

Molecular Coding Format manual

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

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

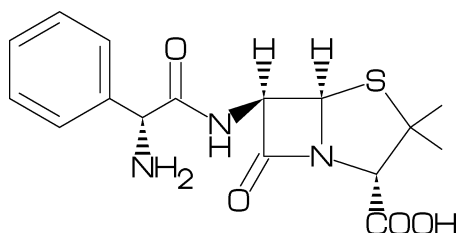
(Molecular definition file)

```
%-----
input mcf2graph.mf;                                % input macro
%-----
sw_auxout:=1;          % aux(information) file output on > Gloval setting
sw_numberA:=0;         % numbering atom off           >
sw_numberB:=0;         % numbering bond off           >
sw_expand:=0;          % substituent expand mode off  >
sw_start_vector:=0;    % start vector output off      >
sw_font_frame:=0;      % font frame off               >
font_wd#:=60mm#;       % font width                  >
font_ht#:=40mm#;       % font height                  >
var3:="cal_MW"; tag3:="cMW";                          > AUX file table
var4:="cal_FM"; tag4:="cFM";                          >
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)/Me,                                >
    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)*~Me^60,9:*/H^60,                  >
    10:/*H^180,@(11,-1)/~H^~60,                      >
    -1\^17,/*Me,!4,/Me,! )                          > end MCF
endfont                                                > end font
%-----
bye
```

(Molecular structure output)

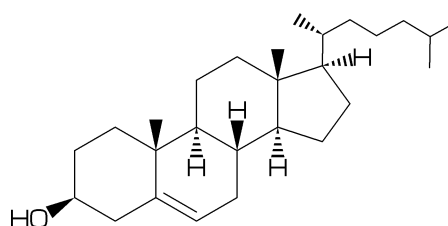
[1]Ampicillin

FM:C16H19N3O4S MW:349.40462



[2]Cholesterol

FM:C27H46O MW:386.6532



(Molecular information output)

'filename'-info.aux : for use in T_EX, it takes over filename, char number, molecular information,etc.

```
(sw_auxfix=0)
F:mcf_man_soc;C:90;cmw:349.40462;cfm:C16H19N3O4S;EN:Ampicillin
F:mcf_man_soc;C:91;cmw:386.6532;cfm:C27H46O;EN:Cholesterol
.....
.....
```

```
(sw_auxfix=1)
F;C;cmw;cfm;EN
mcf_man_soc;90;349.40462;C16H19N3O4S;Ampicillin
mcf_man_soc;91;386.6532;C27H46O;Cholesterol
.....
.....
```

```
( tag : variable )
F : filename   C : char number   NO : serial number   EN : english name
cmw : molecular weight calculated   cfm : molecular formula calculated
MW  : molecular weight from literature data
```

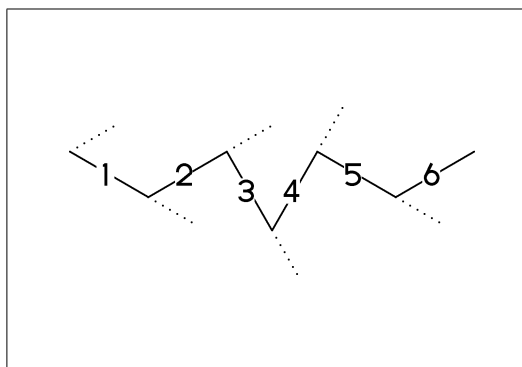
(LaTeX file example)

```
%-----
\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#1\empty\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:90,NO:1,cmw:349.40462,cfm:C16H19N3O4S,EN:Ampicillin}%
\INFO{F:mcf_man_soc,C:91,NO:2,cmw:386.6532,cfm:C27H46O,EN:Cholesterol}%
\end{document}
%-----
```

No.1 Chain(1)

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

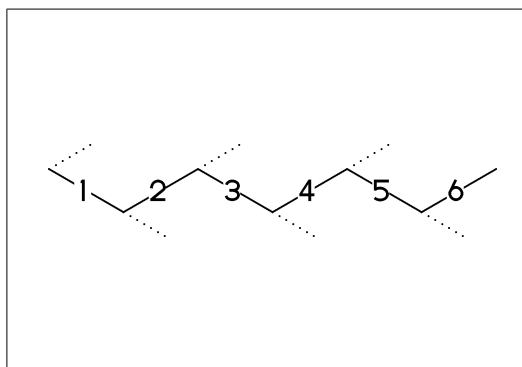
<30,-60,60,-90,120,-90,60



No.2 Chain(2)

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

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

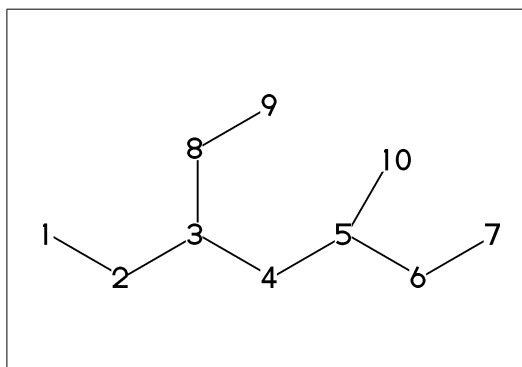


No.3 Jump to atom and branch bond

n* : Jump to An

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

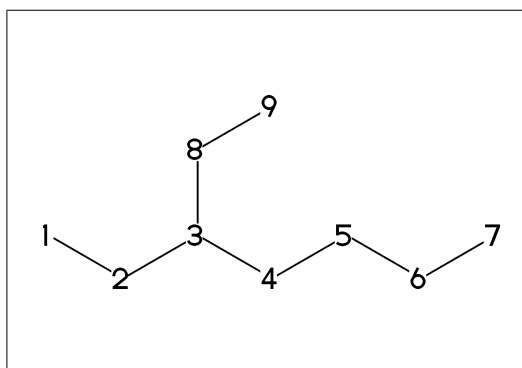
** An(-999<=n<=4095): atom number



No.4 Jump to atom and branch bond

3\ : 3*,0

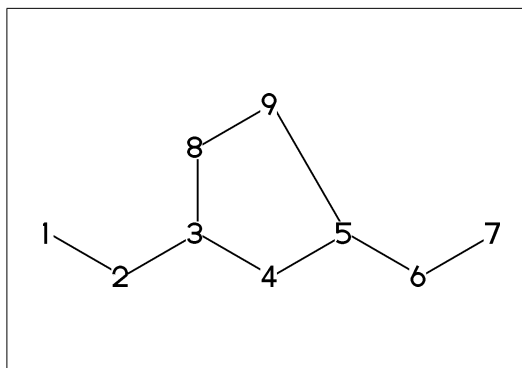
<30,!6,3\,! ,



No.5 Connect atom

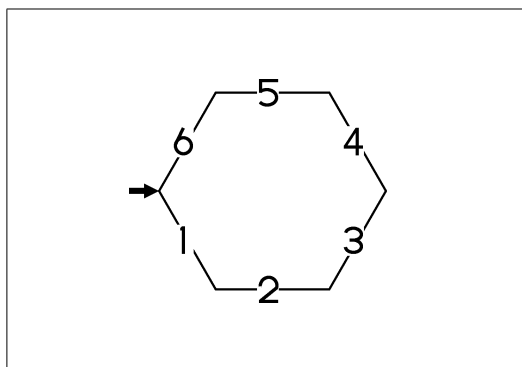
&n : Connect to An

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



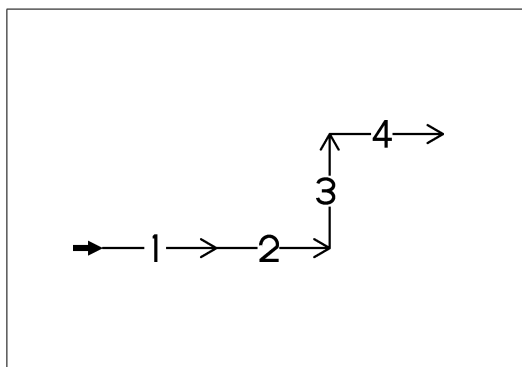
No.6 Ring

?n : n membered ring
?6
** ?6 : <-120,60,60,60,60,60,&1
** ?n(3<=n<=20)
** bold arrow is default angle and position



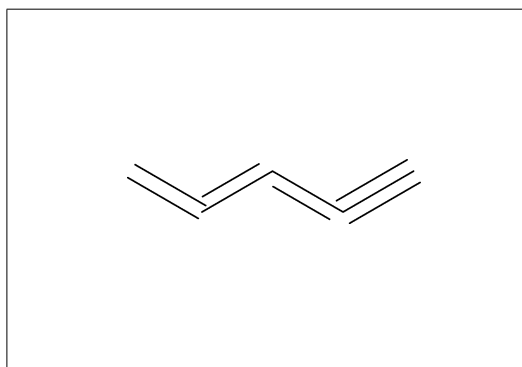
No.7 Rotate current angle

<angle : rotate current angle
‘‘1,
0~vf,0~vf,<90,0~vf,<-90,0~vf



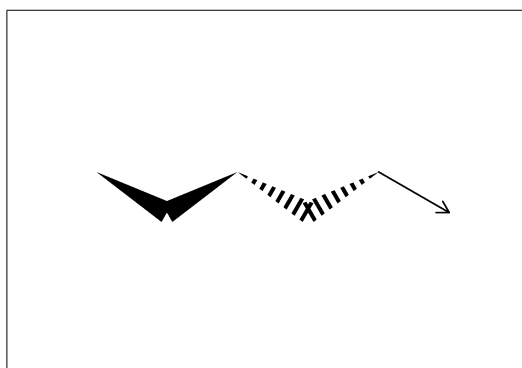
No.8 Change bond type (1)

a~type : ~type,a
dm : double middle
dl : double left side
dr : double right side
tm : triple
<30,!~dm,!~dl,!~dr,!~tm



