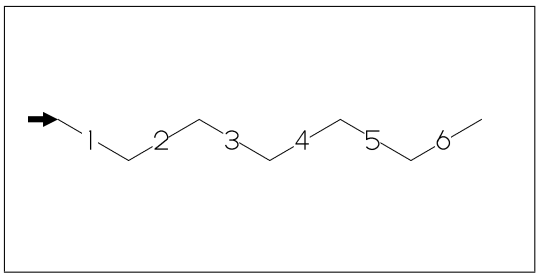
Molecular coding format manual

by Akira Yamaji 2015.7

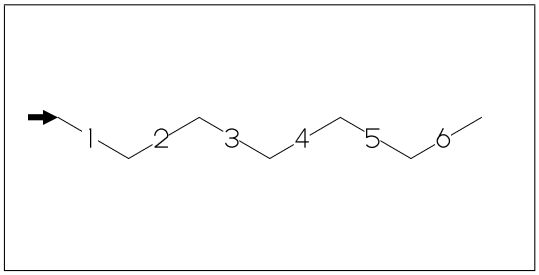
No.1 Chain (1)

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

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



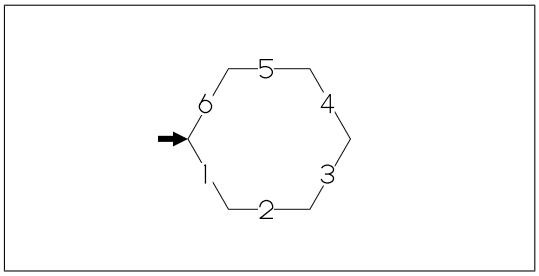
No.2 Chain (2)

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

  !6 (!!6)

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



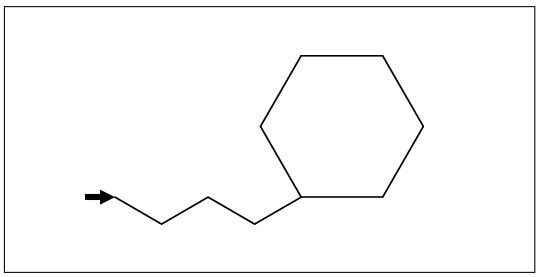
No.3 Ring

```
six membered ring

  ?6 (??6)

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



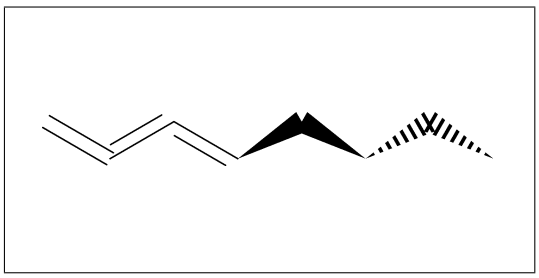
No.4 rotate

```
^^angle:rotate current angle

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



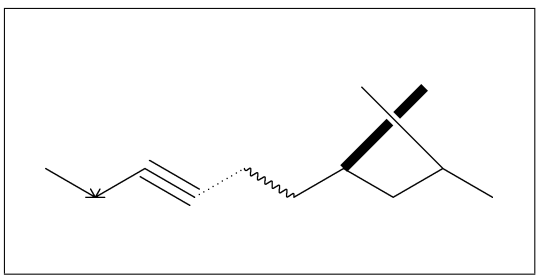
No.5 Change bond (1)

```
~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
```



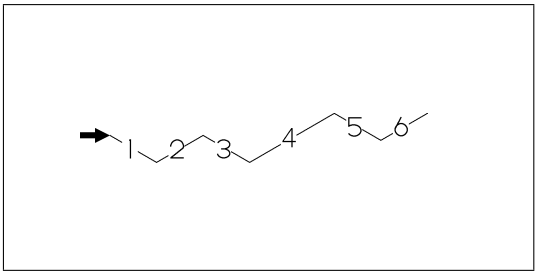
No.6 Change bond (2)

```
 Bn=bond : change bond
  dm:double,dl:double(left),dr:double(right),
  wf:wedge forward,wb:wedge backward,
  zf:wedge dotted,zb:wedge dotted backward

  ^^30,!9,1=vf,2=vb,3=tm,4=dt,5=wv,
  @(7~bd^-45‘2,9~ov^45‘2)/Me
```



