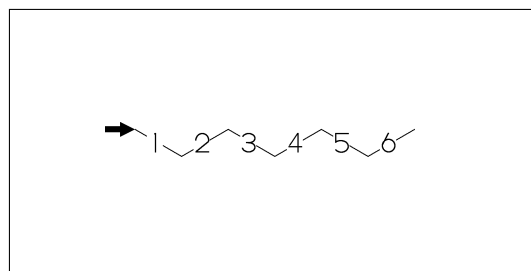


No.1 Chain (1)

plus(+):anticlockwise,minus(-)clockwise
 bold arrow is default angle and position

```
^^30,-60,60,-60,60,-60,60
```

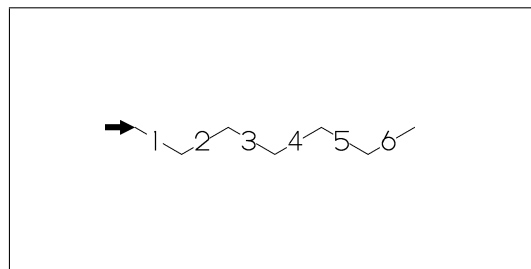
**No.2** Chain (2)

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

```
!6 (!!6)
```

```
** !!6: !,!,!,!,!,!  

!6: {,!!6,}
```

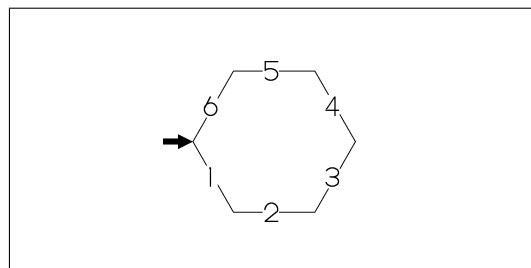
**No.3** Ring

six membered ring

```
?6 (??6)
```

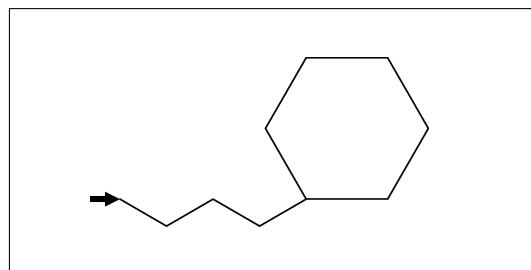
```
** ??6 : ^^ -120,60,60,60,60,60,&(-5)  

?6 : {,??6,}
```

**No.4** rotate

^^angle:rotate current angle

```
^^30,!4,^^30,?6
```

**No.5** Change bond (1)

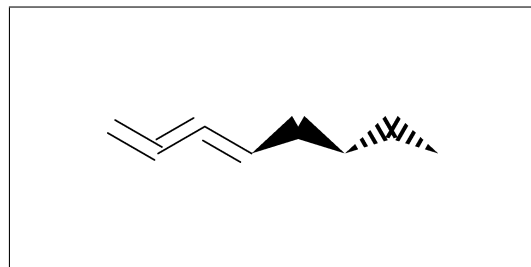
~bond change bond

```
dm:double,dl:double(left),dr:double(right),  

wf:wedge forward,wb:wedge backward,  

zf:wedge dotted,zb:wedge dotted backward
```

```
^^30,!~dm,!~dl,!~dr,!~wf,!~wb,!~zf,!~zb
```

**No.6** Change bond (2)

Bn=bond : change bond

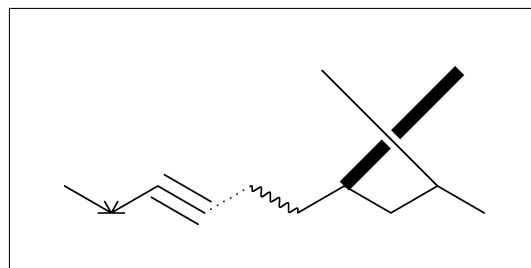
```
vf:vector forward, vb:vector backward,  

tm:triple, wv:waved, bd:broad single,  

ov:over line
```

```
^^30,!9,1=vf,2=vb,3=tm,4=dt,5=wv,  

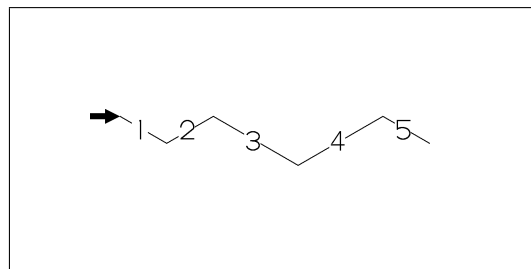
@(7~bd~-45'2,9~ov~45'2)/Me
```



No.7 Change bond length (1)

B'length : change bond length of B

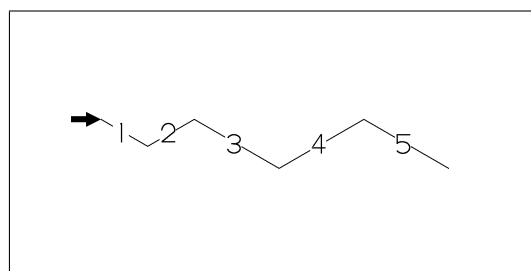
```
^^30,!2,!2'1.2,!
```



No.8 Change bond length (2)