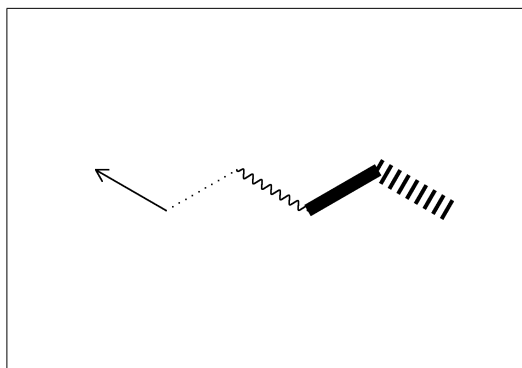
No.9 Change bond type (2)

a~type : ~type,a
wf : wedge forward
wb : wedge backward
zf : wedge dotted
zb : wedge dotted backward
vf : vector forward
vb : vector backward
<30,!~wf,!~wb,!~zf,!~zb,!~vf,!~vb



No.10 Change bond type (3)

Bn=bond type : change bond type at Bn
vb : vector backward
dt : dotted
wv : wave
bd : broad
bz : broad dotted
<30,!5,1=vb,2=dt,3=wv,4=bd,5=bz

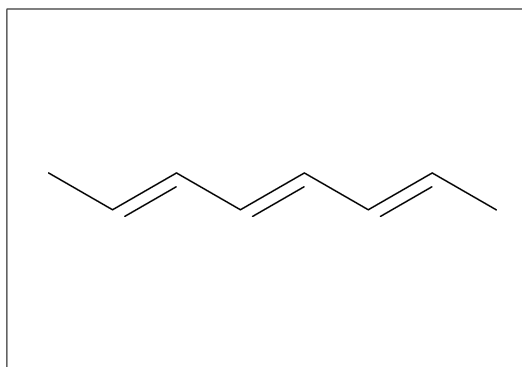


No.11 Change bond type (4)

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

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

`** <30,!7,2=dr,4=dr,6=dr`



No.12 Over line

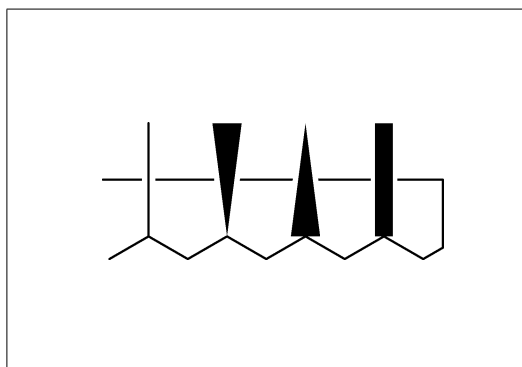
`si_ : single over line`

`wf_ : wedge forward over line`

`wb_ : wedge backward over line`

`bd_ : broad over line`

`<-30,!8'.4,!'.2,60'.6,90'3,
@(2~si_,4~wf_,6~wb_,8~bd_)/Me'1`

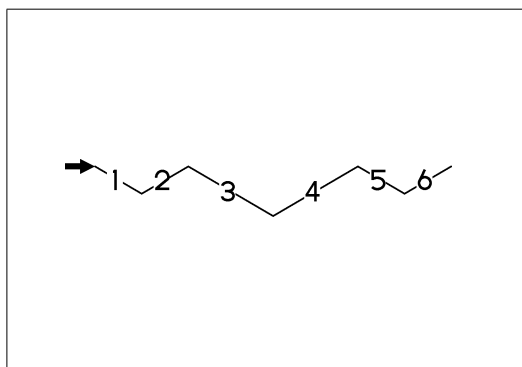


No.13 Change bond length (1)

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

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

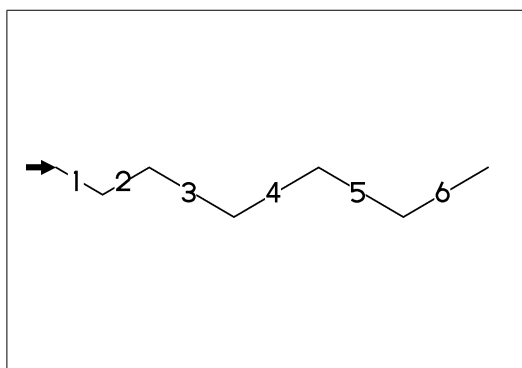
`** !2'1.2 : '1.2,!2`



No.14 Change bond length (2)

`''length : change all bond length after`

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

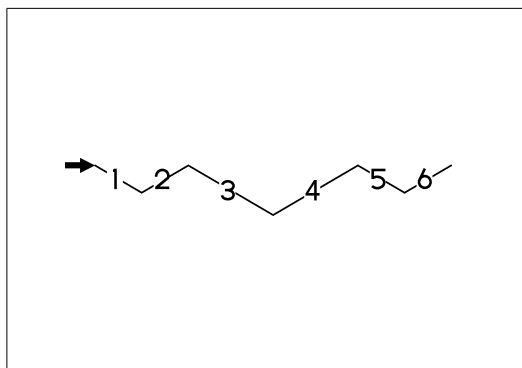


No.15 Make block

`{ : start brock`

`} : end brock`

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

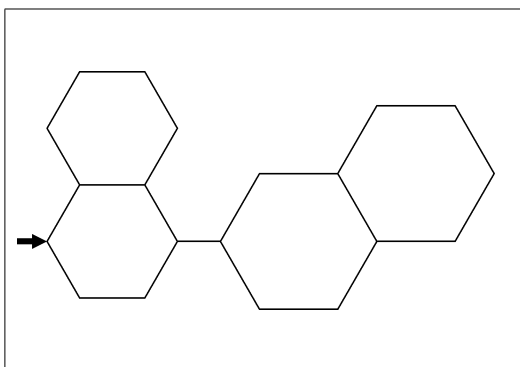


No.16 Change ring length

?n'length : change ring length

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

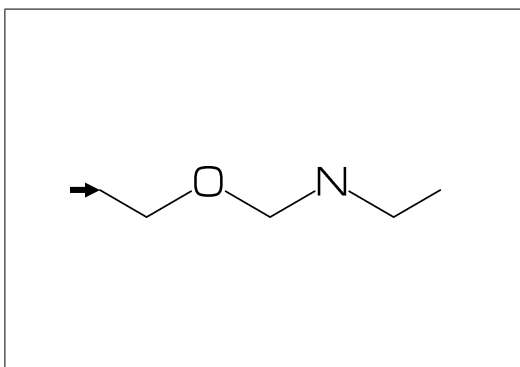
** fused ring size depend on
attached bond length



No.17 Change atom (1)

Insert hetero atom

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

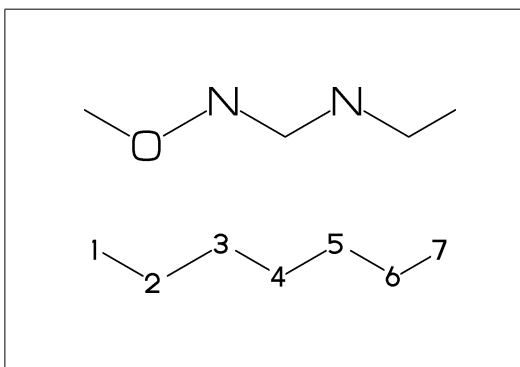


No.18 Change atom (2)

2:0 : change A2 C to O

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

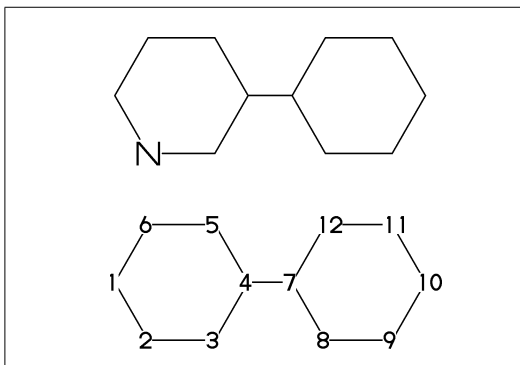
<30,!6,2:0,@(3,5)N



No.19 Change atom (3)

2:N : change A2 C to N

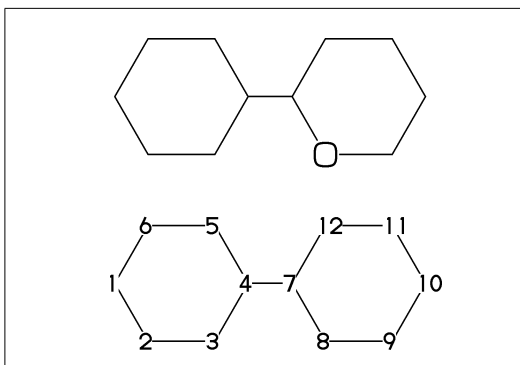
?6,4\,?6,2:N



No.20 Change atom (brock address 1)

| : divide brock

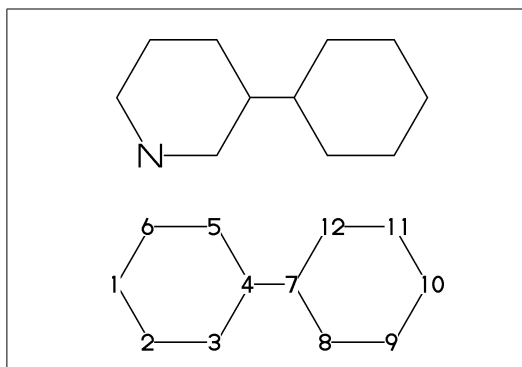
?6,4\,|,?6,2:0



No.21 Change atom (brock address 2)

|| : reset brock address

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

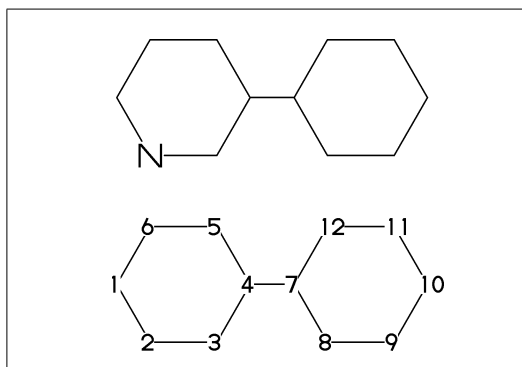


No.22 Change atom (absolute address)