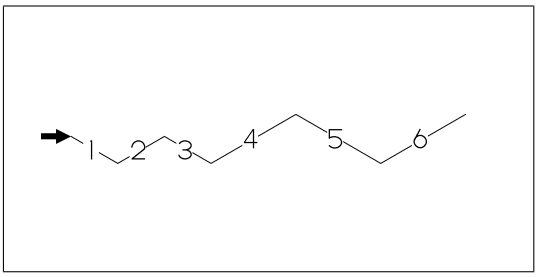
No.7 Change bond length (1)

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

  ^^30,!3,!‘1.2,!2
```



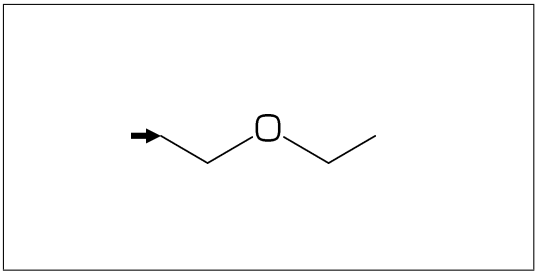
No.8 Change bond length (2)

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

  ^^30,!3,‘‘1.2,!3
```



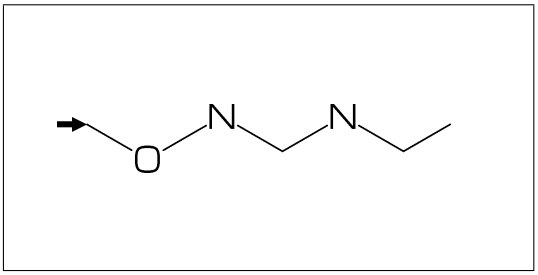
No.9 Change atom (1)

```
Insert hetero atom

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



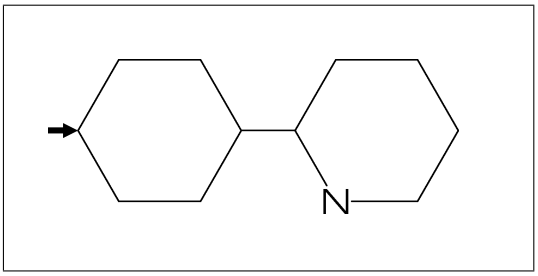
No.10 Change atom (2)

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

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



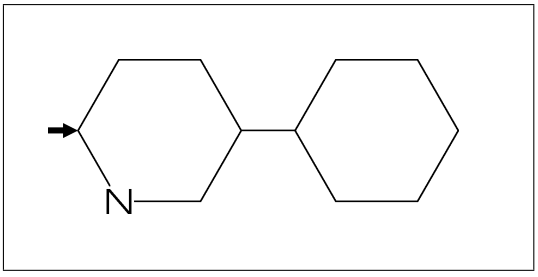
No.11 Change atom (3)

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

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



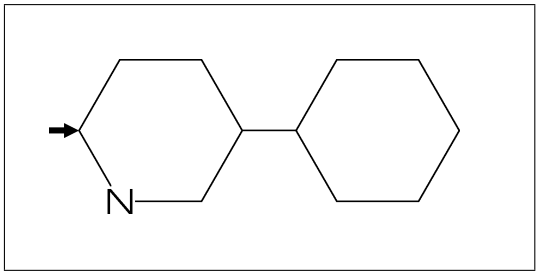
No.12 Change atom (4)

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



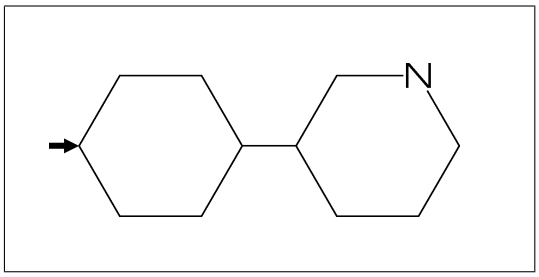
No.13 Change atom (5)

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

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



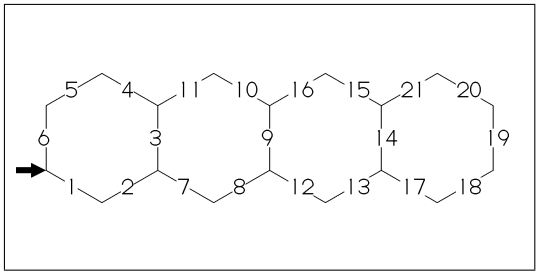
No.14 Change atom (6)

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

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



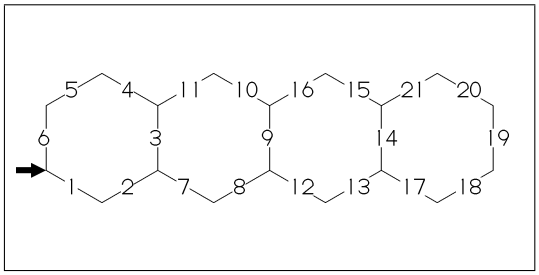
No.15 Fused ring (1)

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



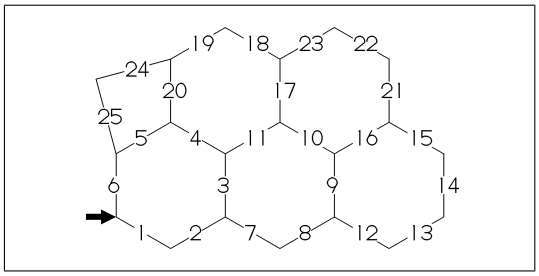
No.16 Fused ring (2)

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



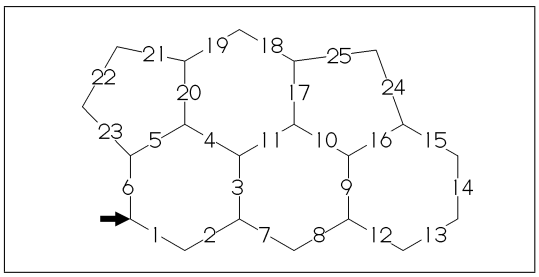
No.17 Fused ring (3)

