

Molecular Coding Format manual

Author : Akira Yamaji Date : June 11, 2016
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 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:85;cMW:335.37805;cFM:C15H17N3O4S;EN:Ampicillin
F:mcf_man_soc;C:86;cMW:386.6532;cFM:C27H46O;EN:Cholesterol
.....
```

```
(sw_auxfix=1)
F;C;cMW;cFM;EN
mcf_man_soc;85;335.37805;C15H17N3O4S;Ampicillin
mcf_man_soc;86;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)

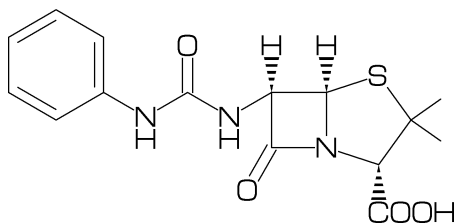
```
%-----
\documentclass[a4paper]{article}
\usepackage{graphicx}
\pagestyle{empty}
\makeatletter%
%-----
\def\@F{F}\def\@C{C}\def\@EN{EN}\def\@NO{NO}\def\@MW{MW}\def\@FMc{FMc}%
\def\@fst@param#1:#2;{#1}\def\@sec@param#1:#2;{#2}%
\def\mol@sel#1{%
\if#1\empty\relax\else%
\edef\@tag{\expandafter\@fst@param#1;}%
\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}(120,45)%
\put(10,35){\bf [\MOLnum] \MOLnameE}%
\put(16,30){\sf MW:\CALmw}%
\put(16,25){\sf FM:\CALfm}%
\put(20,0){\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:85,NO:1,cMW:335.37805,cFM:C15H17N3O4S,EN:Ampicillin}\\%
\INFO{F:mcf_man_soc,C:86,NO:2,cMW:386.6532,cFM:C27H46O,EN:Cholesterol}%
\end{document}
%-----
```

(Molecular structure output)

[1] Ampicillin

MW:335.37805

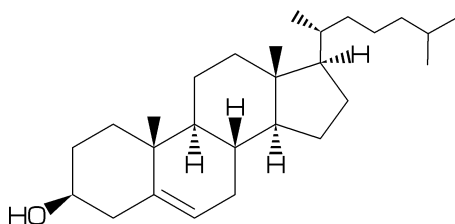
FM:C15H17N3O4S



[2] Cholesterol

MW:386.6532

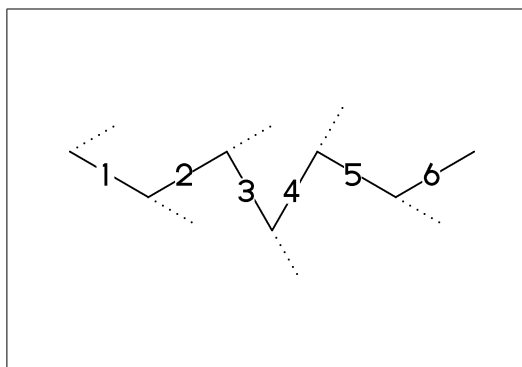
FM:C27H46O



No.1 Chain(1)

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

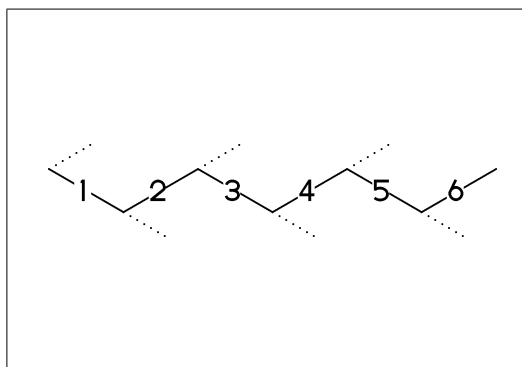
<30,-60,60,-90,120,-90,60



No.2 Chain(2)

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

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

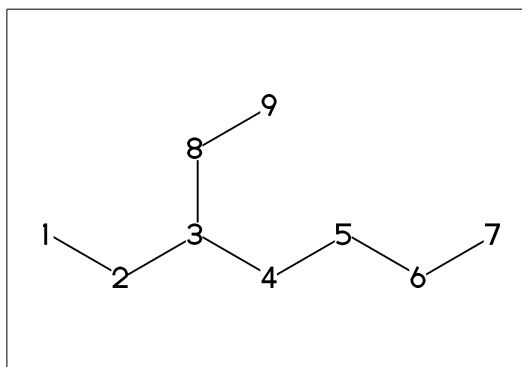


No.3 Jump to atom and branch bond

3* : Jump to A3
3\ : 3*,0

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

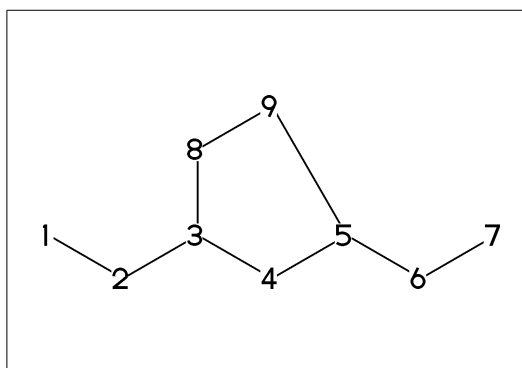
** An(-999<=n<=4095): atom number



No.4 Connect atom

&n : Connect to An

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



No.5 Ring

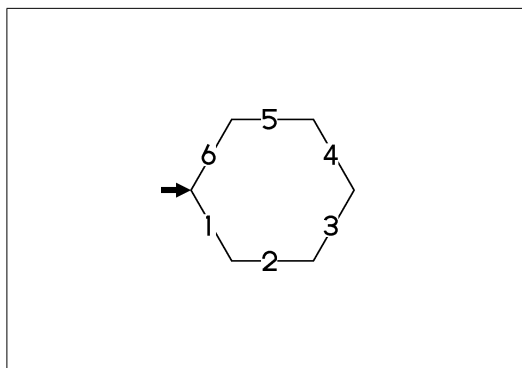
?n : n membered ring

?6

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

** ?n(3<=n<=20)

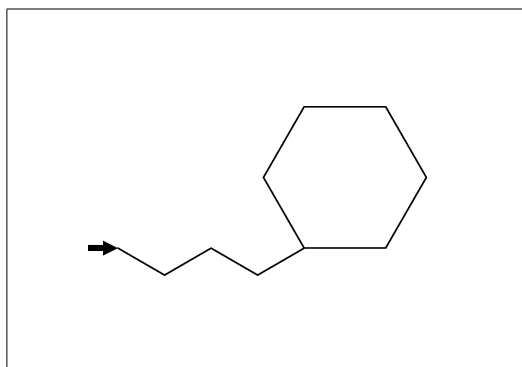
** bold arrow is default angle and position



No.6 Rotate current angle

<angle : rotate current angle

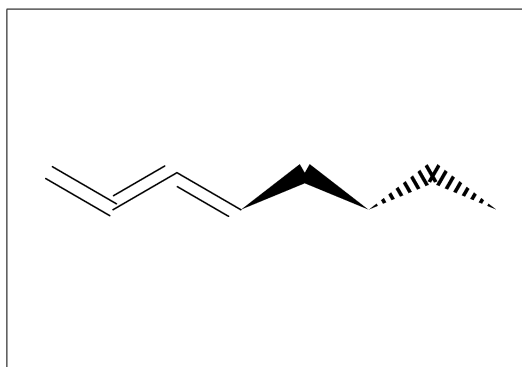
<30,!4,<30,?6



No.7 Change bond type (1)

a~type : ~type,a
dm:double middle,
dl:double left side, dr:double right side,
wf:wedge forward, wb:wedge backward,
zf:wedge dotted, zb:wedge dotted backward