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

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

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

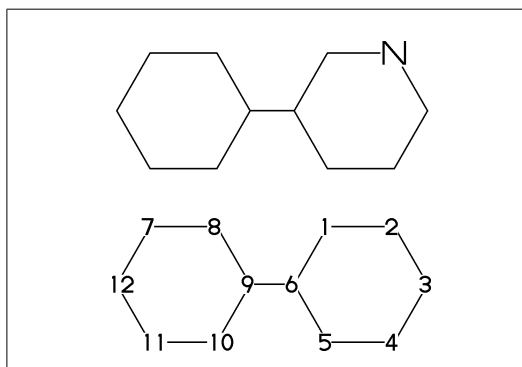


No.23 Change atom (relative address)

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

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

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

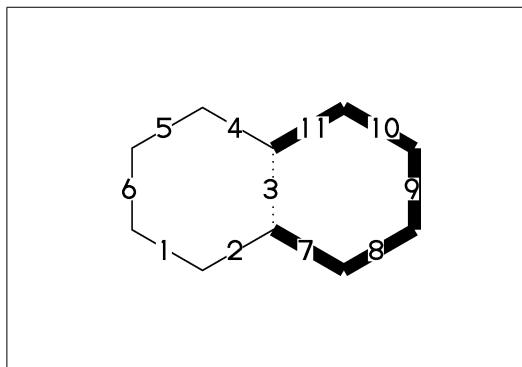


No.24 Fuse ring (attached 1 bond)

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

?6,3=?6

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



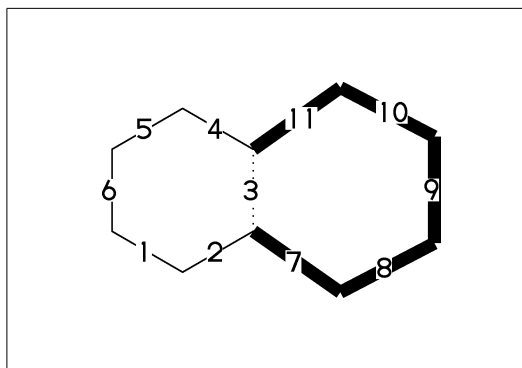
No.25 Fuse large ring (attached 1 bond)

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

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

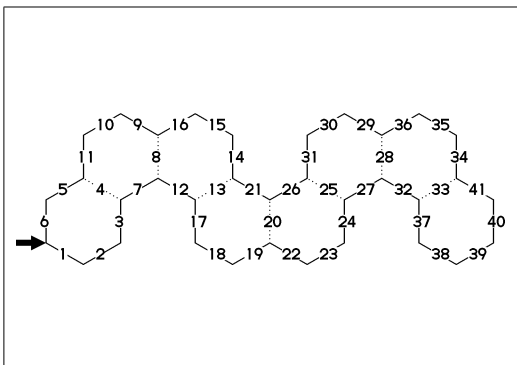
?6,3=?6[13]

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



No.26 Fuse multi ring (attached 1 bond)

```
?6,$(-3,-4,-4,-2,-2,-4,-4)?6
?6,$(4,8,13,20,25,28,33)?6
```

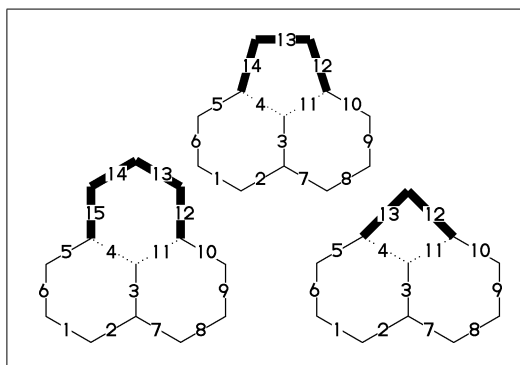


No.27 Fuse ring (attached 2 bond)

```
(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

MCd(1,.7)( 0,0)(<30,?6,3=?6,(11,4)=?6[4])
MCd(1,.6)(.54,1)(<30,?6,3=?6,(11,4)=?5[3])
MCd(1,.6)( 1,0)(<30,?6,3=?6,(11,4)=?4[2])

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

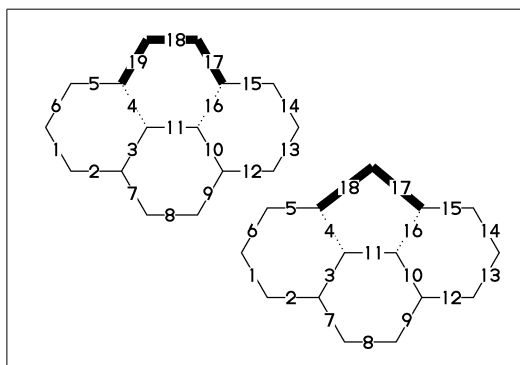


No.28 Fuse ring (attached 3 bond)

```
(16,4)=?6[3] : fuse 3/6 ring to B16..B4
(16,4)=?5[2] : fuse 2/5 ring to B16..B4

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

** ?m[n] (5<=m<=6,n=m-3)
```

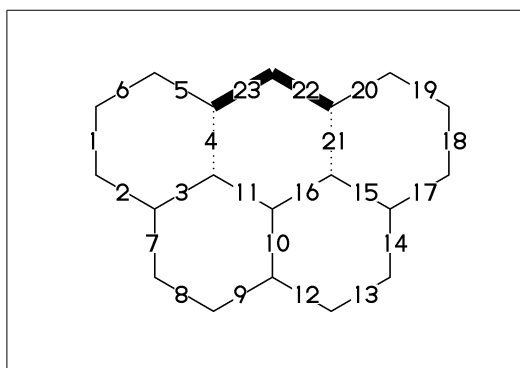


No.29 Fuse ring (attached 4 bond)

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

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

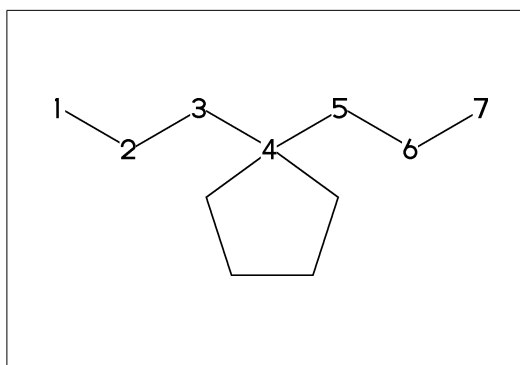
** ?m[n] (m=6,n=2)
```



No.30 Spiro ring

```
4*,?5 : add ?5(5 membered ring) at A4
<30,!6,4*,?5

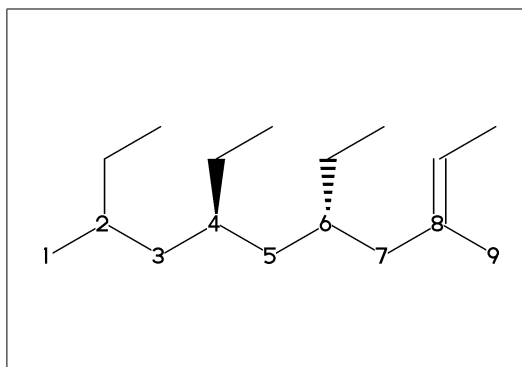
An* : jump to An
```



No.31 Branch bond (1)

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

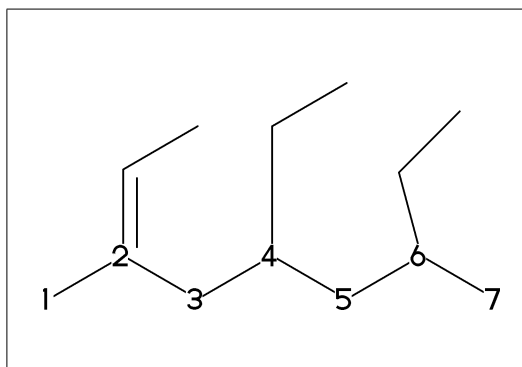
MCf(<30,!8,2\,! ,4*\,! ,6*,! ,8\\,!)



No.32 Branch bond (2)

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

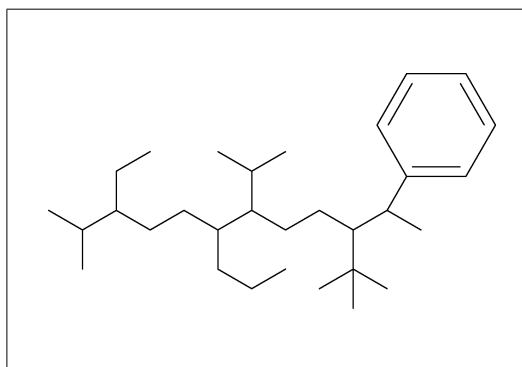
MCf(<-30,
 !6,2\~dr,! ,4\'1.5,! ,6\^15,-60)



No.33 Insert substituent(1)

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

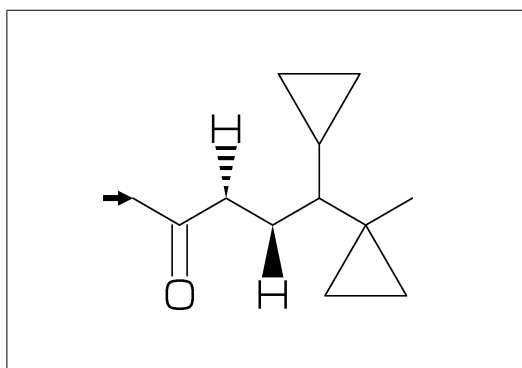
** Me:methyl Et:ethyl
 Pr:propyl iPr:isopropyl
 tBu:tertial buthyl Ph:phenyl



No.34 Insert substituent(2)

/ : single
 // : double
 */ : wedge forward
 /* : wedge dotted forward
 ** : direct

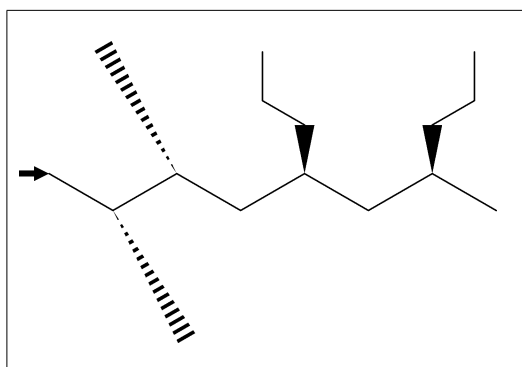
MCf(<30,! ,//0,! ,/*H,! ,*/H,! ,/?3,! ,**?3,!)



