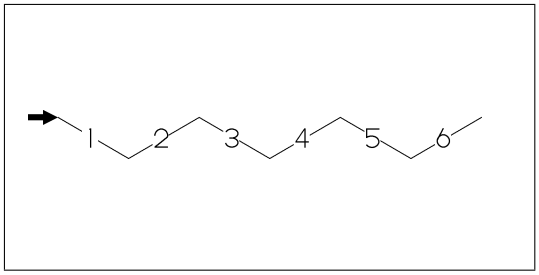
# Molecular Coding Format manual

by Akira Yamaji 2015.7.25

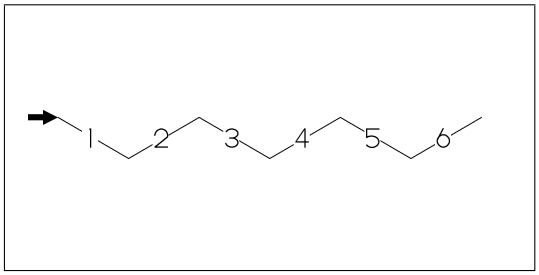
**No.1** Chain (1)

```
plus(+):anticlockwize,minus(-)clockwize
bold arrow is default angle and position

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



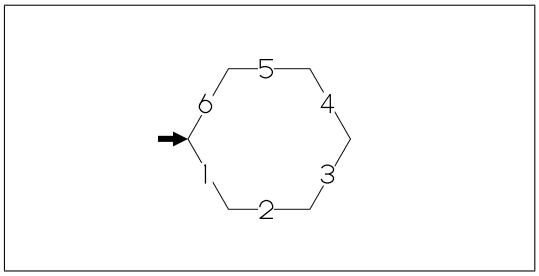

**No.2** Chain (2)

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

  !6 (!!6)

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



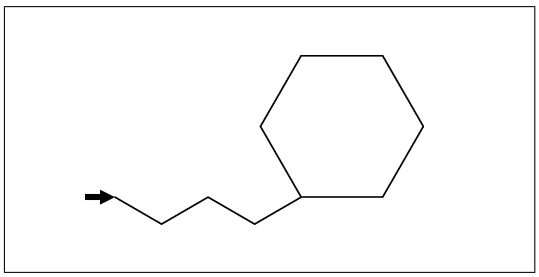

**No.3** Ring

```
six membered ring

  ?6 (??6)

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



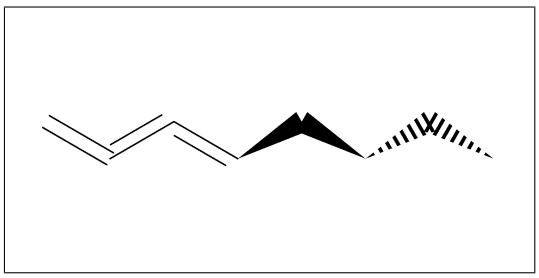

**No.4** rotate

```
^^angle:rotate current angle

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



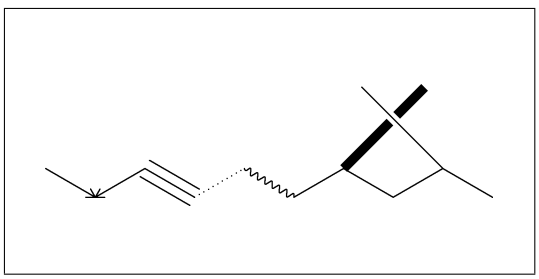
**No.5** Change bond (1)

```
~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
```



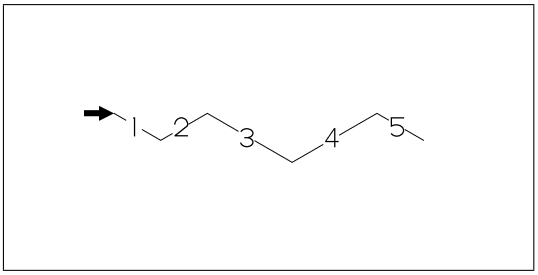
**No.6** Change bond (2)