‘‘length : change all bond length after

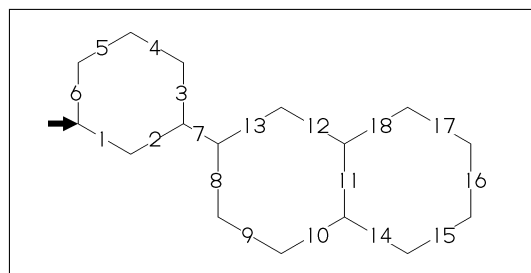
```
^^30,!2,‘‘1.2,!2,!
```



No.9 Change chain length (3)

?n'length : change ring length

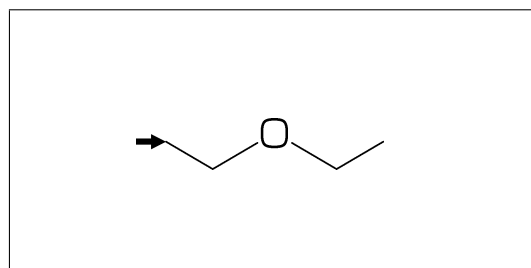
```
^^30,?6,3\,?6'1.2,4=??6
```



No.10 Change atom (1)

Insert hetero atom

```
^^30,!2,0,!2
```

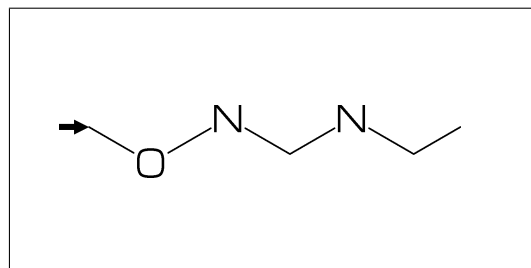


No.11 Change atom (2)

2:0 : change A2 C to O

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

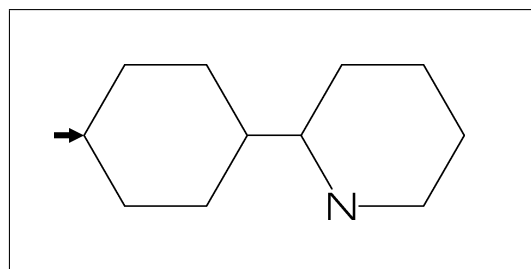
```
^^30,!6,2:0,@(3,5)N
```



No.12 Change atom (3)

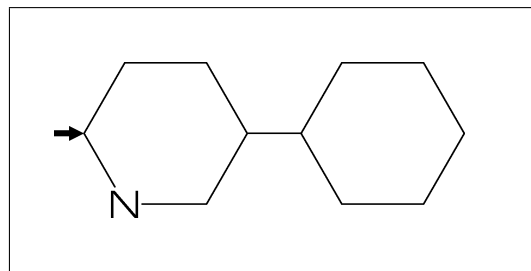
2:N : change A2(brock ahead) C to N

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

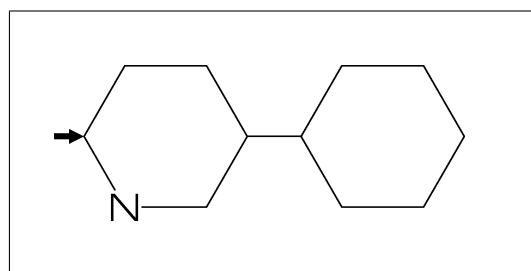


No.13 Change atom (4)

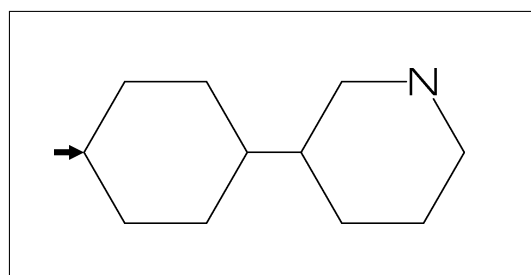
2:N : change A2(brock ahead) C to N
 ??6 is not brock
 ?6,4\,??6,2:N

**No.14** Change atom (5)

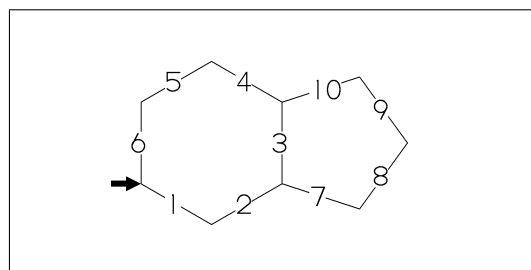
#2:N : change A#2 C to N
 ?6,4\,?6,#2:N

**No.15** Change atom (6)

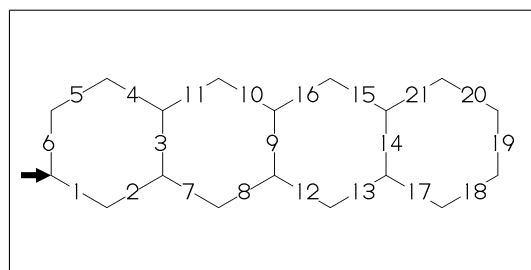
-2:N : change A(-2) C to N
 ?6,4\,?6,-2:N