No.35 Insert substituent(3)

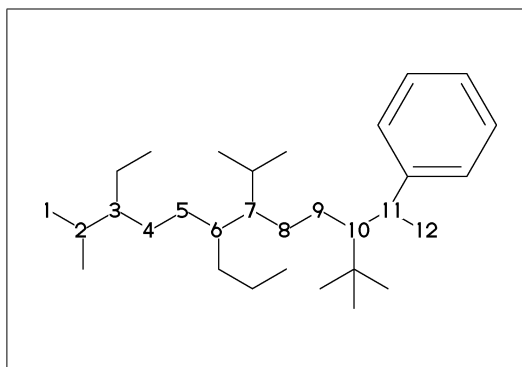
~ : change type
 ^ : change angle
 ' : change length
 > : change enviroment

MCf(<30,'^1,
 ! ,/Me~zf^2^30,! ,/Me~zf^2^30,
 !2,*/Pr>lr,!2,*/Pr>rl,!)



No.36 Add substituent(1)

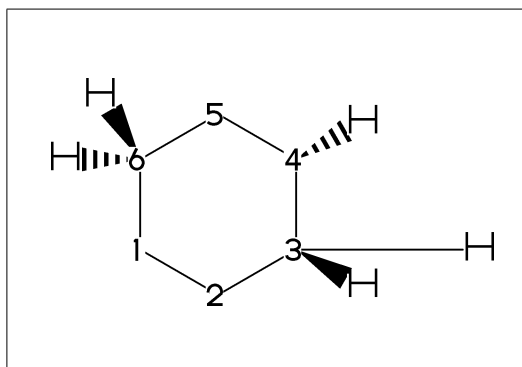
```
sw_numberA:=1; numberA_end:=12;
MCf(<30,!11,
  2:/Me,3:/Et,6:/Pr,7:/iPr,
  10:/tBu,11:/Ph^-30)
```



No.37 Add substituent(2)

```
~,^,' : change type,angle,length
        of substituent
```

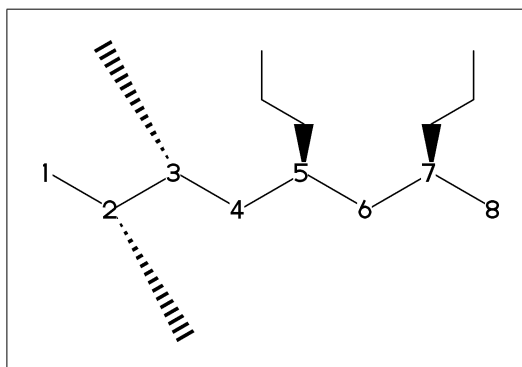
```
MCf(<30,?6,
  @(3'2^30,3~wf,4~zf,6~wf^-30,6~zf^30)/H)
```



No.38 Add substituent(3)

```
~,^,',> : change type,angle,length,
            environment of substituent
```

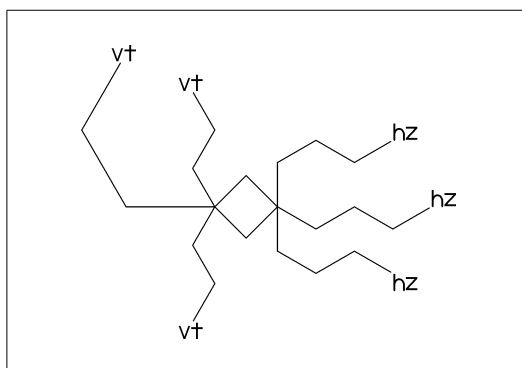
```
MCf(<30,!7'1,
  @(2,3)/*Me'2^30,5:*/Pr>lr,7:*/Pr>rl)
```



No.39 Chain stretch direction environment (1)

```
>hz : horizontal enviroment (default)
>vt : vertical enviroment
```

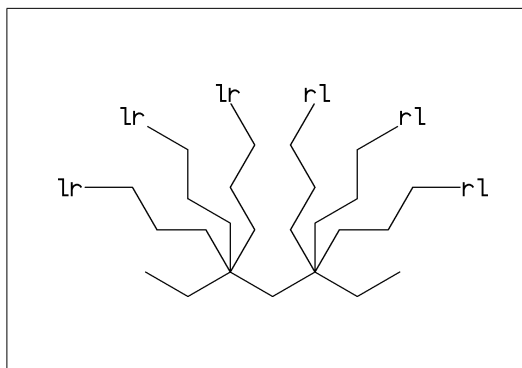
```
?4,
  @(3^-90,3^-30,3^90)/'(!3,"{hz}")>hz,
  @(1^-60,1'2,1^60)/'(!2,"{vt}")>vt
```



No.40 Chain stretch direction environment (2)

```
>lr : left-right enviroment
>rl : right-left enviroment
```

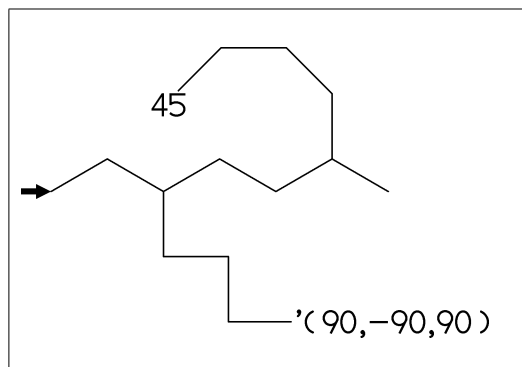
```
<30,!6,
  @(3^-30,3,3^30)/'(!3,"{lr}")>lr,
  @(5^-30,5,5^30)/'(!3,"{rl}")>rl
```



No.41 Chain stretch direction environment (3)

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

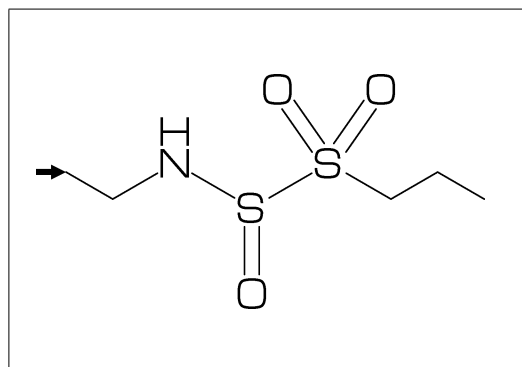
<-30,!6,@(2>45)/'(!3,"{45}"),
@ (6>'(-90,90,-90))/'(!3,"{(-90,90,-90)}")
```



No.42 Change atom and Substituent

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

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

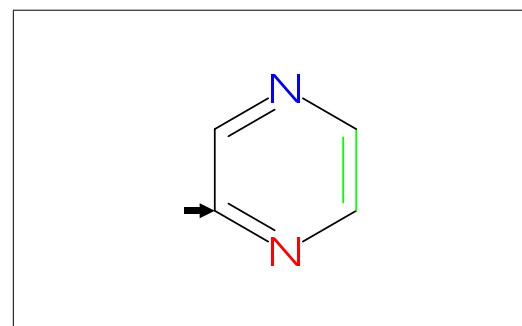


No.43 Change color

@(5)green : change color of A5 green
\$(3)red : change color of B3 red

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

** METAFONT ignore color command

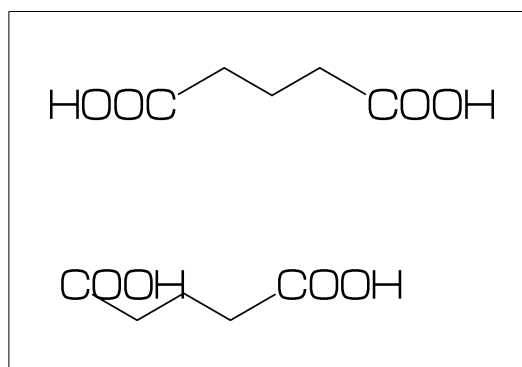


No.44 Chain start multiple characters

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

