >
    14:*/_,@(1^60,4^60)*H)                             > end MCF
endfont;                                                 > end font
%-----
bye
```

## 7.2 Information auxfile output

(Insert option parameter setting)

```
sw_auxout:=1;
** default : sw_auxout=0
```

(Command line)

```
>mpost -s ahangle=0 FILENAME (molecular definition file)
```

(Output)

```
(sw_auxfix=0)
F:mcf_man_soc;C:1;cMW:349.40462;cFM:C16H19N3O4S;EN:Ampicillin
F:mcf_man_soc;C:2;cMW:386.6532;cFM:C27H46O;EN:Cholesterol
F:mcf_exa_soc;C:3;cMW:470.5113;cFM:C26H30O8;EN:Limonin
F:mcf_exa_soc;C:4;cMW:536.8722;cFM:C40H56;EN:beta-Carotene
F:mcf_exa_soc;C:5;cMW:346.3742;cFM:C19H22O6;EN:Gibberellin A3
.....
.....
```

```
(sw_auxfix=1)
F;C;cMW;cFM;EN
mcf_man_soc;1;349.40462;C16H19N3O4S;Ampicillin
mcf_man_soc;2;386.6532;C27H46O;Cholesterol
mcf_exa_soc;3;470.5113;C26H30O8;Limonin
mcf_exa_soc;4;536.8722;C40H56;beta-Carotene
mcf_exa_soc;5;346.3742;C19H22O6;Gibberellin A3
.....
.....
```

( Tag )

```
F   : filename
C   : char number
NO  : serial number
EN  : english name
JN  : japanese name
FM  : formula from literature data
MW  : molecular weight from literature data
USE : the use
cMW : molecular weight calculated
cMI : monoisotopic mass calculated
cFM : molecular formula calculated
```



### 7.3 Report output

(Insert option parameter setting)

```
sw_report:=1;
** default : sw_report=0
```

(Command line)

```
>mpost -s ahandle=0 -s ahandle=2 FILENAME (molecular definition file)
```

(Output)

```
%-----
% Molecular name = Caffeine
% Warnings = 0 / Expanded command = 80
% Width * Height = 54.31772 * 50.43338
% Shift width * height = -12.59462 * -17.49146
% Bond length = 12.75589 Atom size = 5.38914
% Atom count= 14 Bond count= 15 Ring count= 2 Hide H count= 10
%-----
%< NO. >( x axis , y axis )< atom >< bond >< hide_H >
% A1 ( 0 , 0 ) C 4
% A2 ( 0.866 , -0.5 ) N 3
% A3 ( 1.732 , 0 ) C 4
% A4 ( 1.732 , 1 ) C 4
% A5 ( 0.866 , 1.5 ) C 4
% A6 ( 0 , 1 ) N 3
% A7 ( 2.683 , -0.309 ) N 3
% A8 ( 3.271 , 0.5 ) C 3 1
% A9 ( 2.683 , 1.309 ) N 3
% A10 ( 0.866 , -1.371 ) C 1 3
% A11 ( -0.776 , 1.448 ) C 1 3
% A12 ( -0.776 , -0.448 ) O 2
% A13 ( 0.866 , 2.371 ) O 2
% A14 ( 2.955 , 2.147 ) C 1 3
%-----
%< NO. >< bond (sdt)><angle + ( +- )><length ( pt )>
% B1 1 -> 2 ( 1 ) 330 ( -30 ) 1 ( 12.76)
% B2 2 -> 3 ( 1 ) 30 ( 30 ) 1 ( 12.76)
% B3 3 -> 4 ( 2 ) 90 ( 90 ) 1 ( 12.76)
% B4 4 -> 5 ( 1 ) 150 ( 150 ) 1 ( 12.76)
% B5 5 -> 6 ( 1 ) 210 ( -150 ) 1 ( 12.76)
% B6 6 -> 1 ( 1 ) 270 ( -90 ) 1 ( 12.76)
% B7 3 -> 7 ( 1 ) 342 ( -18 ) 1 ( 12.76)
% B8 7 -> 8 ( 2 ) 54 ( 54 ) 1 ( 12.76)
% B9 8 -> 9 ( 1 ) 126 ( 126 ) 1 ( 12.76)
% B10 9 -> 4 ( 1 ) 198 ( -162 ) 0.66 ( 8.42)
% B11 2 -> 10 ( 1 ) 270 ( -90 ) 0.66 ( 8.42)
% B12 6 -> 11 ( 1 ) 150 ( 150 ) 0.66 ( 8.42)
% B13 1 -> 12 ( 2 ) 210 ( -150 ) 0.66 ( 8.42)
% B14 5 -> 13 ( 2 ) 90 ( 90 ) 0.66 ( 8.42)
% B15 9 -> 14 ( 1 ) 72 ( 72 ) 0.66 ( 8.42)
%-----
% C ( 12.0107 ) * 8 = 96.08557
% H ( 1.00793 ) * 10 = 10.07935
% N ( 14.0067 ) * 4 = 56.0268
% O ( 15.9994 ) * 2 = 31.99881
% Monoisotopic mass: 194.08038
% Weight Calc: 194.1905 / Input: 194.194 / weight gap= -0.00348
% Formula Calc: C8H10N4O2 / Input:
%=====
```

## 7.4 Molfile output

(Insert option parameter setting)

```
sw_MOLout:=1;  
** default : sw_MOLout=0
```

(Command line)