**No.16** Fused ring (1)

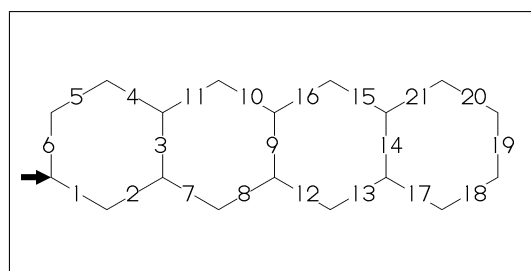
?6,3=?6 : fuse ?6 at B3
 ?6,3=?6

**No.17** Fused ring (2)

?6,\$(3,3,3)??6 NG
 ?6,\$(3,9,14)??6 OK
 ?6,\$(-4,-3,-3)??6 OK
 ?6,\$(#3,#9,#14)??6 OK

**No.18** Fused ring (3)

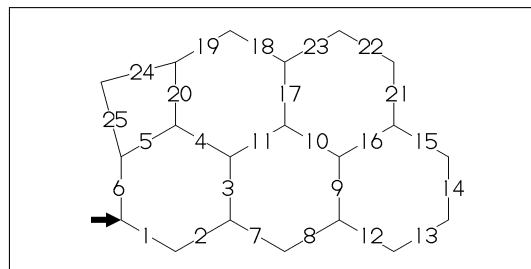
?6,\$(3,3,3)?6 OK
 ?6,\$(3,9,14)?6 NG
 ?6,\$(-4,-3,-3)?6 OK
 ?6,\$(#3,#9,#14)?6 OK



No.19 Fused ring (4)

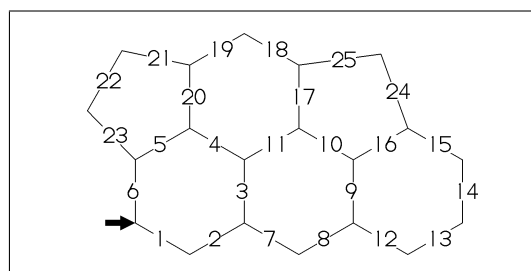
(4,11)=??6[4] : fuse 4/6 ring to B4 ..B11
 (16,17)=??6[3] : fuse 3/6 ring to B16..B17
 (20,5)=??4[2] : fuse 2/4 ring to B20.. B5

```
^^30,?6,$(3,9)??6,(4,11)=??6[4],
      (16,17)=??6[3],(20,5)=??4[2]
```

**No.20** Fused ring (5)

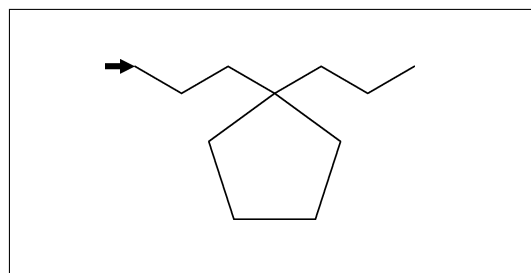
(20,5)=??5[3] : fuse 3/5 ring to B20..B5
 (16,17)=??5[2] : fuse 2/5 ring to B16..B17

```
^^30,?6,$(3,9)??6,(4,11)=??6[4],
      (20,5)=??5[3],(16,17)=??5[2]
```

**No.21** Spiro ring

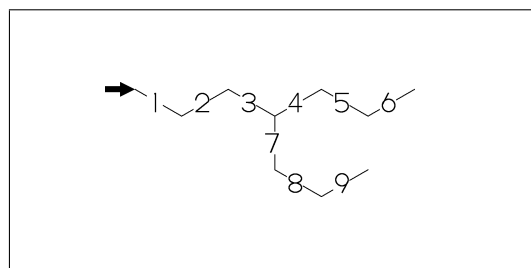
4*,?5 : add ?5(5 membered ring) to A4

```
^^30,!6,4*,?5
```

**No.22** Branch (1)

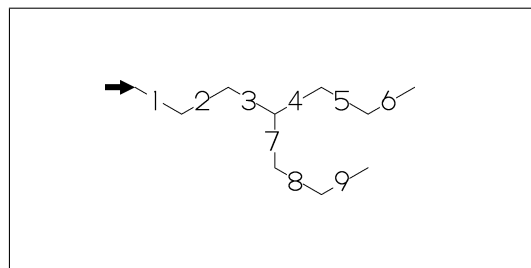
/ : branch bond
 / : process at last

```
^^30,!3,/!2,!3
```

**No.23** Branch (2)

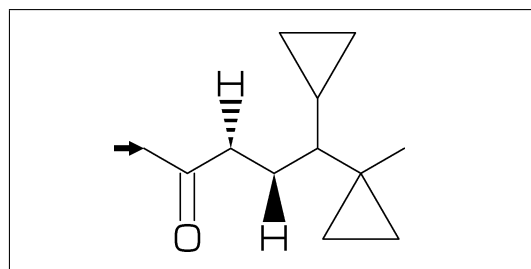
4\ : branch bond at A4

```
^^30,!6,4\,!2
```