```
MCd( 1,1)(0 ,0.9)(<30,COOH,!0,!3,COOH)
```

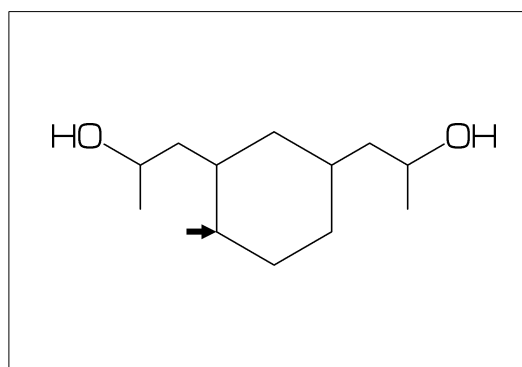
```
MCd(.8,1)(0.3,0.1)(<30,COOH,!4,COOH)
```



No.45 User definition

iBuOH : user defined substructure

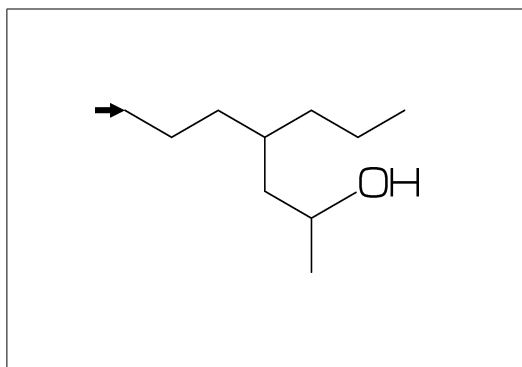
```
iBuOH:= '(!,/Me,! ,OH)
MCf(<30,?6,@(4,6)/iBuOH)
```



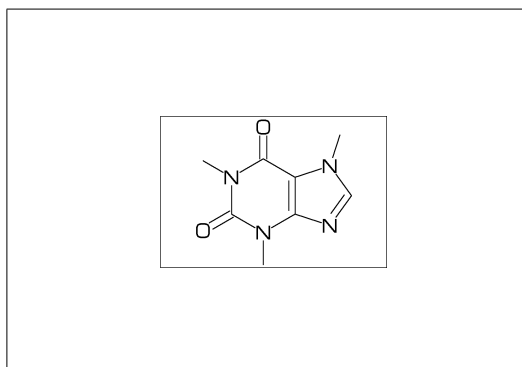
No.46 Inline definition

Insert user defined substructure

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

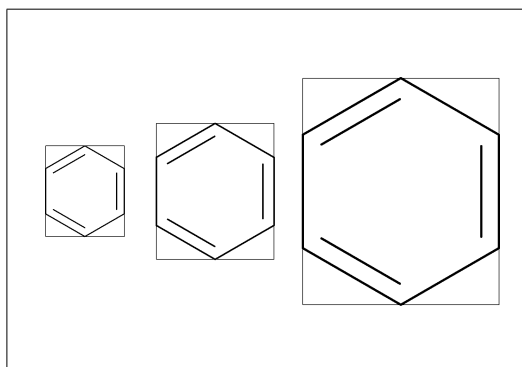
**No.47 Font size**

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

**No.48 Max ratio bond/width length**

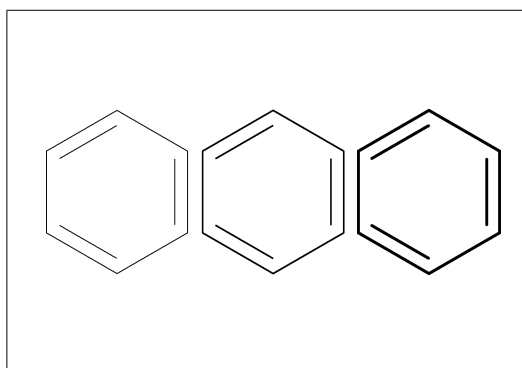
```
max_bond_width:=0.10;
MCd(1,1)( 0, .5)(<30,Ph)
max_bond_width:=0.15;
MCd(1,1)(.33,.5)(<30,Ph)
max_bond_width:=0.25;
MCd(1,1)( 1, .5)(<30,Ph)
```

```
** default: max_bond_width=0.15
```

**No.49 Ratio thickness/bond length**

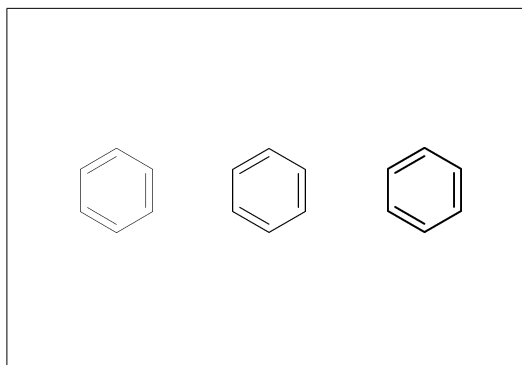
```
ratio_thickness_bond:= 0.005;
MCd(1,.6)(0, .5)(<30,Ph)
ratio_thickness_bond:= 0.015;
MCd(1,.6)(.5,.5)(<30,Ph)
ratio_thickness_bond:= 0.030;
MCd(1,.6)(1, .5)(<30,Ph)
```

```
** default: ratio_thickness_bond=0.015
```

**No.50 Offset thickness of bond**

```
beginfont() offset_thickness#:=0pt#;
MCd(1,.3)(0, .5)(<30,Ph) endfont
beginfont() offset_thickness#:=0.2pt#;
MCd(1,.3)(.5,.5)(<30,Ph) endfont
beginfont() offset_thickness#:=0.5pt#;
MCd(1,.3)(1, .5)(<30,Ph) endfont
```

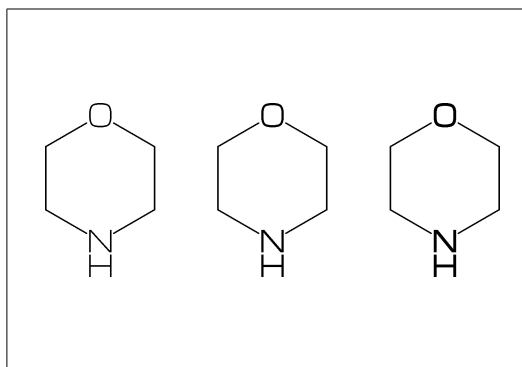
```
** default: offset_thickness#:=0.2pt#
```



No.51 Ratio char/bond thickness

```
ratio_char_bond:=1.0;  
MCd(1,.6)(0, .5)(<30,?6,5:0,2:NH)  
ratio_char_bond:=1.5;  
MCd(1,.6)(.5, .5)(<30,?6,5:0,2:NH)  
ratio_char_bond:=2.0;  
MCd(1,.6)(1, .5)(<30,?6,5:0,2:NH)
```

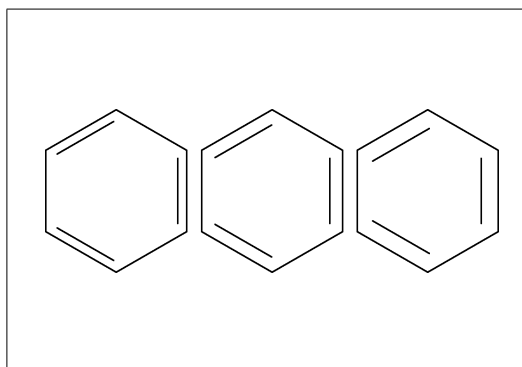
**** default: ratio_char_bond=1.5**



No.52 Ratio bondgap/bond length

```
ratio_bondgap_bond:= 0.10;  
MCd(1,.6)(0, .5)(<30,Ph)  
ratio_bondgap_bond:= 0.15;  
MCd(1,.6)(.5, .5)(<30,Ph)  
ratio_bondgap_bond:= 0.20;  
MCd(1,.6)(1, .5)(<30,Ph)
```

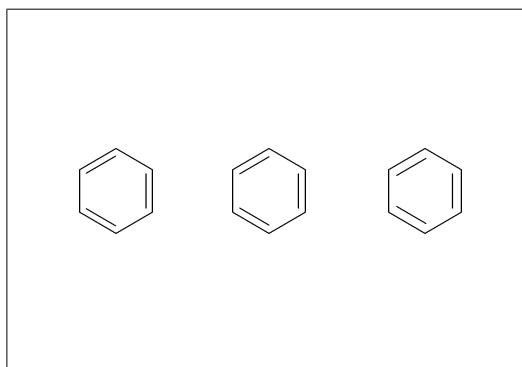
**** default: ratio_bondgap_bond=0.15**



No.53 Offset of doublebond gap

```
beginfont() offset_bond_gap#:=0.0pt#;  
MCd(1,.3)(0, .5)(<30,Ph) endfont  
beginfont() offset_bond_gap#:=0.3pt#;  
MCd(1,.3)(.5, .5)(<30,Ph) endfont  
beginfont() offset_bond_gap#:=1.0pt#;  
MCd(1,.3)(1, .5)(<30,Ph) endfont
```

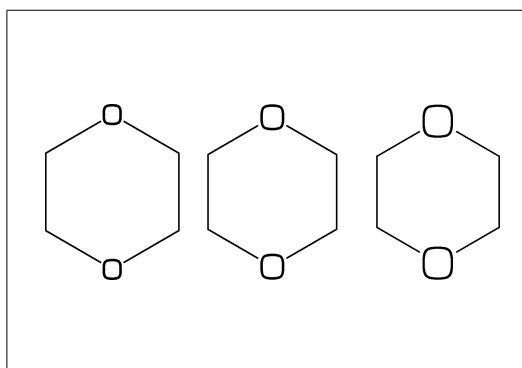
**** default: offset_bond_gap#=0.3pt#**



No.54 Ratio atom/bond length

```
ratio_atom_bond:= 0.25;  
MCd(1,.6)(0, .5)(<30,?6,@(2,5)O)  
ratio_atom_bond:= 0.36;  
MCd(1,.6)(.5, .5)(<30,?6,@(2,5)O)  
ratio_atom_bond:= 0.45;  
MCd(1,.6)(1, .5)(<30,?6,@(2,5)O)
```

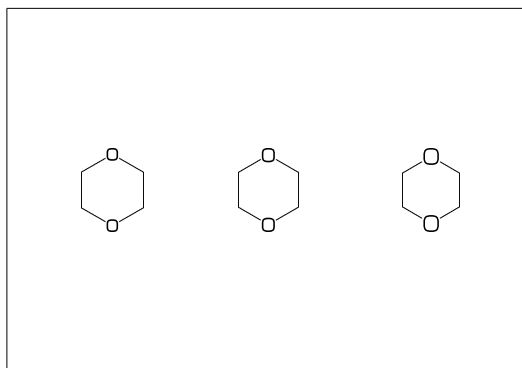
**** default: ratio_atom_bond=0.36**



No.55 Offset of atom width