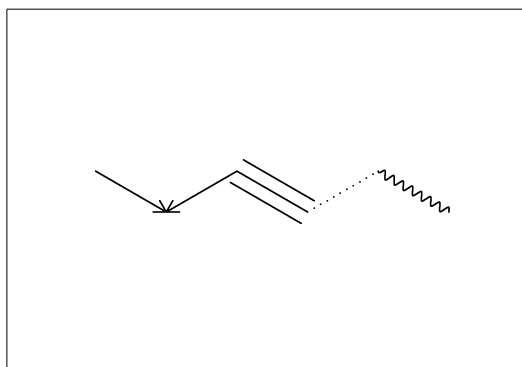
<30,!~dm,!~dl,!~dr,!~wf,!~wb,!~zf,!~zb



No.8 Change bond type (2)

Bn=bond type : change bond type at Bn
vf : vector forward
vb : vector backward
tm : triple
dt : dotted
wv : wave

<30,!6,1=vf,2=vb,3=tm,4=dt,5=bz,5=wv

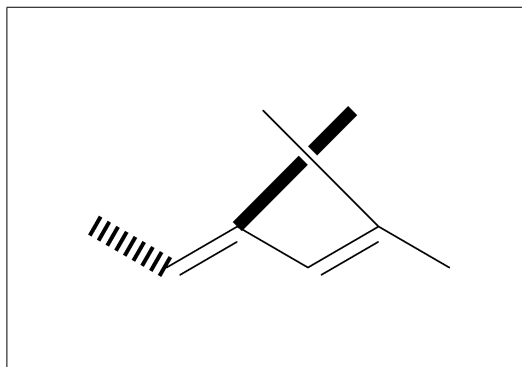


No.9 Change bond type (3)

bd : broad single
bz : broad dotted
ov : over line
\$(2,4)dr : 2=dr,4=dr

<30,!5,1=bz,\$(2,4)dr,
@(3~bd^-45'2,5~ov^45'2)/Me

** 3~bd^-45'2 : ~bd,^^-45,'2,3

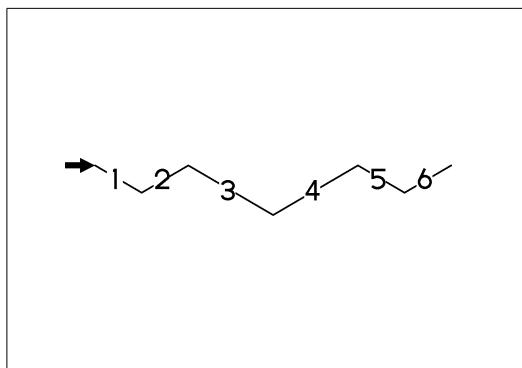


No.10 Change bond length (1)

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

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

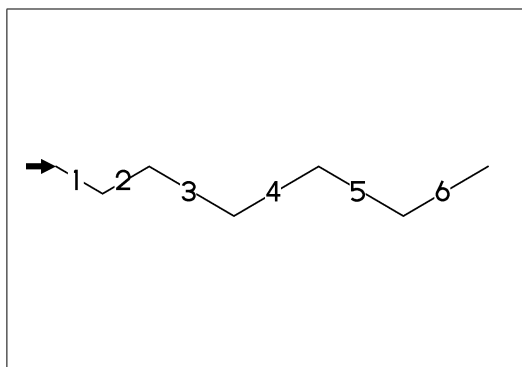
** !2'1.2 : '1.2,!2



No.11 Change bond length (2)

“length : change all bond length after

<30,!2,“1.2,!4

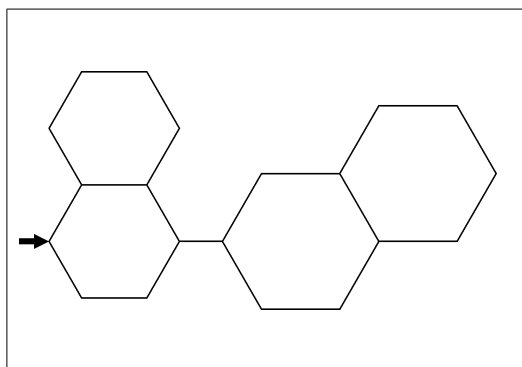


No.12 Change ring length

?n'length : change ring length

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

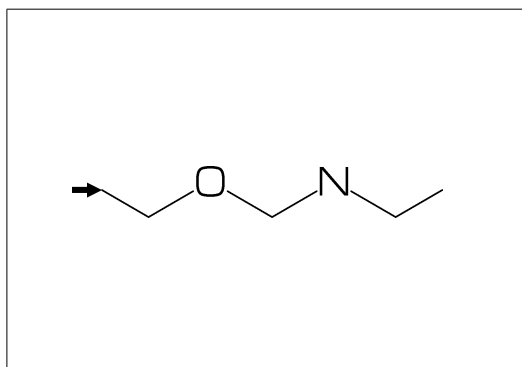
** fused ring size depend on
attached bond length



No.13 Change atom (1)

Insert hetero atom

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

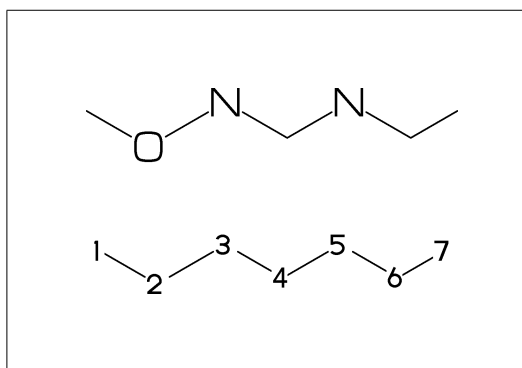


No.14 Change atom (2)

2:0 : change A2 C to O

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

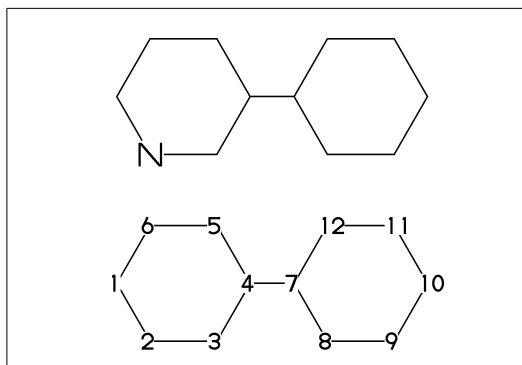
<30,!6,2:0,@(3,5)N



No.15 Change atom (3)

2:N : change A2 C to N

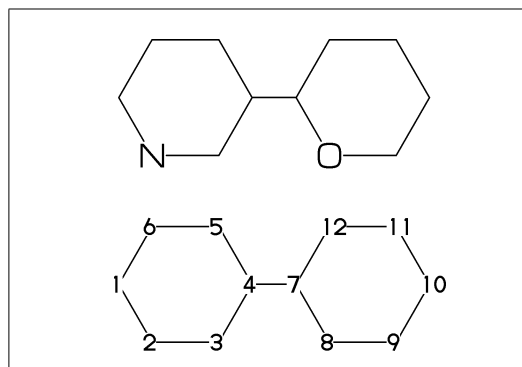
?6,4\,?6,2:N



No.16 Change atom (brock address)

| : divide brock
|| : reset brock address

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

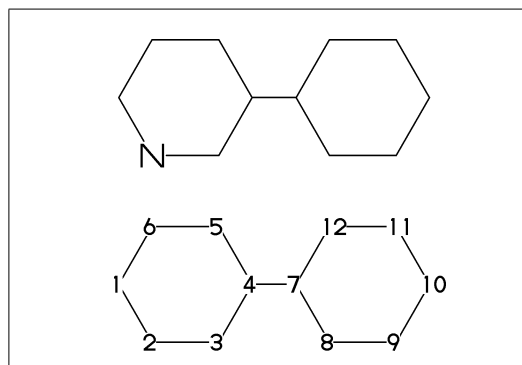


No.17 Change atom (absolute address)