```
 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
```



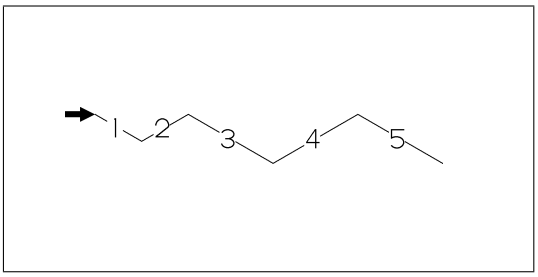
**No.7** Change bond length (1)

```
B‘length : change bond length of B

  ^^30,!2,!2‘1.2,!
```



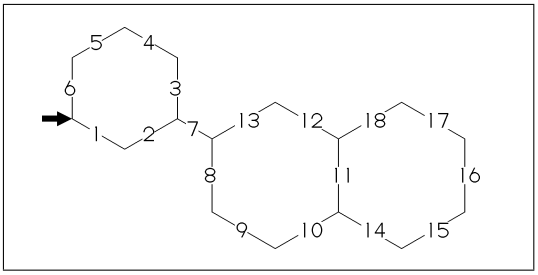

**No.8** Change bond length (2)

```
‘‘length : change all bond length after

  ^^30,!2,‘‘1.2,!2,!
```



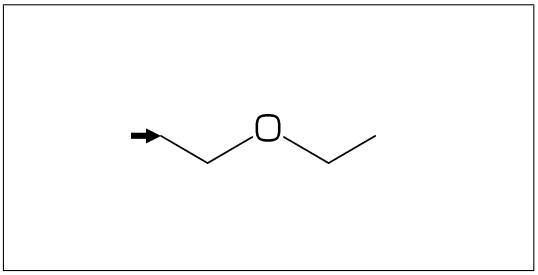

**No.9** Change chain length (3)

```
?n‘length : change ring length

  ^^30,?6,3\,?6‘1.2,4=??6
```



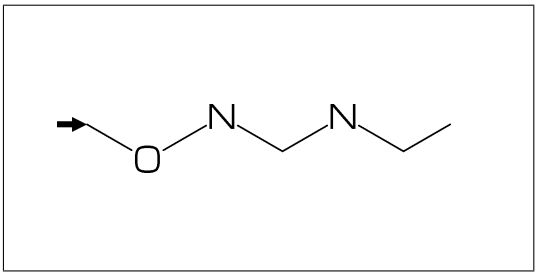

**No.10** Change atom (1)

```
Insert hetero atom

  ^^30,!2,O,!2
```



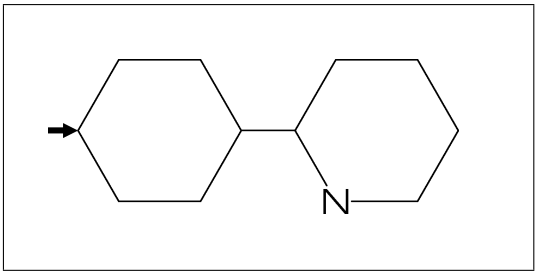

**No.11** Change atom (2)

```
2:O : change A2 C to O
@(3,5)N : change  A3,A5 C to N

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



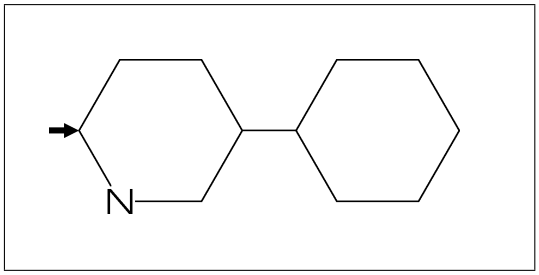

**No.12** Change atom (3)

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

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



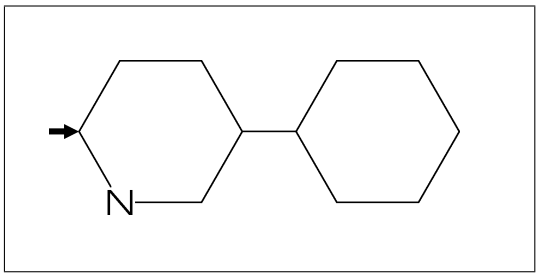
**No.13** Change atom (4)