```
beginfont() offset_atom#:=0.0pt#;  
MCd(1,.3)(0, .5)(<30,Ph,@(2,4,6)N) endfont  
beginfont() offset_atom#:=0.8pt#;  
MCd(1,.3)(.5, .5)(<30,Ph,@(2,4,6)N) endfont  
beginfont() offset_atom#:=2.0pt#;  
MCd(1,.3)(1, .5)(<30,Ph,@(2,4,6)N) endfont
```

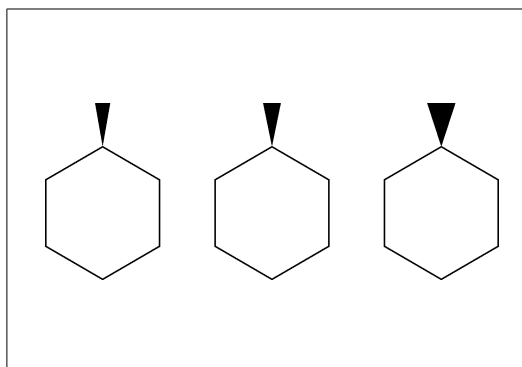
**** default: offset_atom#=0.8pt#**



No.56 Ratio wedge/bond length

```
ratio_wedge_bond:=0.10;
MCd(1,.6)(0,.5)(<30,?6,5:*/Me)
ratio_wedge_bond:=0.12;
MCd(1,.6)(.5,.5)(<30,?6,5:*/Me)
ratio_wedge_bond:=0.20;
MCd(1,.6)(1,.5)(<30,?6,5:*/Me)

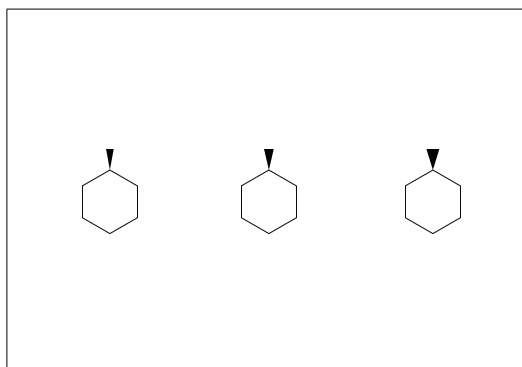
** default: ratio_wedge_bond=0.12
```



No.57 Offset of wedge width

```
beginfont() offset_wedge#:=0.0pt#;
MCd(1,.3)(0,.5)(<30,?6,5:*/Me) endfont
beginfont() offset_wedge#:=0.4pt#;
MCd(1,.3)(.5,.5)(<30,?6,5:*/Me) endfont
beginfont() offset_wedge#:=1.0pt#;
MCd(1,.3)(1,.5)(<30,?6,5:*/Me) endfont

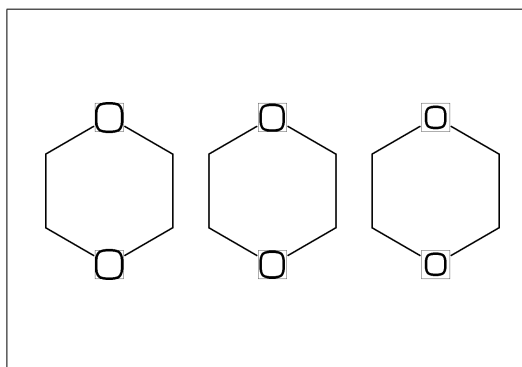
** default: offset_wedge#:=0.4pt#
```



No.58 Ratio font atom gap/atom length

```
ratio_atmgap_atom:=0.0;
MCd(1,.6)(0,.5)(<30,?6,@(2,5)0)
ratio_atmgap_atom:=0.050;
MCd(1,.6)(.5,.5)(<30,?6,@(2,5)0)
ratio_atmgap_atom:=0.12;
MCd(1,.6)(1,.5)(<30,?6,@(2,5)0)

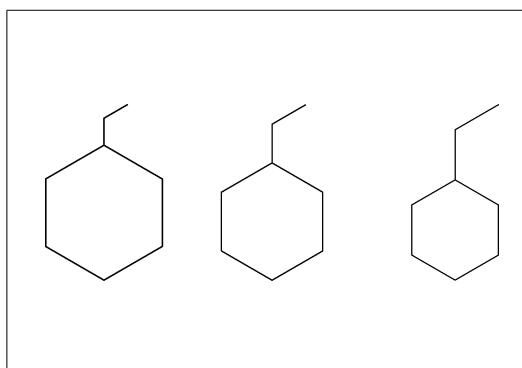
** default: ratio_atmgap_atom=0.050
```



No.59 Ratio chain/ring length

```
ratio_chain_ring:= 0.4;
MCd(1,.6)(0,.5)(<30,?6,5:/Et)
ratio_chain_ring:= 0.66;
MCd(1,.6)(.5,.5)(<30,?6,5:/Et)
ratio_chain_ring:= 1.0;
MCd(1,.6)(1,.5)(<30,?6,5:/Et)

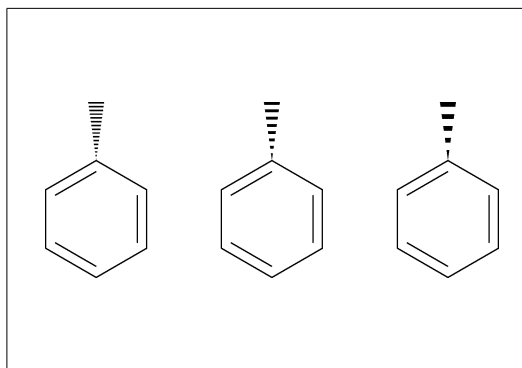
** default: ratio_chain_ring=0.66
```



No.60 Ratio zebra gap/bond length

```
ratio_zebragap_bond:=0.06;
MCd(1,.6)(0,.5)(<30,Ph,5:/*Me'1)
ratio_zebragap_bond:=0.12;
MCd(1,.6)(.5,.5)(<30,Ph,5:/*Me'1)
ratio_zebragap_bond:=0.20;
MCd(1,.6)(1,.5)(<30,Ph,5:/*Me'1)

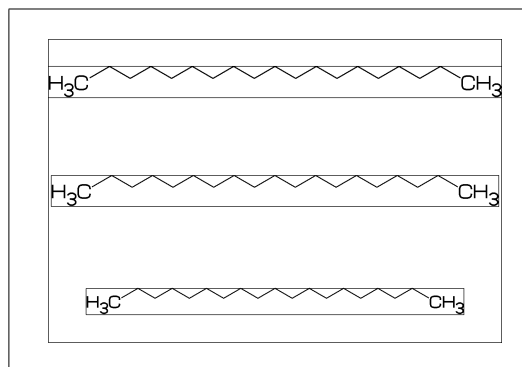
** default: ratio_zebragap_bond=0.12
```



No.61 Margin left and right

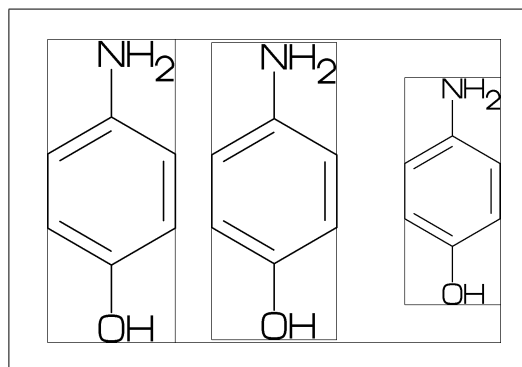
```
margin_left_right:=0mm;
MCd(1,1)(0.5,0.9)(<30,CH3,!0,!17,CH3)
margin_left_right:=0.4mm;
MCd(1,1)(0.5,0.5)(<30,CH3,!0,!17,CH3)
margin_left_right:=5mm;
MCd(1,1)(0.5,0.1)(<30,CH3,!0,!17,CH3)
```

**** default:** margin_left_right=0.4mm

**No.62 Margin top and bottom**

```
margin_top_bottom:=0mm;
MCd(1,1)(0.1,0.5)(<30,Ph,2:/OH,5:/NH2)
margin_top_bottom:=0.4mm;
MCd(1,1)(0.5,0.5)(<30,Ph,2:/OH,5:/NH2)
margin_top_bottom:=5mm;
MCd(1,1)(0.9,0.5)(<30,Ph,2:/OH,5:/NH2)
```

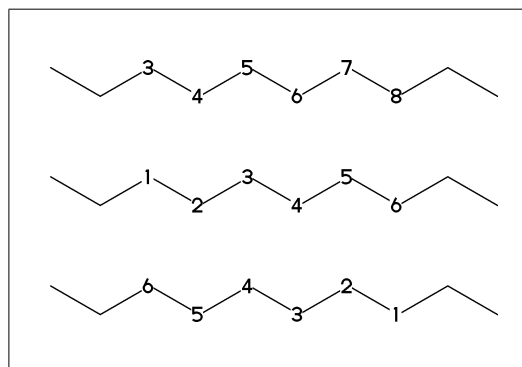
**** default:** margin_top_bottom=0.4mm

**No.63 Switch numbering atom**

```
numberA_start:=3; numberA_end:=8;
```

```
sw_numberA:=1; MCd(1,1)(.5,.9)(<30,!9)
sw_numberA:=2; MCd(1,1)(.5,.5)(<30,!9)
sw_numberA:=3; MCd(1,1)(.5,.1)(<30,!9)
```

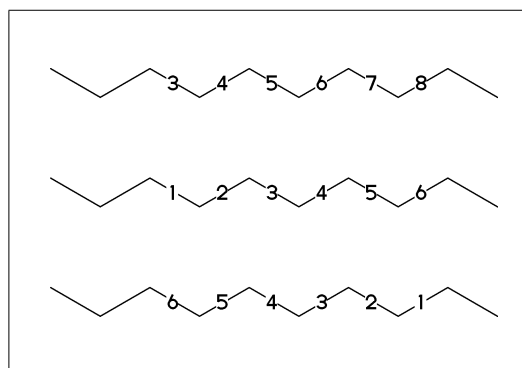
**** default:** numberA_start=1 numberA_end=4095

**No.64 Switch numbering bond**