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

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

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

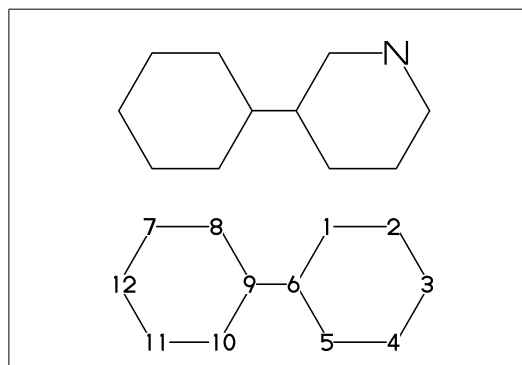


No.18 Change atom (relative address)

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

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

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

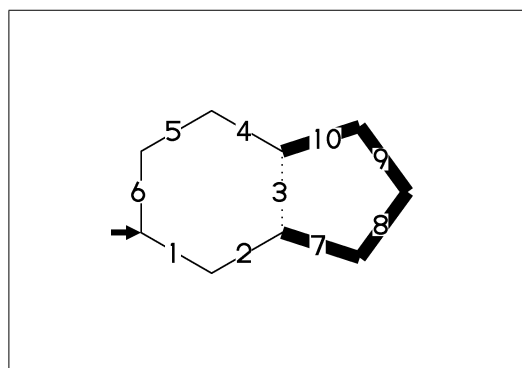


No.19 Fuse ring (attached 1 bond)

?6,3=?5 : fuse ?5 at B3

?6,3=?5

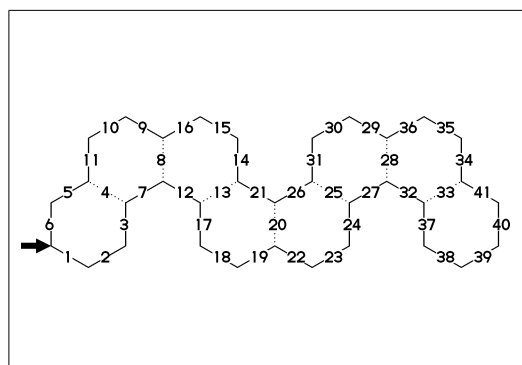
** Bn(n:-999<=n<=4095): bond number



No.20 Fuse multi ring (attached 1 bond)

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

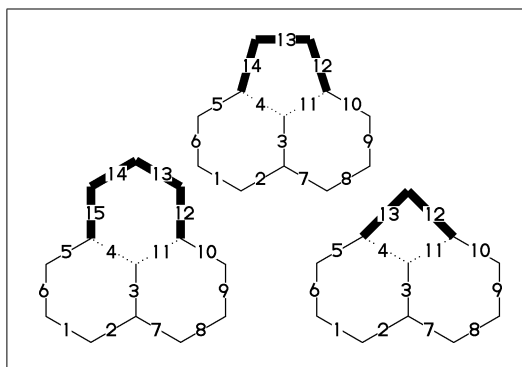
?6,\$(4,8,13,20,25,28,33)?6



No.21 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

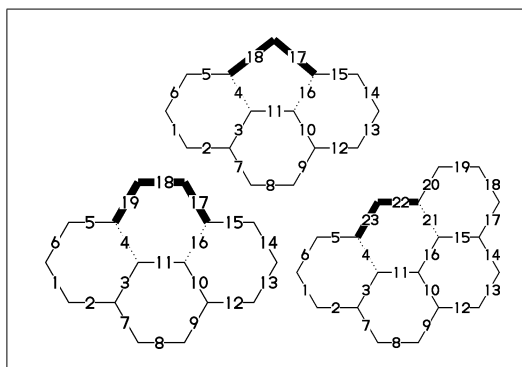
MCd(1,.7)(0,0)(<30,?6,3=?6,(11,4)=?6[4])
 MCd(1,.6)(.54,1)(<30,?6,3=?6,(11,4)=?5[3])
 MCd(1,.6)(1,0)(<30,?6,3=?6,(11,4)=?4[2])



No.22 Fuse ring (attached 3,4 bond)

(16,4)=?6[3] : fuse 3/6 ring to B16..B4
 (16,4)=?5[2] : fuse 2/5 ring to B16..B4
 (21,4)=?6[2] : fuse 2/6 ring to B21..B4

MCd(1,.55)(0,0)(?6,\$(3,10)?6,(16,4)=?6[3])
 MCd(1,.55)(.5,1)(?6,\$(3,10)?6,(16,4)=?5[2])
 MCd(1,.68)(1, 0)(?6,\$(3,10,15)?6,(21,4)=?6[2])

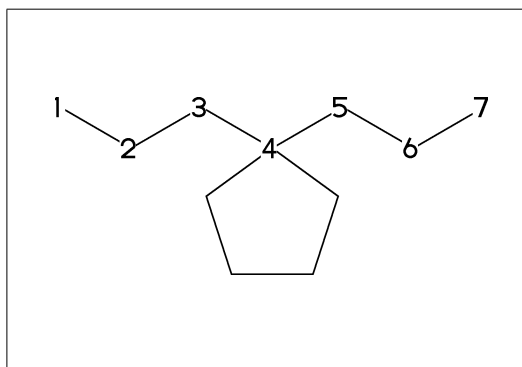


No.23 Spiro ring

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

<30,!6,4*,?5

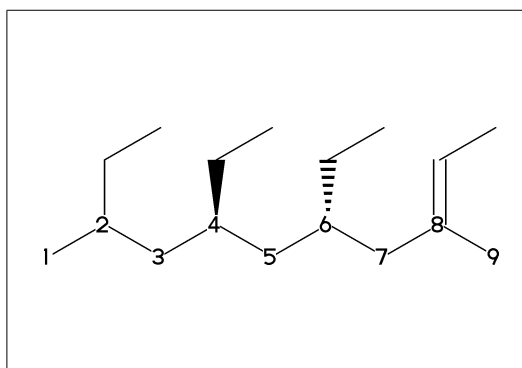
An* : jump to An



No.24 Branch bond (1)

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

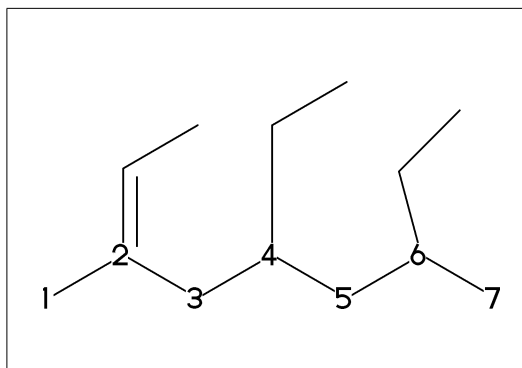
MCf(<30,!8,2\,! ,4*\,! ,6*,! ,8\\,!)



No.25 Branch bond (2)

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

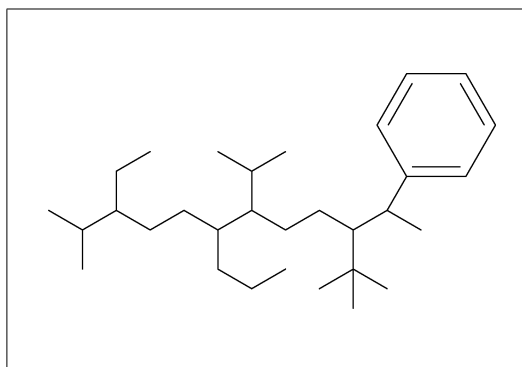
MCf(<-30,
 !6,2~dr,! ,4^1.5,! ,6~15,-60)



No.26 Insert substituent(1)

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

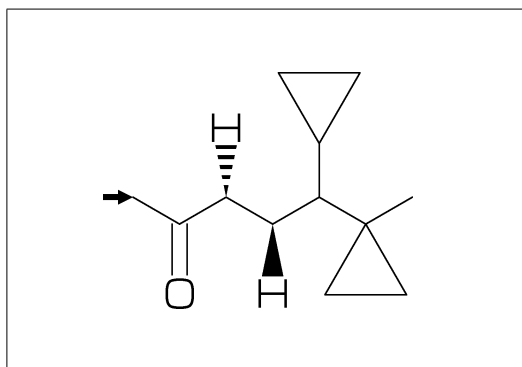
** Me:methyl Et:ethyl
Pr:propyl iPr:isopropyl
tBu:tertial buthyl Ph:phenyl



No.27 Insert substituent(2)

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

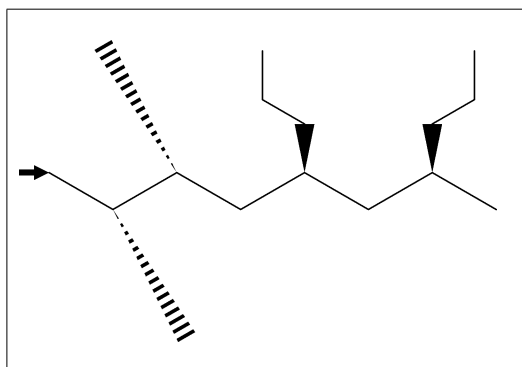
MCf(<30,!,//O,!,/*H,!,*/H,!,/?3,!,**?3,!)