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



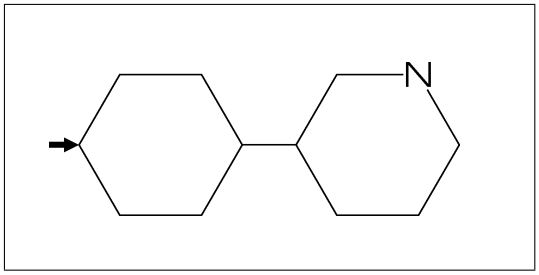

**No.14** Change atom (5)

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

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



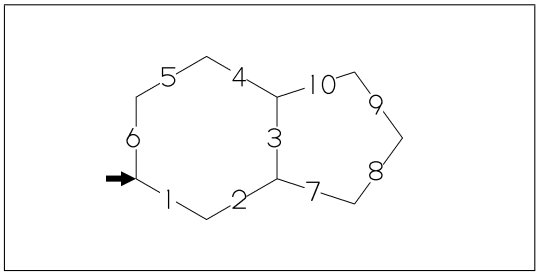

**No.15** Change atom (6)

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

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



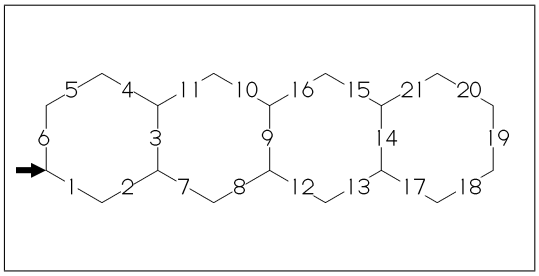

**No.16** Fused ring (1)

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

  ?6,3=?6
```



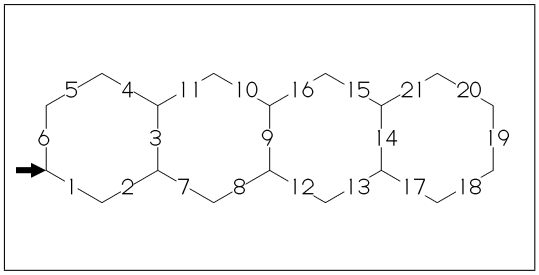

**No.17** Fused ring (2)

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



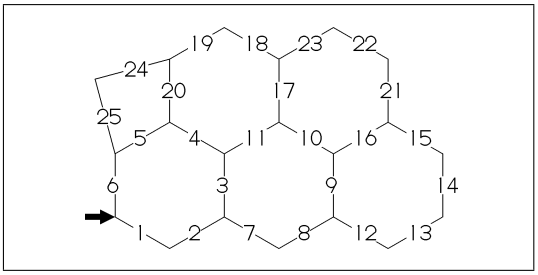

**No.18** Fused ring (3)

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



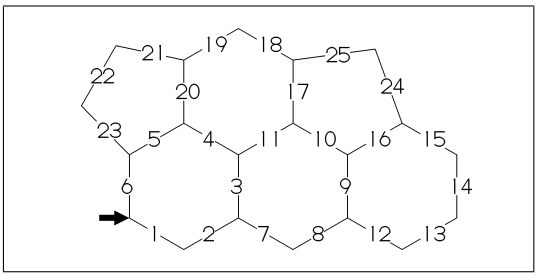
**No.19** Fused ring (4)