```
numberB_start:=3; numberB_end:=8;
```

```
sw_numberB:=1; MCd(1,1)(.5,.9)(<30,!9)
sw_numberB:=2; MCd(1,1)(.5,.5)(<30,!9)
sw_numberB:=3; MCd(1,1)(.5,.1)(<30,!9)
```

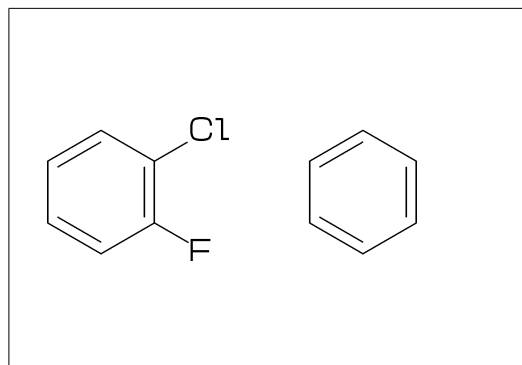
**** default:** numberB_start=1 numberB_end=4095

**No.65 Switch substituent off**

```
MCd(1,.5)( 0,0.5)(<30,Ph,4:/Cl,3:/F)
```

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

**** default:** sw_subst_off=0

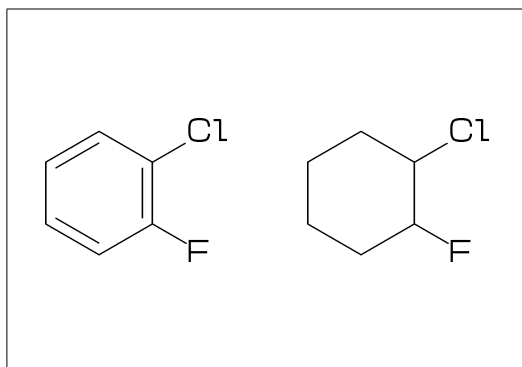


No.66 Switch all bond single

```
MCd(1,.5)( 0,0.5)(<30,Ph,4:/Cl,3:/F)

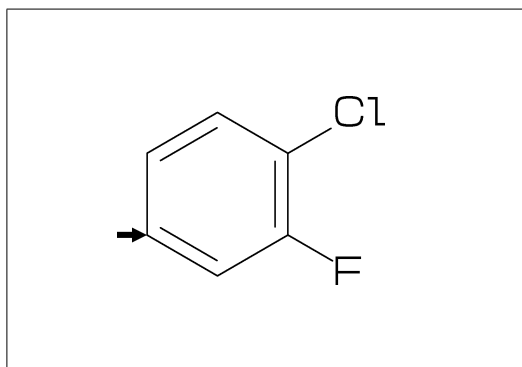
sw_bond_single:=1;
MCd(1,.5)( 1,0.5)(<30,Ph,4:/Cl,3:/F)

** default: sw_bond_single=0
```

**No.67 Switch start vector**

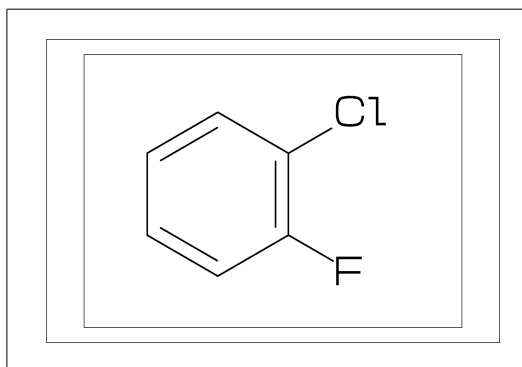
```
sw_start_vector:=1;
MCf(<30,Ph,4:/Cl,3:/F)

** default: sw_start_vector=0
```

**No.68 Switch font frame**

```
sw_font_frame=0 : no frame **default
sw_font_frame=1 : draw frame of font
sw_font_frame=2 : draw frame inside margin
sw_font_frame=3 : draw both

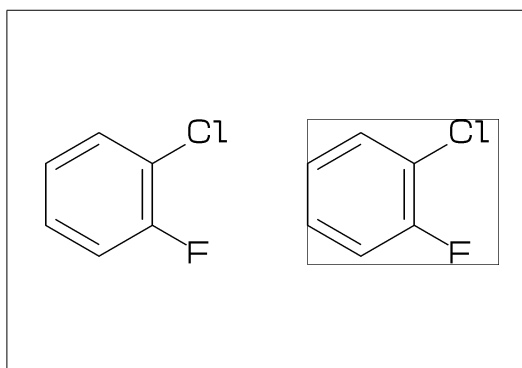
sw_font_frame:=3;
margin_left_right:=5mm; margin_top_bottom:=2mm;
MCf(<30,Ph,4:/Cl,3:/F)
```

**No.69 Switch molecular frame**

```
MCd(1,.5)(0,0.5)(<30,Ph,4:/Cl,3:/F)

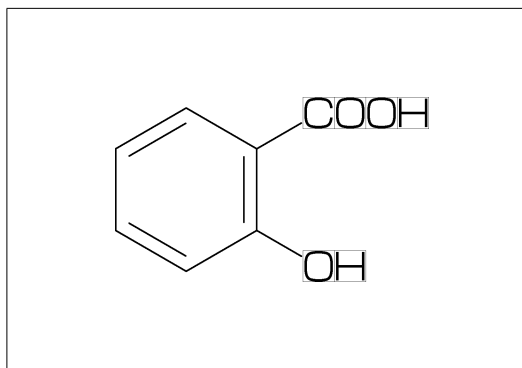
sw_mol_frame:=1;
MCd(1,.5)(1,0.5)(<30,Ph,4:/Cl,3:/F)

** default: sw_mol_frame=0
```

**No.70 Switch atom frame**

```
sw_atom_frame:=1;
MCf(<30,Ph,4:/COOH,3:/OH)

** default: sw_atom_frame=0
```

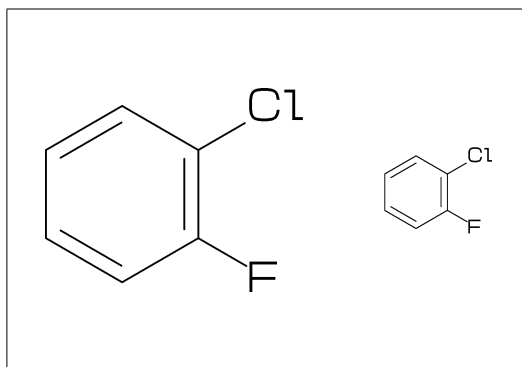


No.71 Switch solid mode

```
MCd(1,.8)( 0,0.5)(<30,Ph,4:/Cl,3:/F)

sw_solid:=1;
ratio_bond_width:=0.08;
MCd(1,.8)( 1,0.5)(<30,Ph,4:/Cl,3:/F)

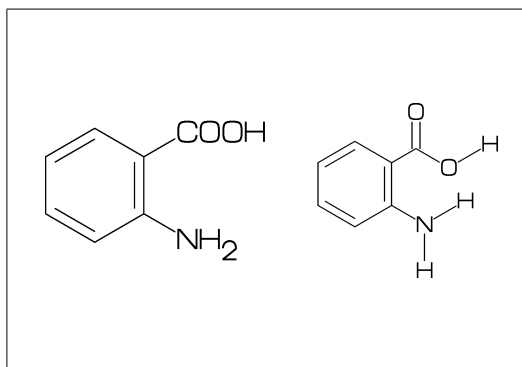
** default: sw_solid=0
```

**No.72 Switch Expand**

```
MCd(1,.5)(0,0.5)(<30,Ph,4:/COOH,3:/NH2)

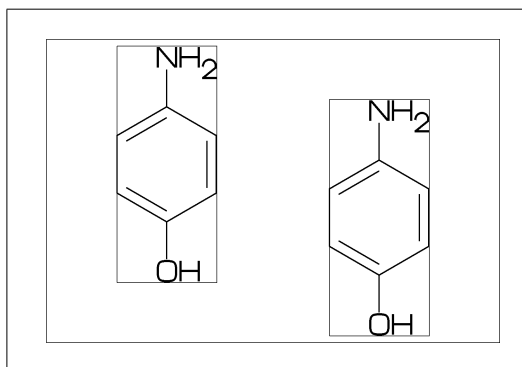
sw_expand:=1;
MCd(1,.5)(1,0.5)(<30,Ph,4:/COOH,3:/NH2)

** default: sw_expand=0
```

**No.73 Function MCd (draw)**

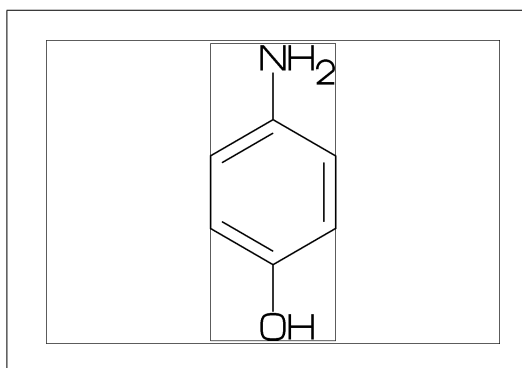
```
MCd(a,b)(c,d)(...)
  a: ratio molecular width/font width
  b: ratio molecular height/font height
  c: x axis position
  d: y axis position