```
(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]
```



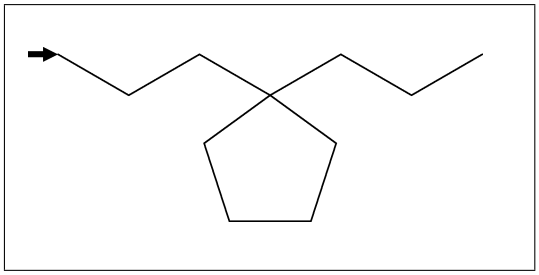
No.18 Fused ring (4)

```
(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]
```



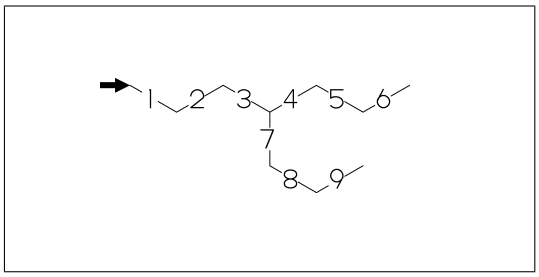
No.19 Spiro ring

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

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



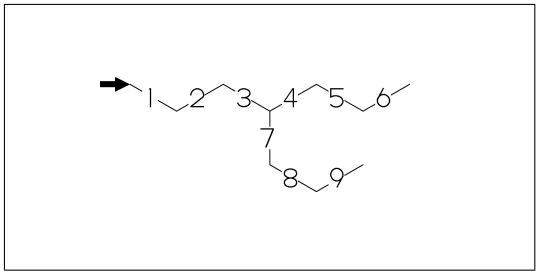
No.20 Branch (1)

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

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



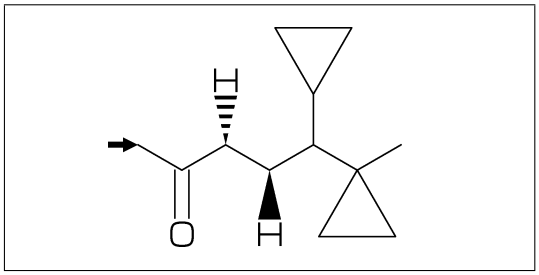
No.21 Branch (2)