```
(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]
```



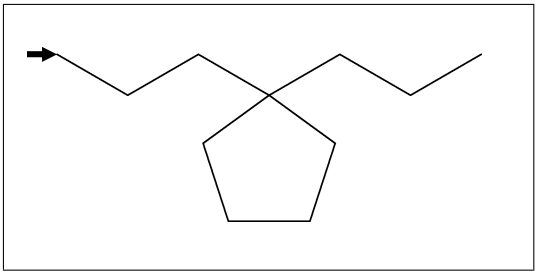

**No.20** Fused ring (5)

```
(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]
```



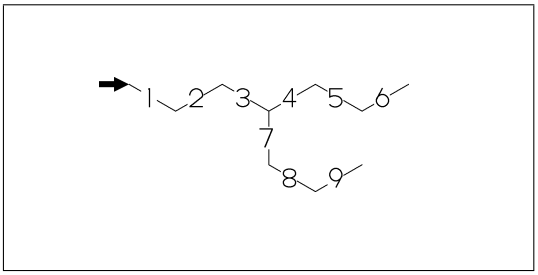

**No.21** Spiro ring

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

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



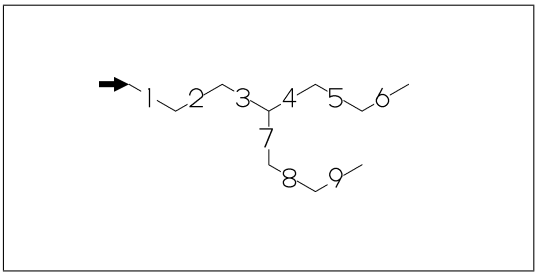
**No.22** Branch (1)

```
/ : branch bond
/ : process at last

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



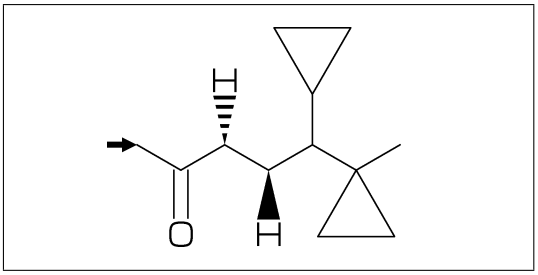

**No.23** Branch (2)

```
4\ : branch bond at A4

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



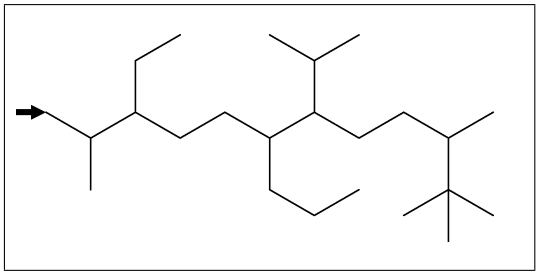

**No.24** Substituent (1)

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

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



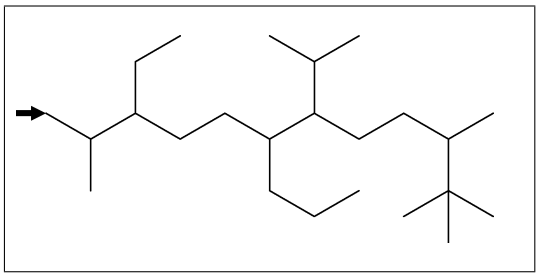
**No.25** Substituent (2)