**No.24** Substituent (1)

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

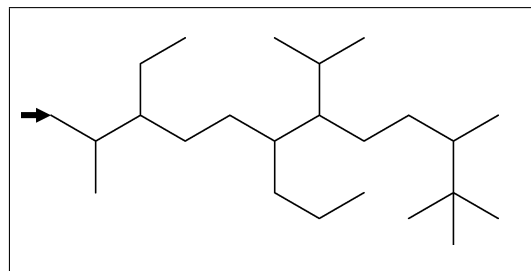
```
^^30,!,,/O,!,*H,!,*H,!,,/?3,!,**?3,!
```



No.25 Substituent (2)

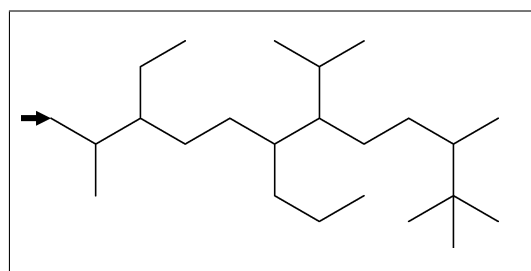
Insert substituent

```
^^30,! ,/Me,! ,/Et,!3,/Pr,! ,/iPr,!3,/tBu,!
```

**No.26** Substituent (3)

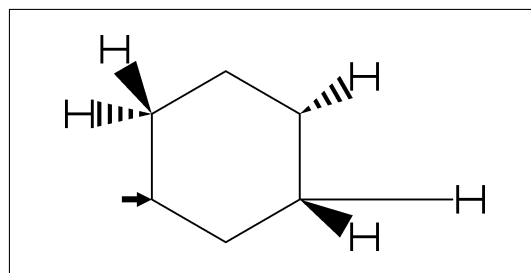
Add substituent

```
^^30,!10,2:/Me,3:/Et,6:/Pr,7:/iPr,10:/tBu
```

**No.27** Substituent (4)

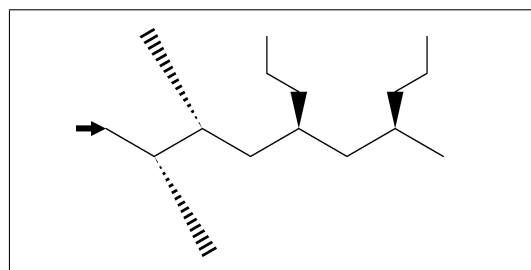
~,^,','> : change type,angle,length,enviroment
of substituent

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

**No.28** Substituent (5)

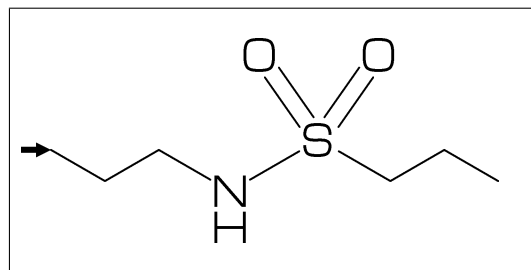
~,^,','> : change type,angle,length,enviroment
of substituent

```
^^30,!7'1,  
@(2,3)/*Me'2^30,5:*/Pr>lr,7:*/Pr>r1
```

**No.29** Change atom and Substituent

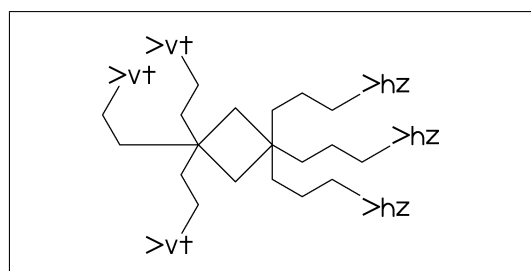
NH,S00 : inset hetero atom and substituent
simultaneously

```
^^30,!3,NH,! ,S00,!3
```

**No.30** Chain stretch direction environment (1)

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

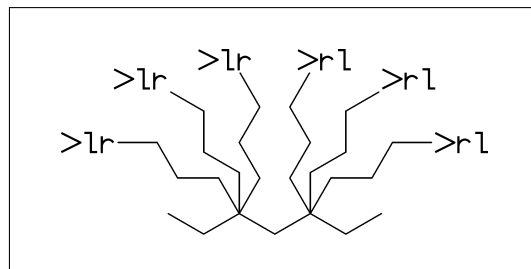
```
?4,  
@(3^-90,3^-30,3^90)/'(!3,"{>hz}")>hz,  
@(1^-60,1'1.5,1^60)/'(!2,"{>vt}")>vt
```



No.31 Chain stretch direction environment (2)