No.28 Insert substituent(3)

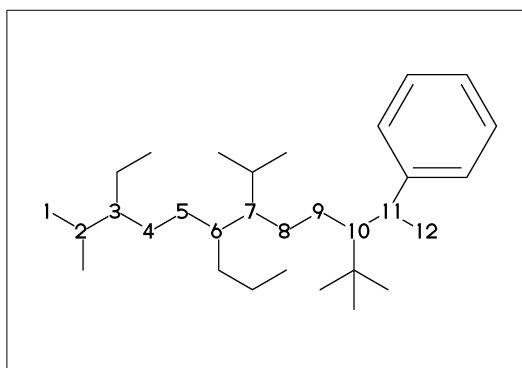
~ : change type
^ : change angle
' : change length
> : change enviroment

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



No.29 Add substituent(1)

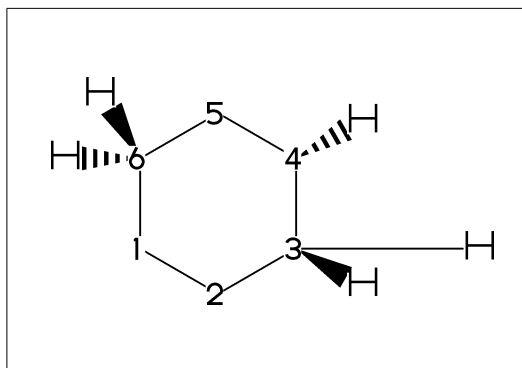
sw_numberA:=1; numberA_end:=12;
MCf(<30,!11,
2:/Me,3:/Et,6:/Pr,7:/iPr,
10:/tBu,11:/Ph~-30)



No.30 Add substituent(2)

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

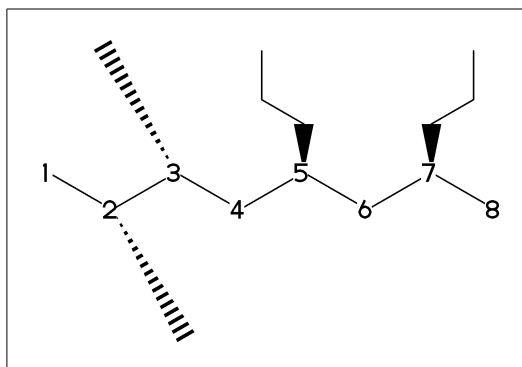
MCf(<30,?6,
@(3'2^30,3~wf,4~zf,6~wf~-30,6~zf^30)/H)



No.31 Add substituent(3)

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

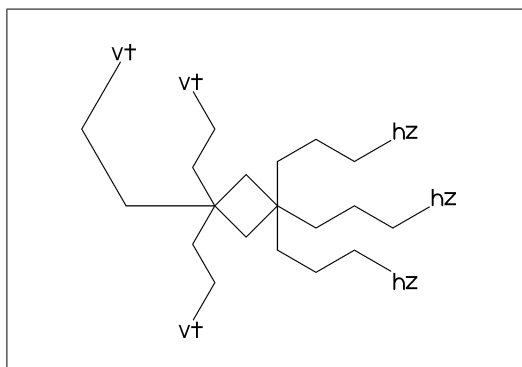
```
MCF(<30,!7'1,
@ (2,3)/*Me'2^30,5:*/Pr>lr,7:*/Pr>rl)
```



No.32 Chain stretch direction environment (1)

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

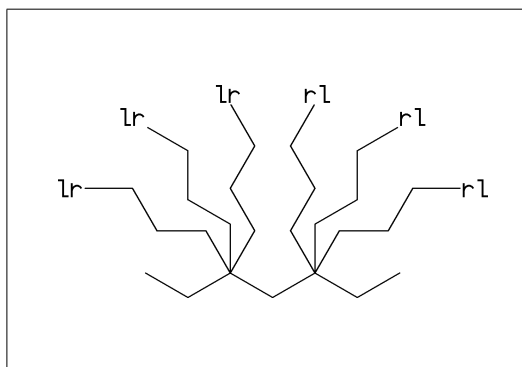
```
?4,
@ (3^-90,3^-30,3^90)/'(!3,"{hz}")>hz,
@ (1^-60,1'2,1^60)/'(!2,"{vt}")>vt
```



No.33 Chain stretch direction environment (2)

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

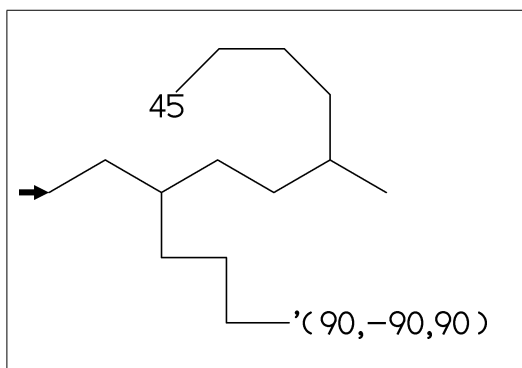
```
<30,!6,
@ (3^-30,3,3^30)/'(!3,"{lr}")>lr,
@ (5^-30,5,5^30)/'(!3,"{rl}")>rl
```



No.34 Chain stretch direction environment (3)

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

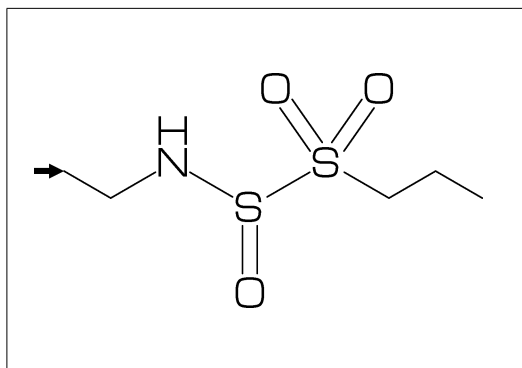
```
<-30,!6,@ (2>45)/'(!3,"{45}"),
@ (6>'(-90,90,-90))/'(!3,"{(-90,90,-90)}")
```