```
Insert substituent

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



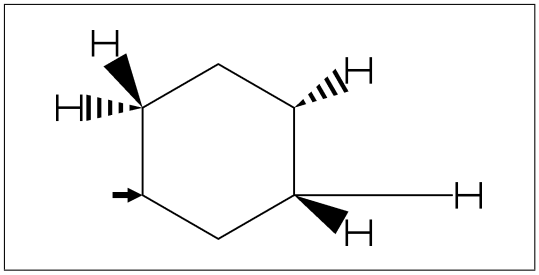
**No.26** Substituent (3)

```
Add substituent

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



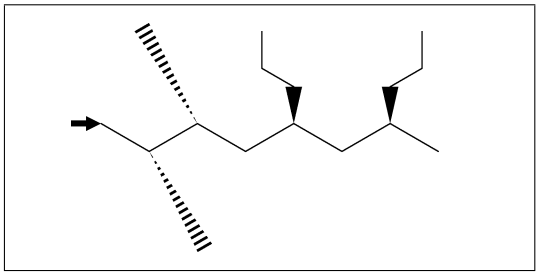
**No.27** Substituent (4)

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

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



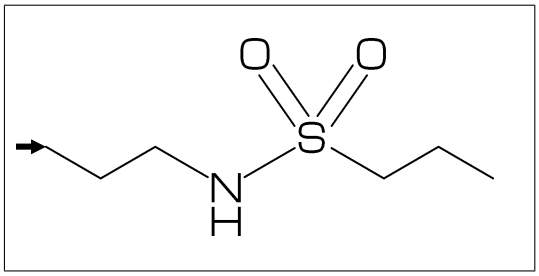

**No.28** Substituent (5)

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

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



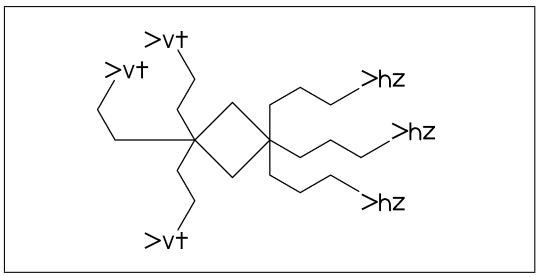
**No.29** Change atom and Substituent

```
NH,SOO : inset hetero atom and substituent
         simultaneously

  ^^30,!3,NH,!,SOO,!3
```



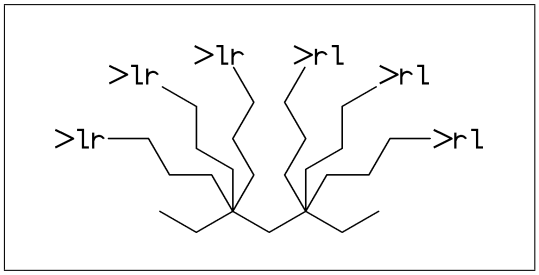

**No.30** Chain strech direction environment (1)

```
>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
```



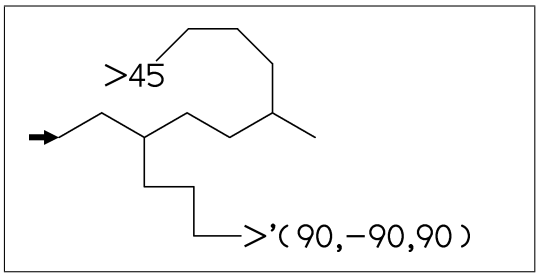
**No.31** Chain strech direction environment (2)

```
>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
```



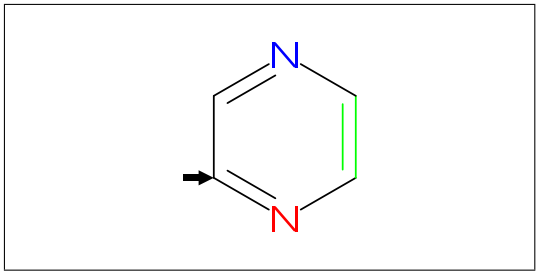

**No.32** Chain strech direction environment (3)

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

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



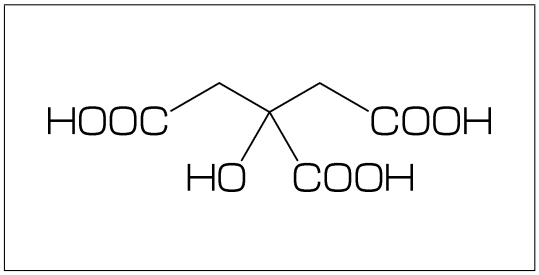

**No.33** Change color