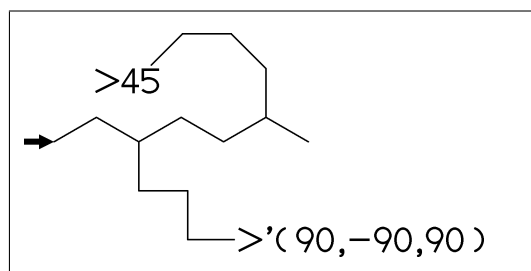
```
>lr : left-right enviroment
>rl : right-left enviroment

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

**No.32** Chain stretch direction environment (3)

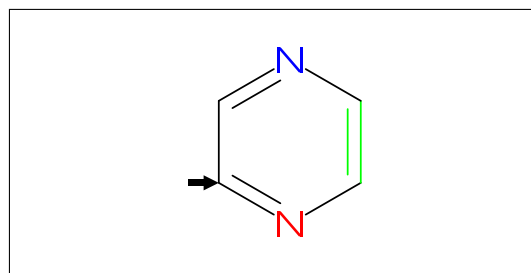
```
>45 : fixed angle enviroment
>'(-90,90,-90) : multi angle enviroment

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

**No.33** Change color

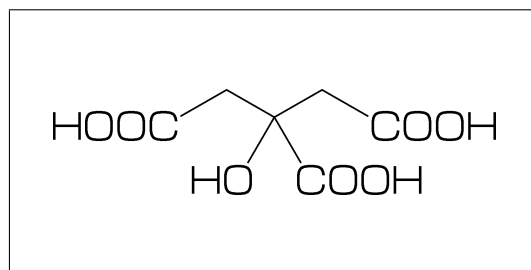
```
@(5)green : change color of A5 green
$(3)red : change color of B3 red

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

**No.34** Chain start multiple characters

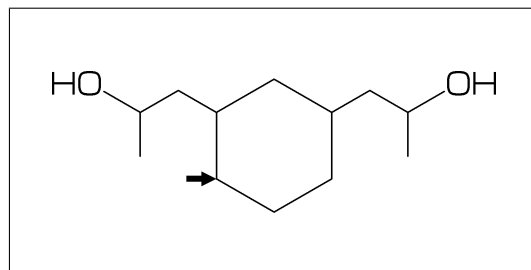
```
Use !0 instead of !,
if begin with multi charactor string

^^30,COOH,!0,!,/OH^-30,/COOH^30,!2,COOH
```

**No.35** User definition

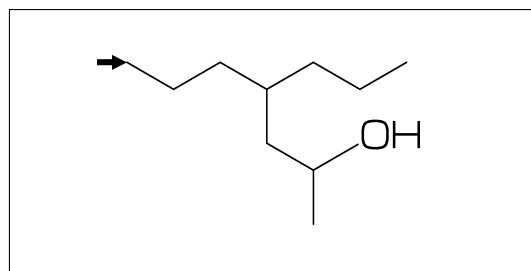
```
iBuOH : user defined substructure

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

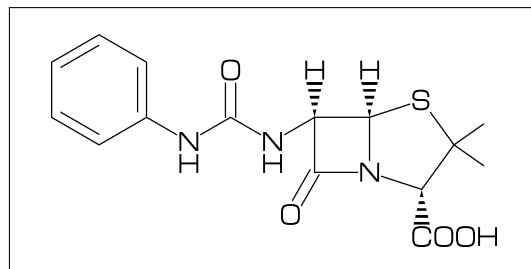
**No.36** Inline definition

```
Insert user defined substructure

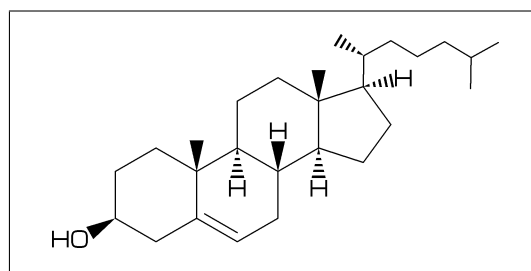
^^30,!3,/ '(!,/Me,! ,OH),!3
```



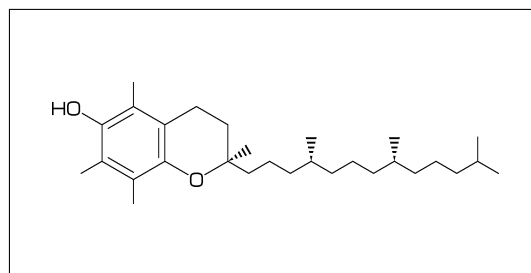
No.37 Example(1) Ampicillin

$$\begin{aligned} & \sim 45, \\ & 74, 2: N, 2 = ? 75, -1: S, \\ & @ (3 \sim 45, 4 \sim 45) / * H, 1: // O \sim 15, \\ & 5: / * COOH \sim 18, @ (6 \sim 35, 6 \sim 35) / Me, \\ & 4 \sim 75, NH, !, // O, !, NH, !, Ph \end{aligned}$$