No.35 Change atom and Substituent

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

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

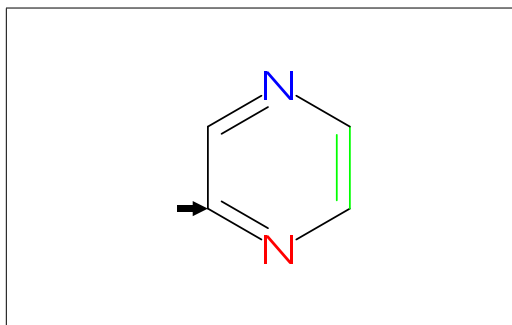


No.36 Change color

@(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
```

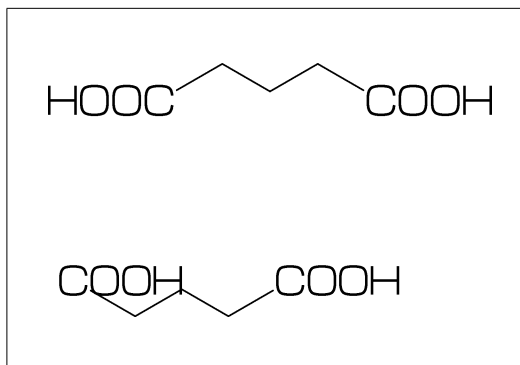
** METAFONT ignore color command

**No.37 Chain start multiple characters**

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

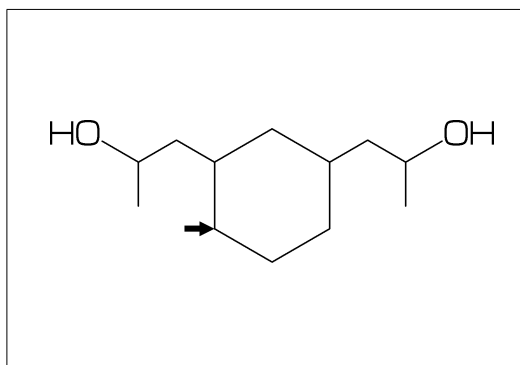
```
MCd( 1,1)(0 ,0.9)<30,COOH,!0,!3,COOH)
```

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

**No.38 User definition**

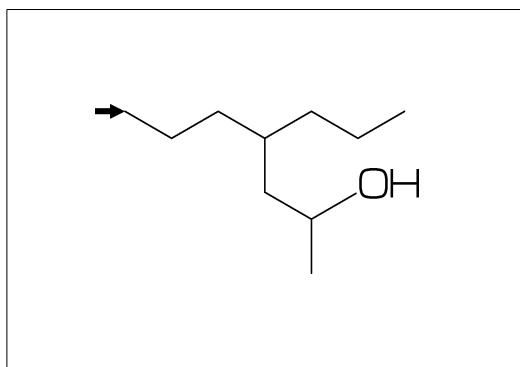
iBuOH : user defined substructure

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

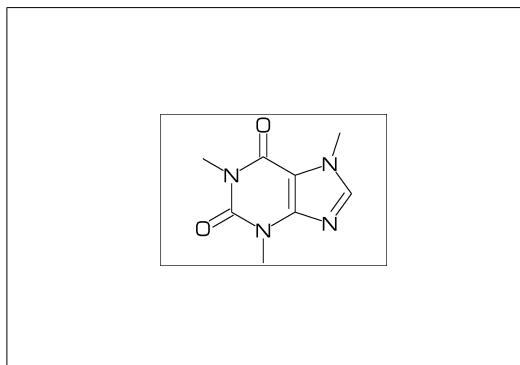
**No.39 Inline definition**

Insert user defined substructure

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

**No.40 Font size**

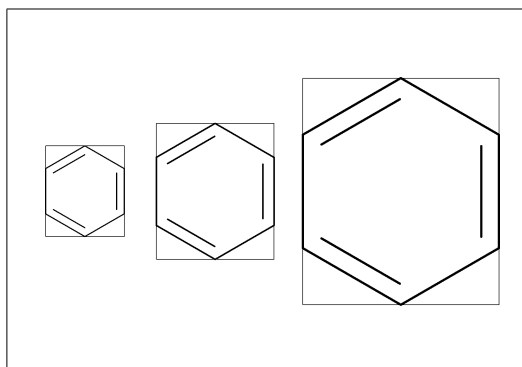
```
beginfont("EN:Caffeine")
font_wd#:=30mm#; %<==font width
font_ht#:=20mm#; %<==font height
sw_font_frame:=1;
MCf(<30,?6,-4=?5,$(3,8)d1,@(2,6,7,9)N,
    @(2,6,9)/Me,@(1,5)//0)
endfont
```



No.41 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)
```

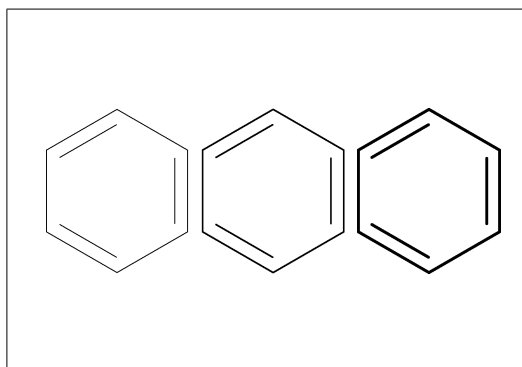
**** default: max_bond_width=0.15**



No.42 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)
```

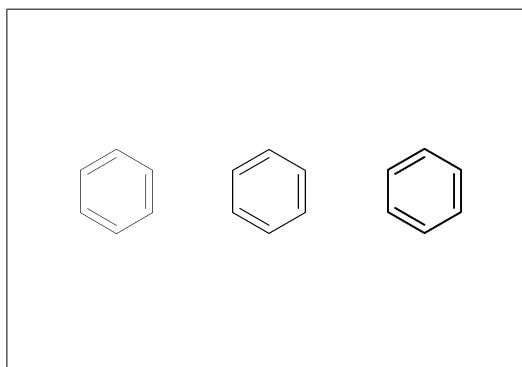
**** default: ratio_thickness_bond=0.015**



No.43 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
```

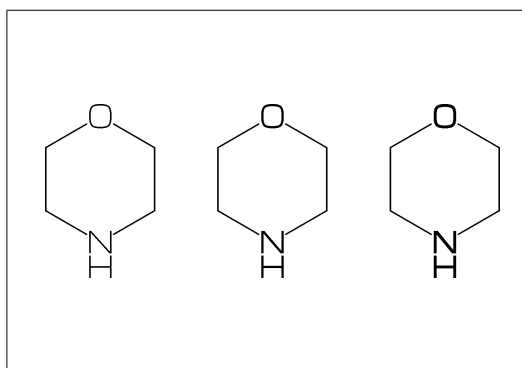
**** default: offset_thickness#=0.2pt#**



No.44 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)
```

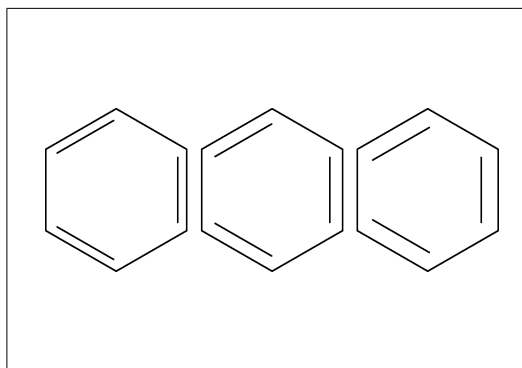
**** default: ratio_char_bond=1.5**



No.45 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)
```

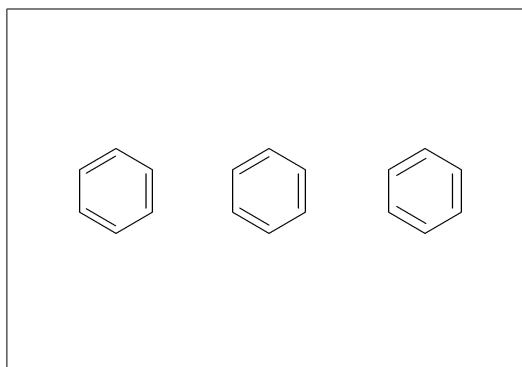
**** default: ratio_bondgap_bond=0.15**



No.46 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
```

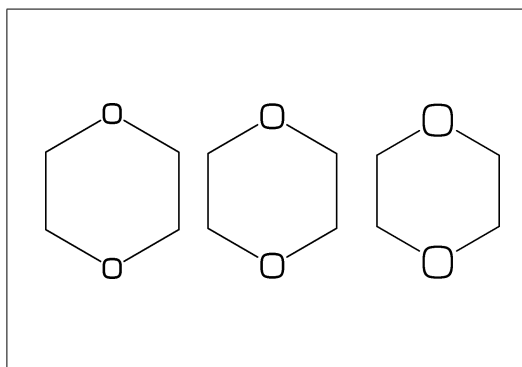
**** default: offset_bond_gap#=0.3pt#**



No.47 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)
```