```
@(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
```



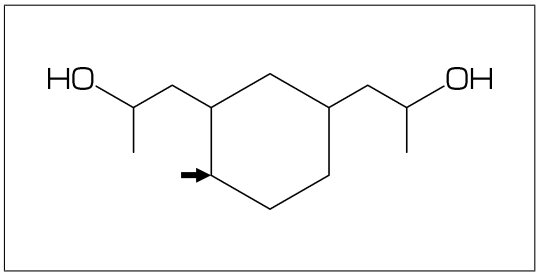

**No.34** Chain start multiple characters

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

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



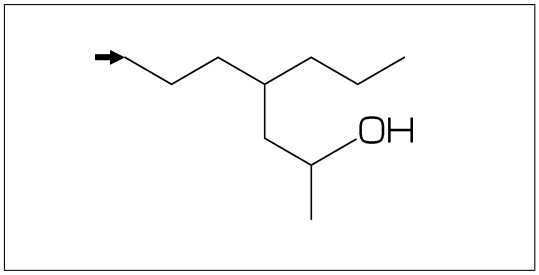

**No.35** User definition

```
iBuOH : user defined substructure

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



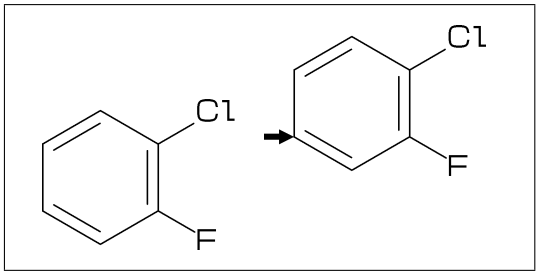

**No.36** Inline definition

```
Insert user defined substructure

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



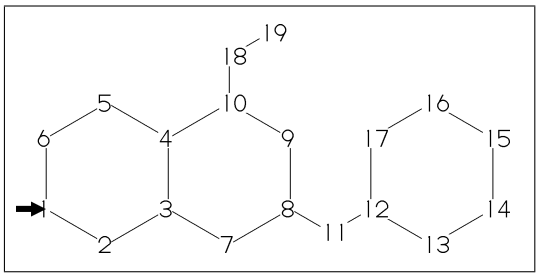
**No.37** Switch Start Vector

```
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)
```



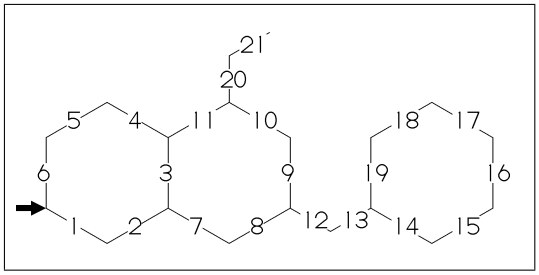

**No.38** Switch NumberingA

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



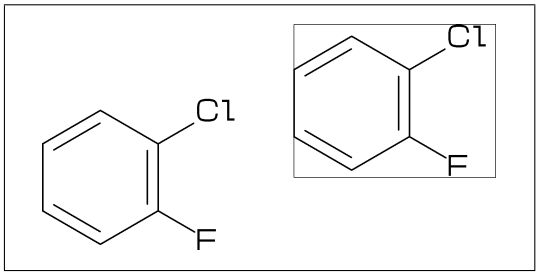

**No.39** Switch NumberingB

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



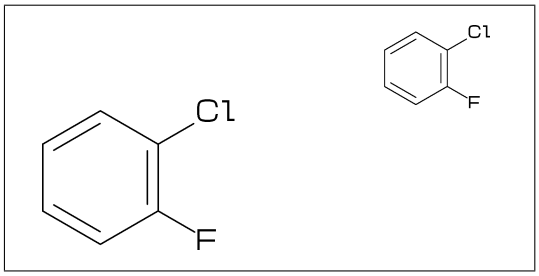

**No.40** Switch Frame

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



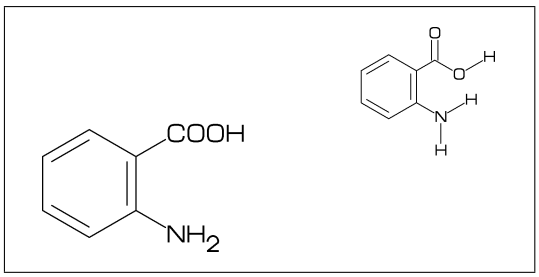

**No.41** Switch Solid ratio