```
4\ : branch bond at A4

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



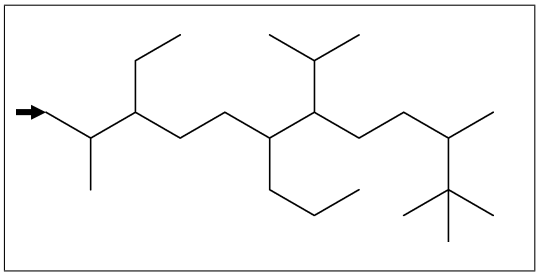
No.22 Substituent (1)

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

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



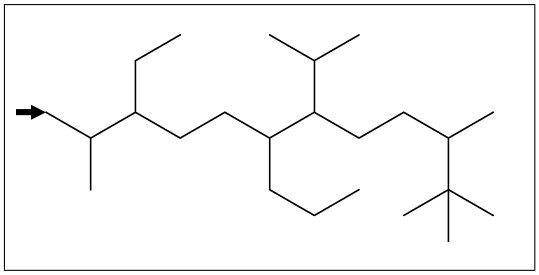
No.23 Substituent (2)

```
Insert substituent

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



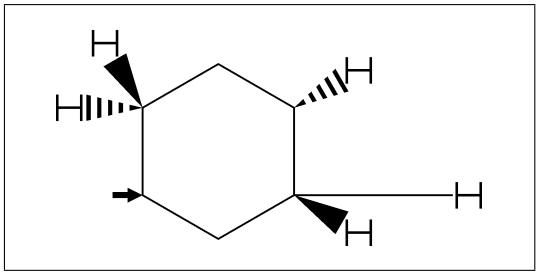
No.24 Substituent (3)

```
Add substituent

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



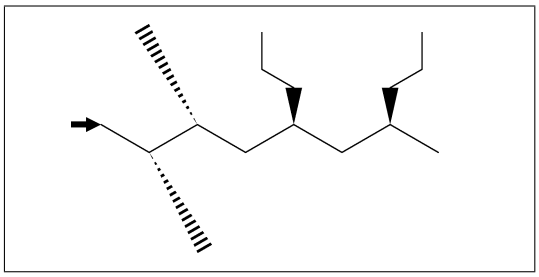
No.25 Substituent (4)

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

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



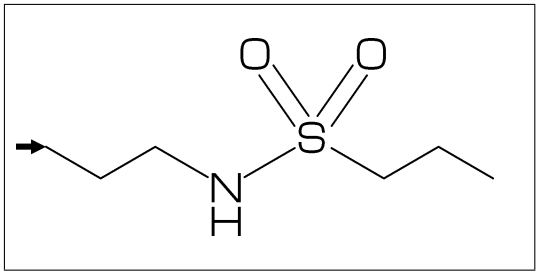
No.26 Substituent (5)

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

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



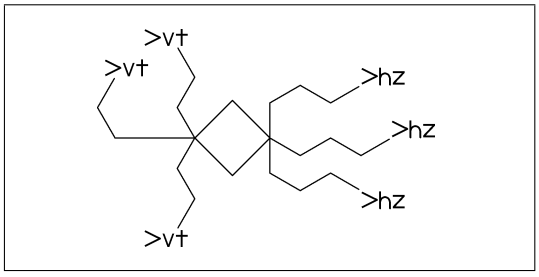
No.27 Change atom and Substituent

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

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



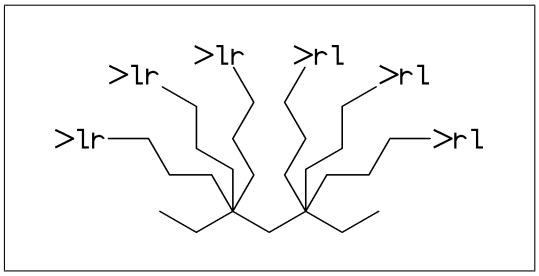
No.28 Chain strech direction environment (1)

```
>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
```



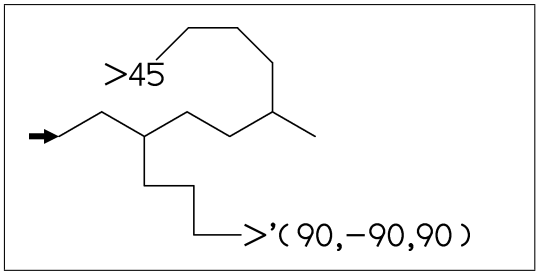
No.29 Chain strech direction environment (2)

```
>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
```