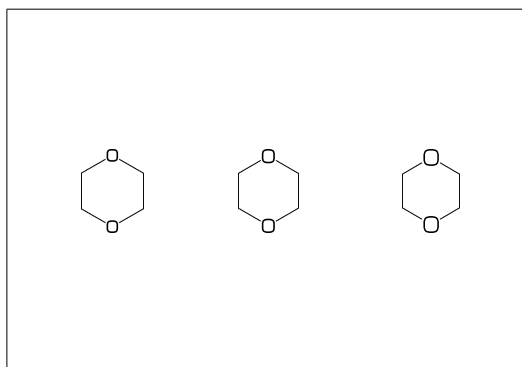
**** default: ratio_atom_bond=0.36**



No.48 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
```

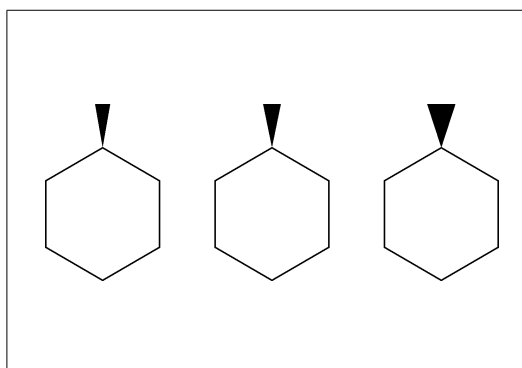
**** default: offset_atom#=0.8pt#**



No.49 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)
```

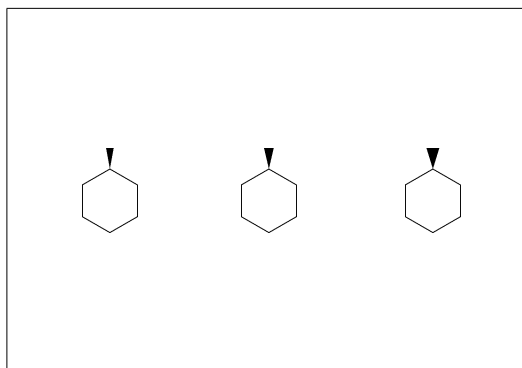
**** default: ratio_wedge_bond=0.12**



No.50 Offset of wedge width

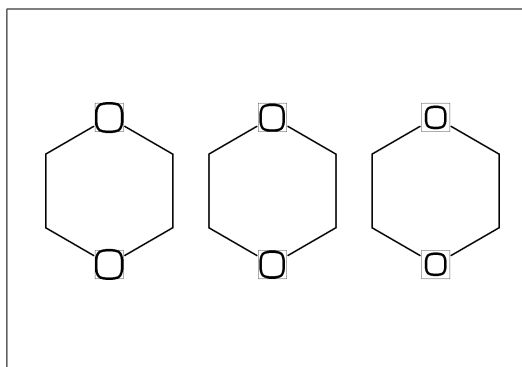
```
beginfont() offset_wedge#:=0.0pt#;  
MCd(1,.3)(0, .5)(<30,?6,5:*/Me) endfont  
beginfont() offset_wedge#:=0.4pt#;  
MCd(1,.3)(.5,.5)(<30,?6,5:*/Me) endfont  
beginfont() offset_wedge#:=1.0pt#;  
MCd(1,.3)(1, .5)(<30,?6,5:*/Me) endfont
```

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



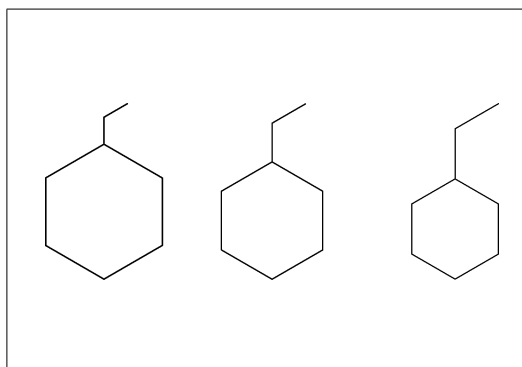
No.51 Ratio font atom gap/atom length

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



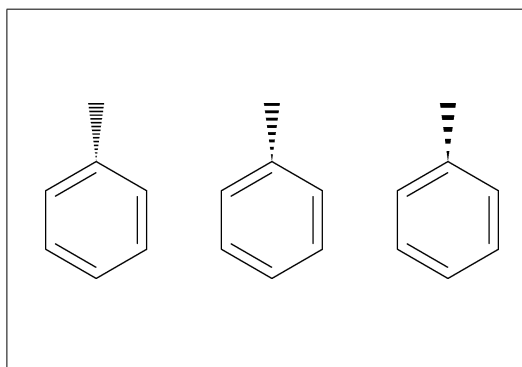
No.52 Ratio chain/ring length

```
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
```



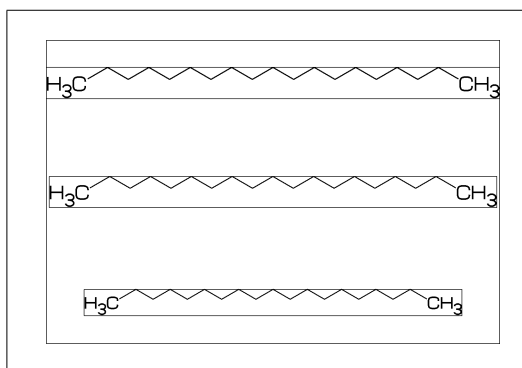
No.53 Ratio zebra gap/bond length

```
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
```



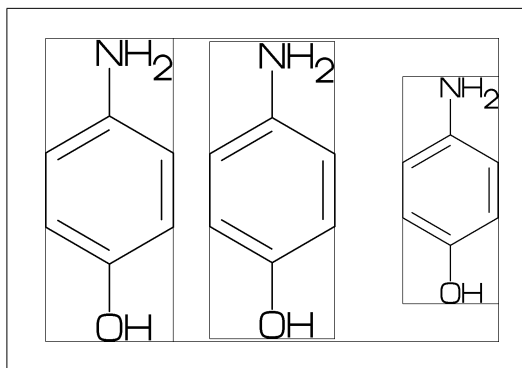
No.54 Margin left and right

```
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.55 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.56 Switch numbering atom

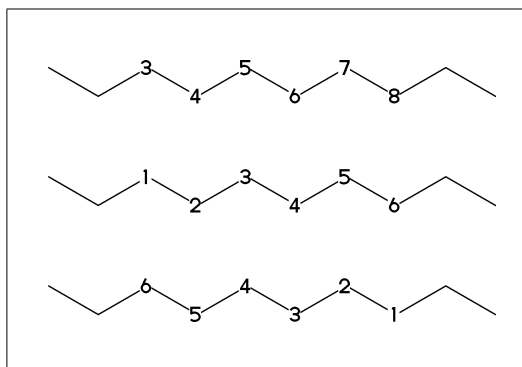
```

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.57 Switch numbering bond**

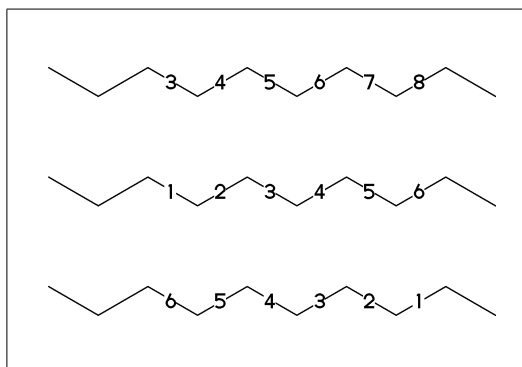
```

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.58 Switch substituent off**

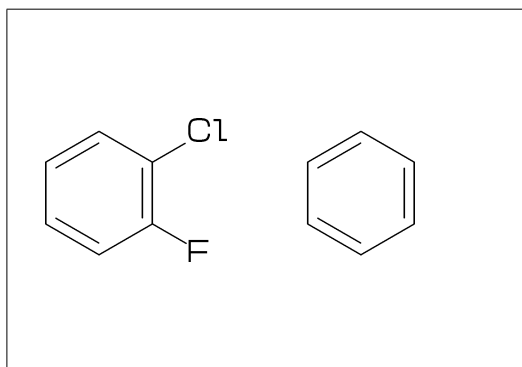
```