MCd(1,0.8)(0.2,0.9)(<30,Ph,2:/OH,5:/NH2)
MCd(1,0.8)(0.8,0.1)(<30,Ph,2:/OH,5:/NH2)
```

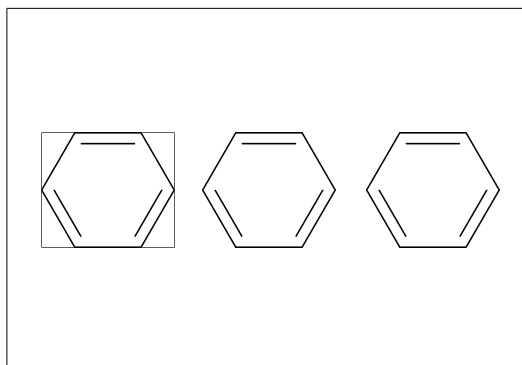
**No.74 Function MCf (fit draw)**

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

sw_font_frame:=1;
sw_mol_frame:=1;
MCf(<30,Ph,2:/OH,5:/NH2)
```

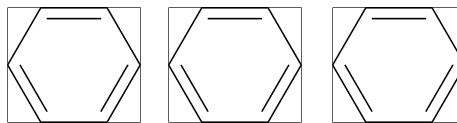
**No.75 Local setting**

```
beginfont()
  sw_mol_frame:=1; % <== Local setting
  MCd(1,.4)( 0,.5)(Ph)
endfont
beginfont() MCd(1,.4)(.5,.5)(Ph) endfont
beginfont() MCd(1,.4)( 1,.5)(Ph) endfont
```



No.76 Global setting

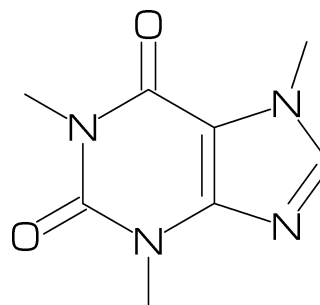
```
sw_mol_frame:=1; % <== Global setting
beginfont() MCd(1,.4)( 0,.5)(Ph) endfont
beginfont() MCd(1,.4)(.5,.5)(Ph) endfont
beginfont() MCd(1,.4)( 1,.5)(Ph) endfont
```



No.77 Output molecular information

```
var3:="calc_weight"; tag3:="cMW";
var4:="calc_formula"; tag4:="cFM";
%% Output to mcf_man_soc-info.aux %%
F:mcf_man_soc;C:85;cMW:194.19174;cFM:C8H10N4O2

cMW:calculated molecular weight
cFM:calculated molecular formula
```

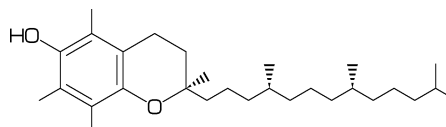


No.78 Output additional information

```
beginfont("EN:Tocopherol","CAS:59-02-9")
MCf(...) endfont

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

*f:filename *C:char number EN:molecular name
CAS:CAS number *:default output
```

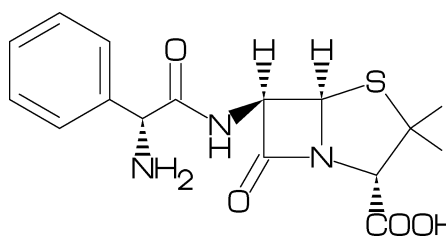


No.79 Change aux information delimiter

```
aux_delimiter:="/";
beginfont("EN:Ampicillin","CAS:69-53-4")
MCf(...) endfont

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

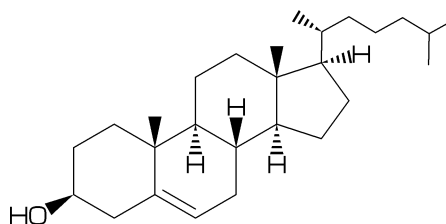
**default aux_delimiter=";"
```



No.80 Fixed aux information

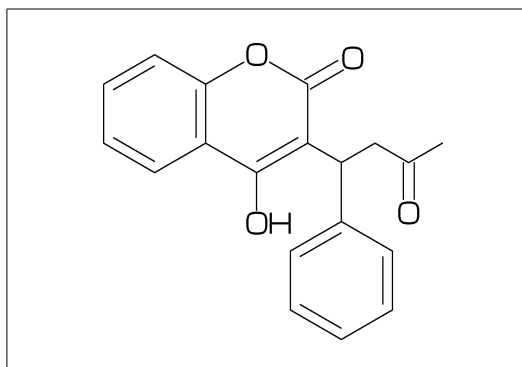
```
tag3:="NO"; var3:="inf_NO";
tag4:="EN"; var4:="inf_EN";
sw_auxfix:=1; auxtag_out;
beginfont("EN:Cholesterol","NO:1") ... endfont

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



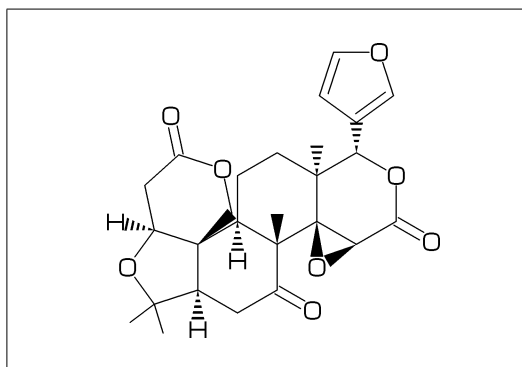
No.81 Example(1) Warfarin

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



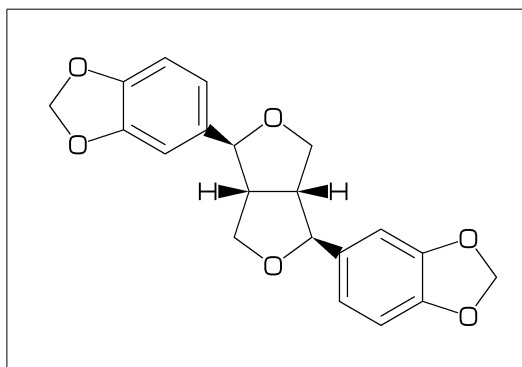
No.82 Example(2) Limonin

<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)/Me,
@(1^60,5^180,16^60)/*H,
14*,|,?5,\$(1,4)d1,3:0



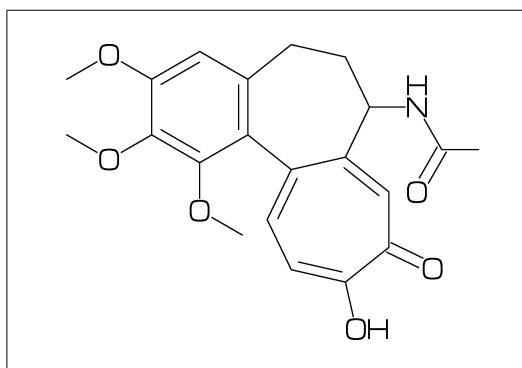
No.83 Example(3) Sesamine

<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



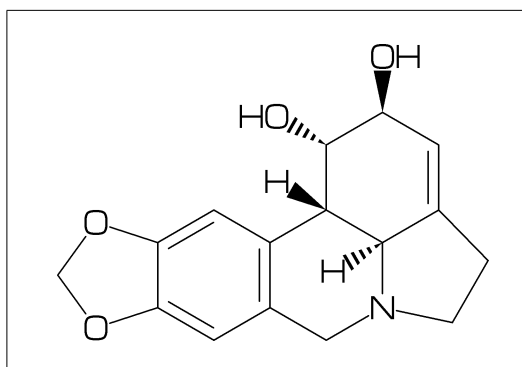
No.84 Example(4) Colchicine

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



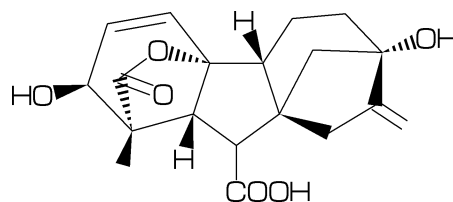
No.85 Example(5) Lycorine

<30,Ph,
-4=?6,-2=?6,6=?5,(9,12)=?5[3],
13=d1,
8:N,@(15,17)0,
9:/*H^180,10:*/H^60,
13:*/OH,14:/*OH



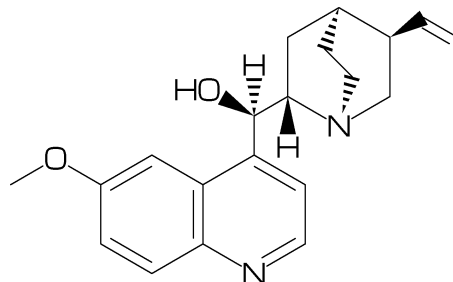
No.86 Example(6) Gibberellin

<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://Me,13:*/OH,8:*/OH,
14:*/Me,@(1^60,4^60)*/H



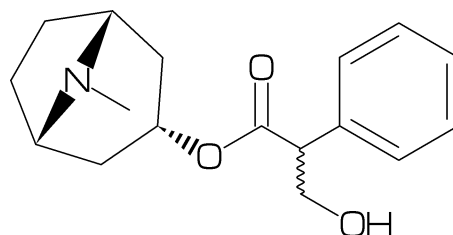
No.87 Example(7) Quinine

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



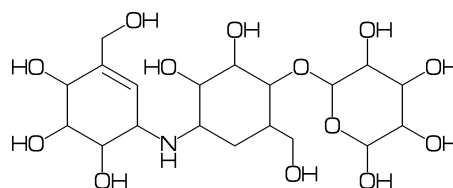
No.88 Example(8) Atoropin

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



No.89 Example(9) Validamycin

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



No.90 Example(10) Paclitaxel

?6,5=d,3*,{,'1,36,45,45,45,45,},,
-4=?6,-4=?4,-1=wb,-3=wf,-1:0,||,
@(4^35,4^~35,6)/Me,@(3^~60,15)*/OH,
8:/*H^~60,9:*/Me^60,10://0,
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