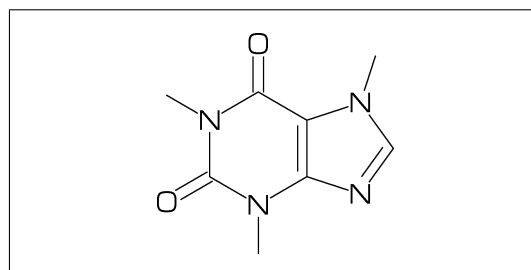
No.38 Example(2) Cholesterol

$$\begin{aligned} & \sim 30, \\ & 76, \$(-4, -2)??6, -4=?5, 7=d1, \\ & 1:*/OH, @(4, 12)*/Me^{60}, 9:*/H^{60}, \\ & 10:/*H^{180}, @(11, -1)/*H^{-60}, \\ & -1\backslash^{17}, /*Me, !4, /Me, !, \end{aligned}$$


No.39 Example(3) alfa-Tocopherol

$$\begin{aligned} & \sim 30, \\ & \text{Ph}_3 = \text{??6}, \\ & 7:0, @ (1, 2, 5) / \text{Me}, 8: / * \text{Me}^{60}, 6: / \text{OH}, \\ & 8: \backslash, 12, @ (4, 8) / * \text{Me}, 12: / \text{Me} \end{aligned}$$


No.40 Example(4) Caffeine

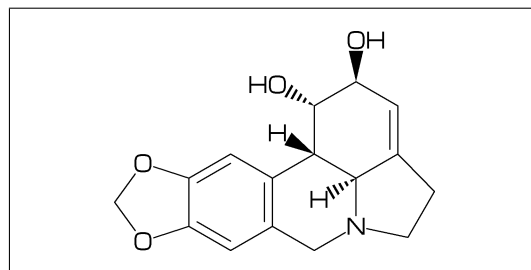
$$\begin{aligned} & \sim 30, \\ & ?6, -4 = ?75, \$ (3, 8) d1, @ (2, 6, 7, 9) N, \\ & @ (2, 6, 9) / \text{Me}, @ (1, 5) // 0 \end{aligned}$$


No.41 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

```

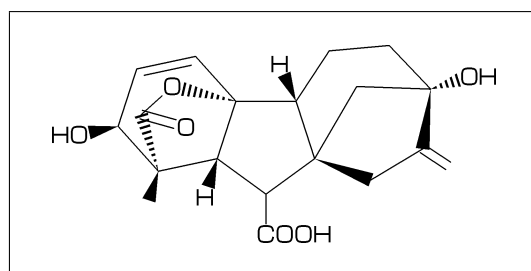


No.42 Example(6) Gibberellin