```
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)
```



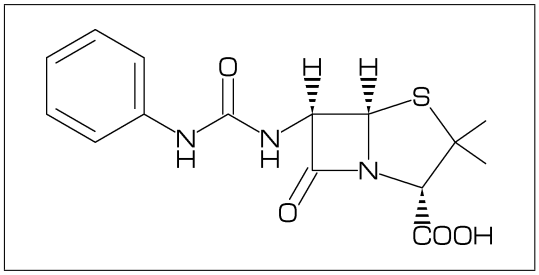

**No.42** Switch Expand

```
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)
```



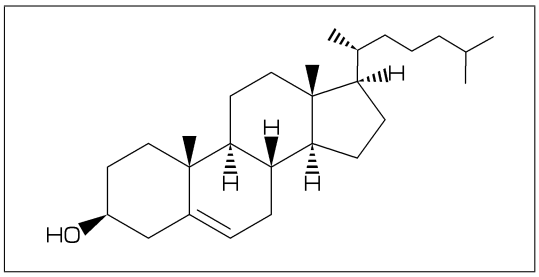
**No.43** Example(1) Ampicillin

```
^^45,
?4,2:N,2=??5,-1:S,
@(3^45,4^-45)/*H,1://O^15,
5:/*COOH^-18,@(6^35,6^-35)/Me,
4\^75,NH,!,//O,!,NH,!,Ph
```



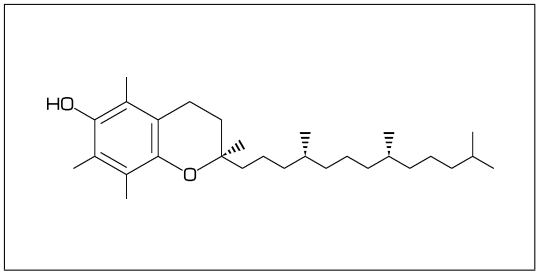
**No.44** Example(2) Cholesterol

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



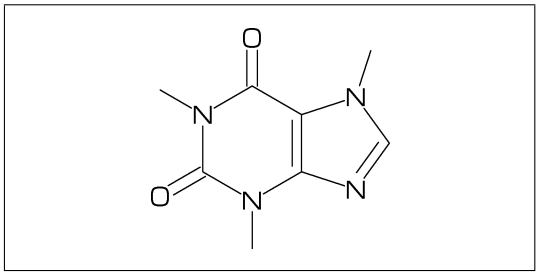
**No.45** Example(3) alfa-Tocopherol

```
^^30,
Ph,3=??6,
7:O,@(1,2,5)/Me,8:/*Me^60,6:/OH,
8\,!12,@(4,8)/*Me,12:/Me
```



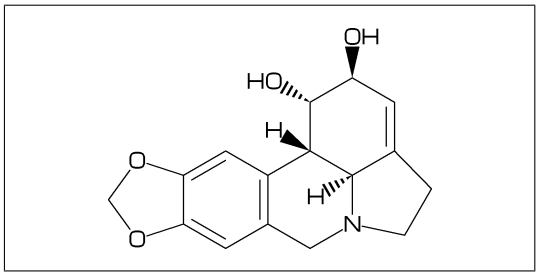
**No.46** Example(4) Caffeine

```
^^30,
?6,-4=??5,$(3,8)dl,@(2,6,7,9)N,
@(2,6,9)/Me,@(1,5)//O
```



**No.47** Example(5) Lycorine

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



**No.48** Example(6) Gibberellin

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