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.59 Switch all bond single**

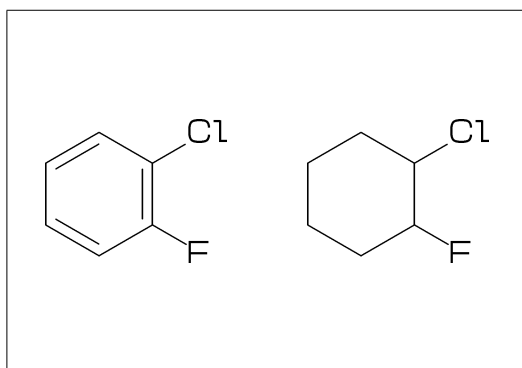
```

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

```

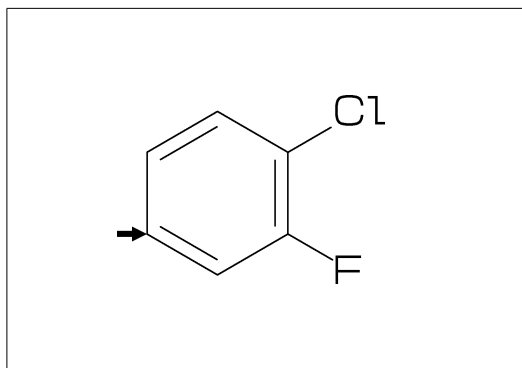
**No.60 Switch start vector**

```

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

** default: sw_start_vector=0

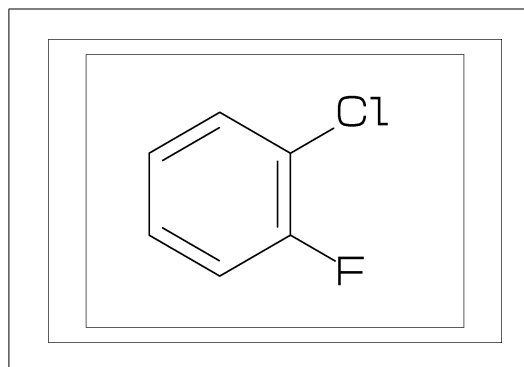
```



No.61 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

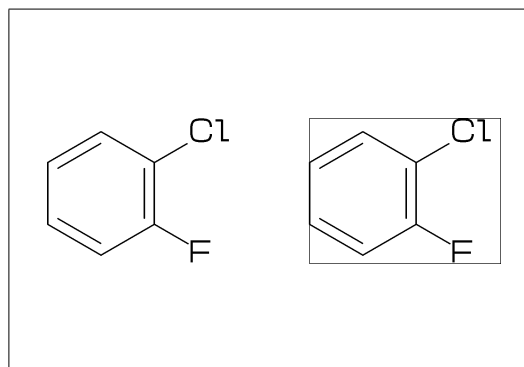
sw_font_frame:=3;
margin_left_right:=5mm; margin_top_bottom:=2mm;
MCf(<30,Ph,4:/Cl,3:/F)
```

**No.62 Switch molecular frame**

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

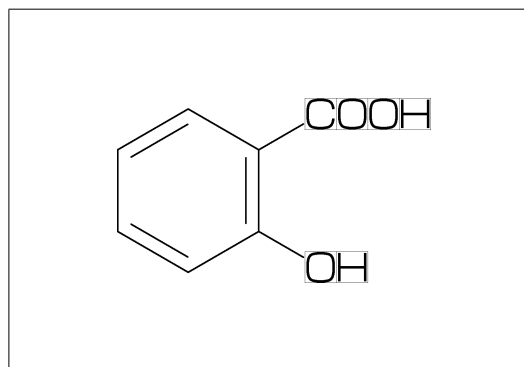
sw_mol_frame:=1;
MCd(1,.5)(1,0.5)(<30,Ph,4:/Cl,3:/F)

** default: sw_mol_frame=0
```

**No.63 Switch atom frame**

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

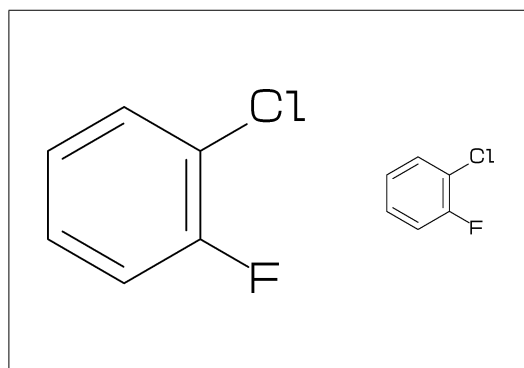
** default: sw_atom_frame=0
```

**No.64 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)

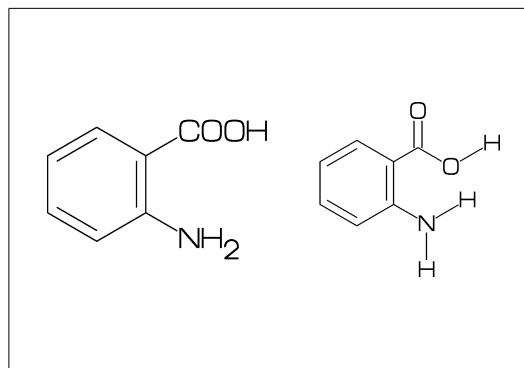
** default: sw_solid=0
```

**No.65 Switch Expand**

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

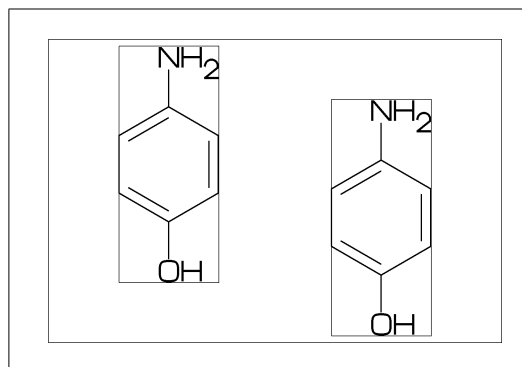
sw_expand:=1;
MCd(1,.5)(1,0.5)(<30,Ph,4:/COOH,3:/NH2)

** default: sw_expand=0
```



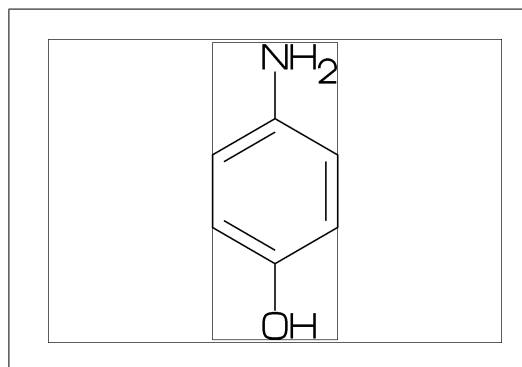
No.66 Function MCd (draw)

```
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)
```



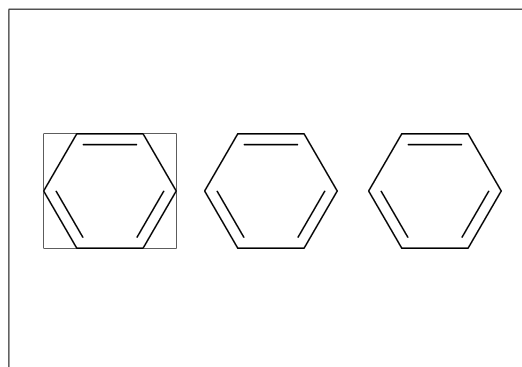
No.67 Function MCf (fit draw)