```

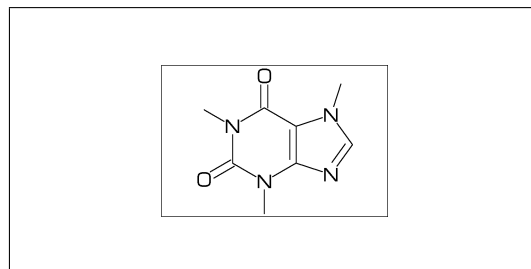
^~12,
76'1.3,3=?75,9=?77,12\^160'1.6,&8,
4\^155~zf'-1.2,0,55,//0^180'1,&2~zb,
5=d1,11=wf,13=wb,7:/COOH,11://Me,1:*/OH,
12:/*OH,2:*/Me,@(3^-60,9^60)*/H

```

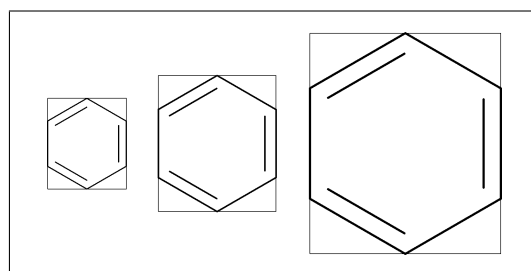


No.43 Font size

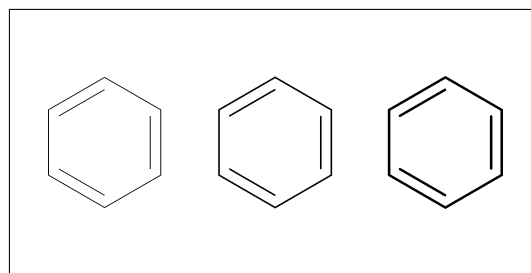
```
font_wd#:=30mm#;
font_ht#:=20mm#;
beginfont("EN:Caffeine")
  sw_font_frame:=1;
  MCf(^30,?6,-4=?5,$(3,8)d1,@(2,6,7,9)N,
    @(2,6,9)/Me,@(1,5)//O)
endfont
```

**No.44** Max ratio bond/width length

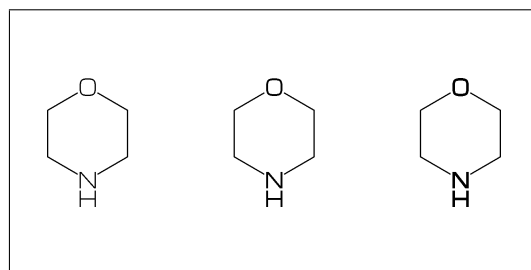
```
max_bond_width:=0.10;
MCd(1,1)(0, .5)(^30,Ph)
max_bond_width:=0.15;          %<== default ==>
MCd(1,1)(.33, .5)(^30,Ph)
max_bond_width:=0.30;
MCd(1,1)(1, .5)(^30,Ph)
```

**No.45** Ratio thickness/bond length

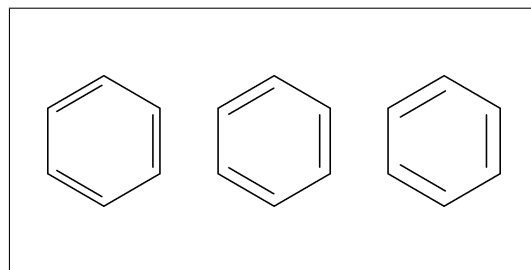
```
ratio_thickness_bond:= 0.005;
MCd(.6,.6)(0, .5)(^30,Ph)
ratio_thickness_bond:= 0.015;   %<== default ==>
MCd(.6,.6)(.5, .5)(^30,Ph)
ratio_thickness_bond:= 0.030;
MCd(.6,.6)(1, .5)(^30,Ph)
```

**No.46** Ratio char/bond thickness

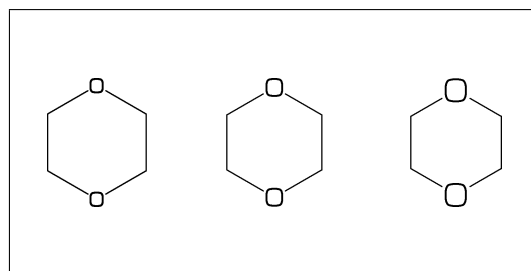
```
ratio_char_bond:=1.0;
MCd(.6,.6)(0, .5)(^30,?6,5:0,2:NH)
ratio_char_bond:=1.5;          %<== default ==>
MCd(.6,.6)(.5, .5)(^30,?6,5:0,2:NH)
ratio_char_bond:=2.0;
MCd(.6,.6)(1, .5)(^30,?6,5:0,2:NH)
```

**No.47** Ratio bondgap/bond length

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

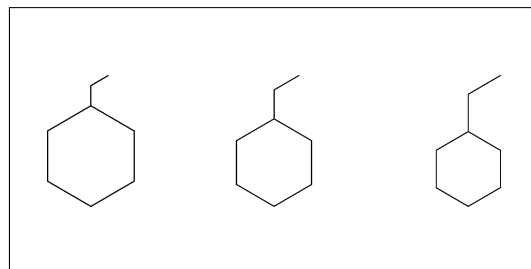
**No.48** Ratio atom/bond length

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

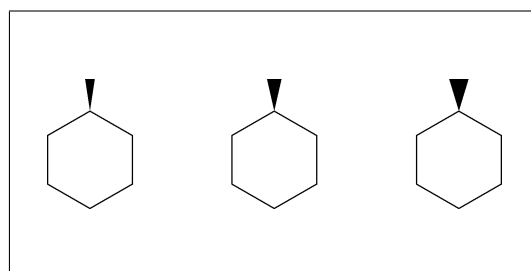


No.49 Ratio chain/ring length

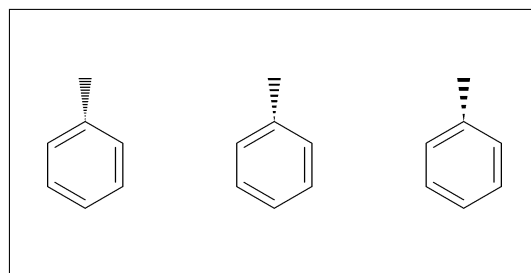
```
ratio_chain_ring:= 0.4;
MCd(.6,.6)(0, .5)(^30,?6,5:/Et)
ratio_chain_ring:= 0.66;          %<<== default ==>>
MCd(.6,.6)(.5, .5)(^30,?6,5:/Et)
ratio_chain_ring:= 1.0;
MCd(.6,.6)(1, .5)(^30,?6,5:/Et)
```

**No.50** Ratio wedge/bond length

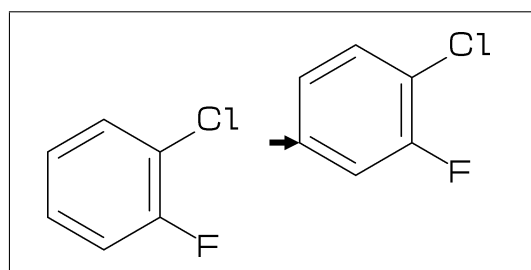
```
ratio_wedge_bond:=0.10;
MCd(.6,.6)(0, .5)(^30,?6,5:*/Me)
ratio_wedge_bond:=0.15;          %<<== default ==>>
MCd(.6,.6)(.5, .5)(^30,?6,5:*/Me)
ratio_wedge_bond:=0.20;
MCd(.6,.6)(1, .5)(^30,?6,5:*/Me)
```

**No.51** Ratio zebra gap/bond length

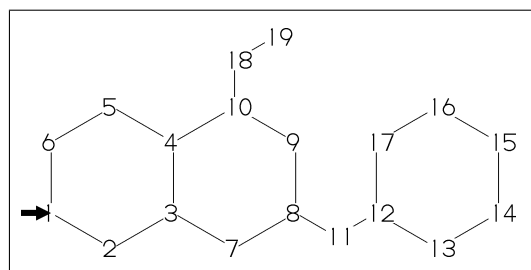
```
ratio_zebra_gap:=0.06;
MCd(.6,.6)(0, .5)(^30,Ph,5:/*Me'1)
ratio_zebra_gap:=0.12;          %<<== default ==>>
MCd(.6,.6)(.5, .5)(^30,Ph,5:/*Me'1)
ratio_zebra_gap:=0.20;
MCd(.6,.6)(1, .5)(^30,Ph,5:/*Me'1)
```

**No.52** Switch Start Vector

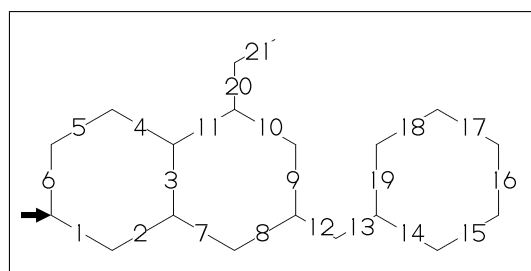
```
MCd(.8,.8)( 0, 0)(^30,Ph,4:/Cl,3:/F)
sw_start_vector:=1;
MCd(.8,.8)( 1, 1)(^30,Ph,4:/Cl,3:/F)
```

**No.53** Switch NumberingA