```
>mpost -s ahandle=3  FILENAME (molecular definition file)
```

(Output)

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%  
-MCFtoMOL- EN:Caffeine  
  
14 15  0  0  0  0  0  0  0  0999 V2000  
      0      0      0 C  0  0  0  0  
0.86603     -0.5      0 N  0  0  0  0  
1.73206      0      0 C  0  0  0  0  
1.73206      1      0 C  0  0  0  0  
0.86603     1.5      0 C  0  0  0  0  
      0      1      0 N  0  0  0  0  
2.6831    -0.30902    0 N  0  0  0  0  
3.27089      0.5      0 C  0  0  0  0  
2.6831     1.30902    0 N  0  0  0  0  
0.86603    -1.36383    0 C  0  0  0  0  
-0.76894     1.44394    0 C  0  0  0  0  
-0.76894    -0.44394    0 O  0  0  0  0  
0.86603     2.36383    0 O  0  0  0  0  
2.95299     2.1396     0 C  0  0  0  0  
1  2  1  0      0  0  
2  3  1  0      0  0  
3  4  2  0      0  0  
4  5  1  0      0  0  
5  6  1  0      0  0  
6  1  1  0      0  0  
3  7  1  0      0  0  
7  8  2  0      0  0  
8  9  1  0      0  0  
9  4  1  0      0  0  
2 10  1  0      0  0  
6 11  1  0      0  0  
1 12  2  0      0  0  
5 13  2  0      0  0  
9 14  1  0      0  0  
M  END  
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

## 7.5 LuaTeX file example

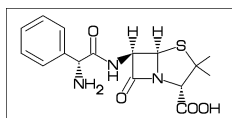
```
%-----
\documentclass{article}
\usepackage{luamplib}%
\mplibcodeinherit{enable}%
\mplibverbatim{enable}%
\everymplib{if unknown Ph1:
    input mcf2graph.mf;
    mp_log_name:="temp-info.aux";
    sw_auxout:=1;
fi}%
%-----
\begin{document}
\noindent%
%-----
\begin{mplibcode}
font_wd:=50mm; font_ht:=50mm;
beginfont("N0:2","EN:Limonin","MW:470.51")
MCf(<30,
    ?6,$(-3,-4)?6,
    -5=?3,-2=wf,-1=wb,6=?5,-4=?6,-5=wf,
    @(13,15,17,20)0,@(3,12,21)//0,
    @(4~wf^60,8~zf^60,18^35,18^-35)/_,
    @(1^60,5^180,16^60)*H,
    14\*,|,?5,$(1,4)d1,3:0
)
endfont
\end{mplibcode}\\
%-----
\begin{mplibcode}
font_wd:=80mm; font_ht:=50mm;
beginfont("N0:3","EN:beta-carotene","MW:536.87")
MCf(<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)/_
)
endfont
\end{mplibcode}\\
%-----
\begin{mplibcode}
font_wd:=50mm; font_ht:=50mm;
beginfont("N0:4","EN:Gibberellin A3","MW:346.37");
MCf(<18,?5,3=?7,5=?6[12],
    8*,160'1.3,&3,13=d1,6=wf,8=wb,
    5*,40~zf'1,0,60,//0^180,&14~zb,
    2:/COOH,7://_,13:*/OH,8:/*OH,
    14:*/_,@(1^60,4^60)*H
)
endfont;
\end{mplibcode}\\
%-----
\end{document}
%-----
```

## 7.6 LaTeX file example

```
%-----
\documentclass[a4paper]{article}
\usepackage{graphicx}
\pagestyle{empty}
\makeatletter%
%-----
\def\@F{F}\def\@C{C}\def\@EN{EN}\def\@NO{NO}\def\@MW{MW}\def\@FMc{FMc}%
\def\@fst@param#1:#2;{#1}\def\@sec@param#1:#2;{#2}%
\def\mol@sel#1{%
\if#1empty\relax\else%
\edef\@tag{\expandafter\@fst@param#1;}%
\edef\@var{\expandafter\@sec@param#1;}%
\ifx\@tag\@F\edef\MOLfile{\@var}\fi%
\ifx\@tag\@C\edef\MOLchar{\@var}\fi%
\ifx\@tag\@EN\edef\MOLnameE{\@var}\fi%
\ifx\@tag\@NO\edef\MOLnum{\@var}\fi%
\ifx\@tag\@MW\edef\CALmw{\@var}\fi%
\ifx\@tag\@FMc\edef\CALfm{\@var}\fi%
\fi}%
\def\put@char{%
\begin{picture}(84,42)%
\put(0,38){\bf [MOLnum]\MOLnameE{ }\small\tt/FM:\CALfm/MW:\CALmw}%
\put(10,0){\font\@strufont=\MOLfile\relax%
\hbox{\@strufont\char\MOLchar}}%
\end{picture}%
\def\INFO#1{\@for\@temp:=#1\do{\mol@sel\@temp}\put@char}%
\makeatother
%-----
\begin{document}
\unitlength=1mm%
\INFO{F:mcf_man_soc,C:115,NO:1,cMW:349.40462,cFM:C16H19N3O4S,EN:Ampicillin}%
\INFO{F:mcf_man_soc,C:116,NO:2,cMW:386.6532,cFM:C27H46O,EN:Cholesterol}%
\end{document}
%-----
```

### [1]Ampicillin

FM:C16H19N3O4S MW:349.40462



### [2]Cholesterol

FM:C27H46O MW:386.6532