```
MCf(...) : MCd(1,1)(0.5,0.5)(...)  
  
sw_font_frame:=1;  
sw_mol_frame:=1;  
MCf(<30,Ph,2:/OH,5:/NH2)
```



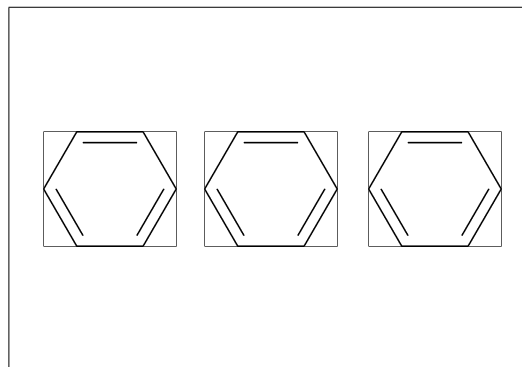
No.68 Local setting

```
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.69 Global setting

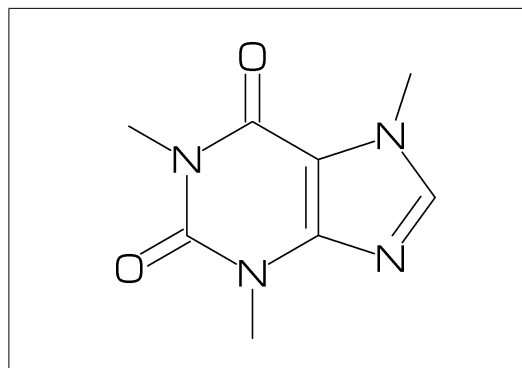
```
sw_mol_frame:=1; % <== Global setting  
beginfont() MCd(1,.4)( 0,.5)(Ph) endfont  
beginfont() MCd(1,.4)(.5,.5)(Ph) endfont  
beginfont() MCd(1,.4)( 1,.5)(Ph) endfont
```



No.70 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.71 Output additional information

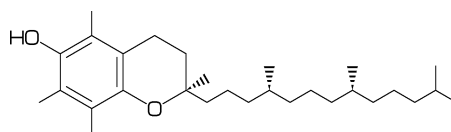
```

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.72 Change aux information delimiter**

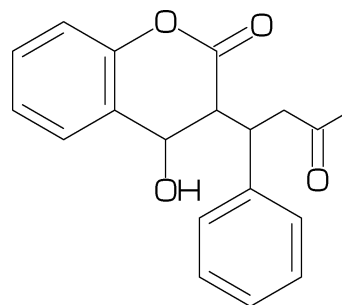
```

aux_delimiter:="/";
beginfont("EN:Warfarin","CAS:81-81-2")
Mcf(...) endfont

%% Output to mcf_man_soc-info.aux %%
F:mcf_man_soc/C:87/EN:Warfarin/CAS:81-81-2

**default aux_delimiter=";"

```

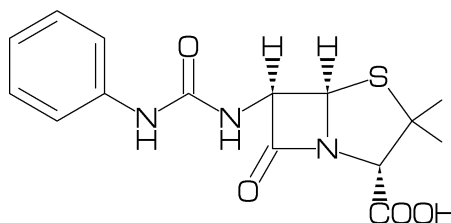
**No.73 Fixed aux information**

```

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

%% Output to mcf_man_soc-info.aux %%
F;C;NO;EN
mcf_man_soc;88;1;Ampicillin

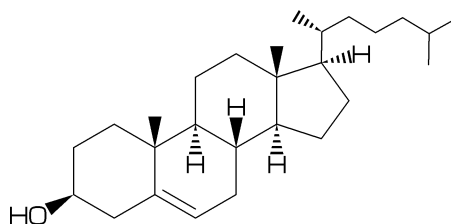
```

**No.74 Example(1) Cholesterol**

```

<30,?6,$(-4,-2)?6,-4=?5,7=d1,
1:*/OH,@(4,12)*/Me^60,9:*/H^60,
10:*/H^180,@(11,-1)*/H^60,
-1^17,/*Me,!4,/Me,!

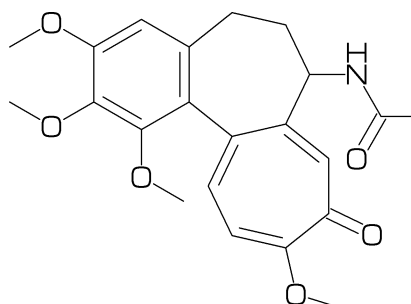
```

**No.75 Example(2) Colchicine**

```

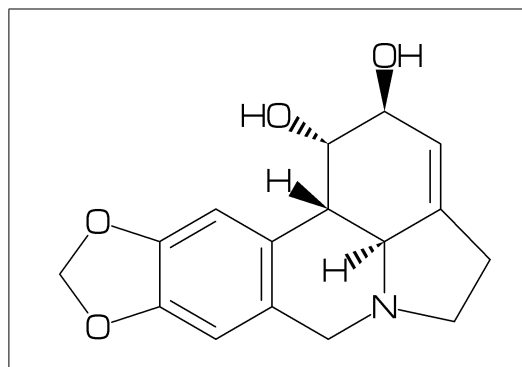
<30,Ph,@(1,2,6)/OMe,l,-4=?7,
l,-5=?7,$(-1,-4,-6)d1,-2://0,-3:/OMe,
#9\,NH,! ,//0,!

```



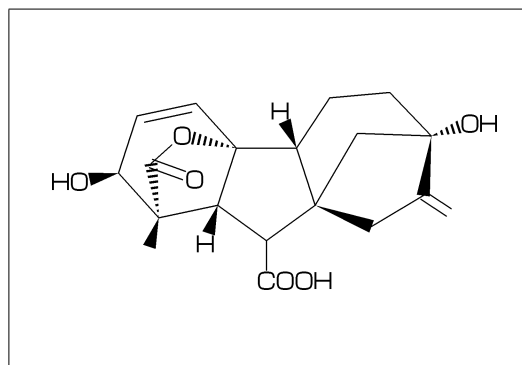
No.76 Example(3) Lycorine

<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:/*OH



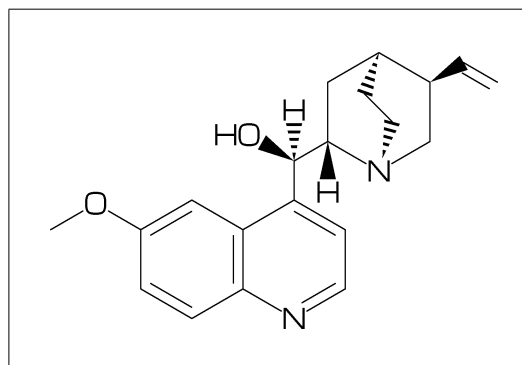
No.77 Example(4) Gibberellin

<12,?6'1.3,3=?5,9=?7,12\^160'1.6,&8,
4\^155~zf'1.2,0,55,//0^180'1,&2~zb,
5=d1,11=wf,13=wb,
7:/COOH,11://Me,1:*/OH,12:/*OH,2:*/Me,
@(3^-60,9^60)*/H



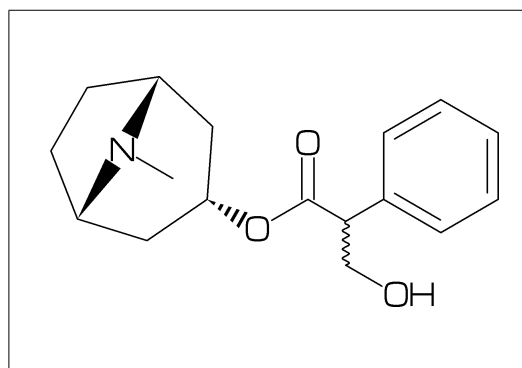
No.78 Example(5) Quinine

<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.79 Example(6) Atoropin

<-30,0,!,//0,!,!,Ph,
#1\~zb^-120,
|,?7'1.1,6*\^190'1.25,N,/Me,&3~wb,
#3\~wv,!,OH



No.80 Example(7) 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