```
sw_numberA:=1;
MCf(^30,
    Ph,-4=Ph1,-3\,! ,Ph,10:/Et)
```

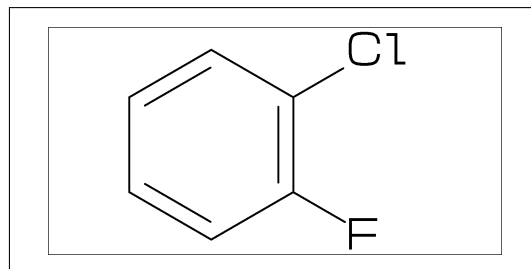
**No.54** Switch NumberingB

```
sw_numberB:=1;
MCf(^30,
    Ph,-4=Ph1,-3\,! ,Ph,10:/Et)
```

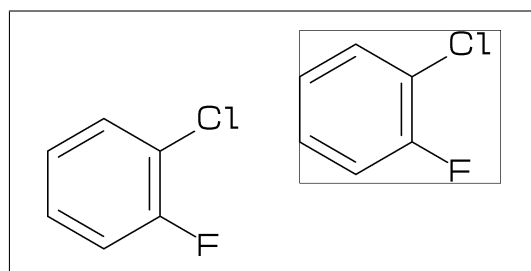


No.55 Switch font frame

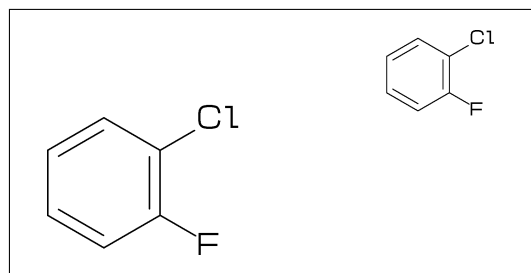
```
sw_font_frame:=1;
MCf(^^30,Ph,4:/Cl,3:/F)
```

**No.56** Switch molecular frame

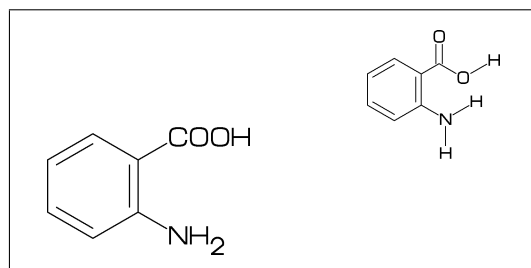
```
MCd(.8,.8)(0,0)(^^30,Ph,4:/Cl,3:/F)
sw_mol_frame:=1;
MCd(.8,.8)(1,1)(^^30,Ph,4:/Cl,3:/F)
```

**No.57** Switch Solid ratio

```
MCd(.8,.8)( 0, 0)(^^30,Ph,4:/Cl,3:/F)
sw_solid:=1; ratio_bond_width:=0.08;
MCd(.8,.8)( 1, 1)(^^30,Ph,4:/Cl,3:/F)
```

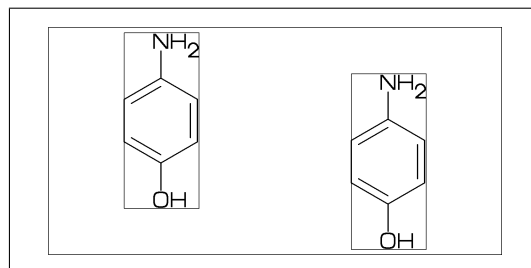
**No.58** Switch Expand

```
MCd(.6,.6)(0,0)(^^30,Ph,4:/COOH,3:/NH2)
sw_expand:=1;
MCd(.6,.6)(1,1)(^^30,Ph,4:/COOH,3:/NH2)
```

**No.59** Function MCd

```
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)
```

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

**No.60** Function MCf

```
MCf(^^30,Ph,2:/OH,5:/NH2)

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