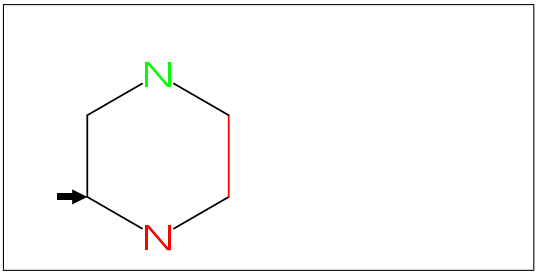
No.30 Chain strech direction environment (3)

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

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



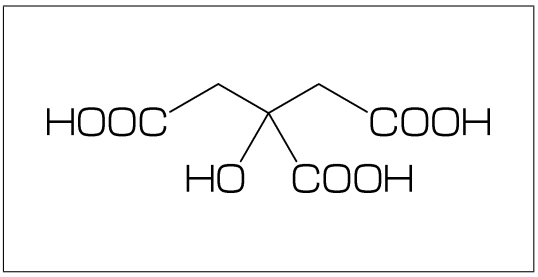
No.31 Change color

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

  ^^30,?6,@(2,5)N,
         2:red,5:green,3=red
```



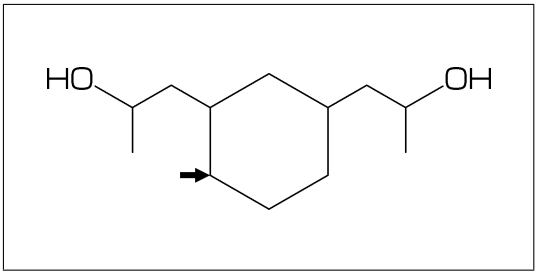
No.32 Chain start multiple characters

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

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



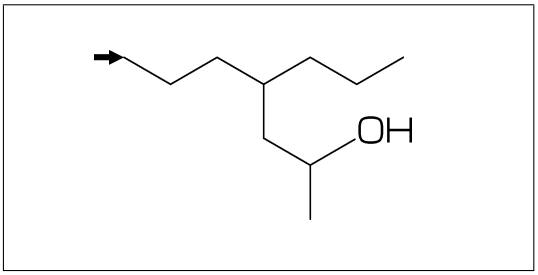
No.33 User definition

```
iBuOH : user defined substructure

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



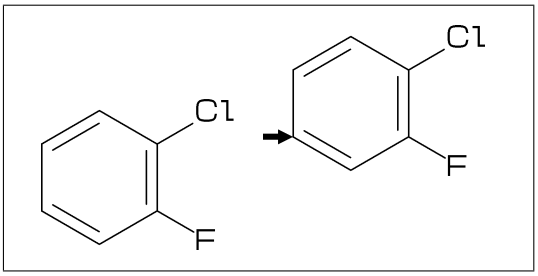
No.34 Inline definition

```
Insert user defined substructure

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



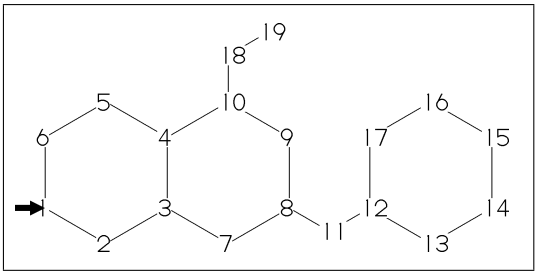
No.35 Switch Start Vector

```
  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)
```



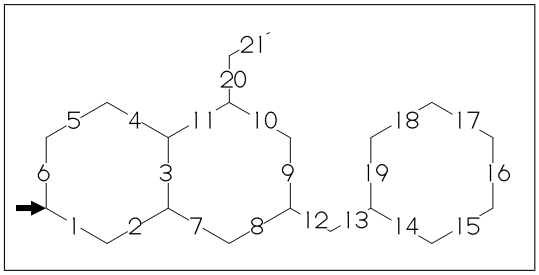
No.36 Switch NumberingA

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



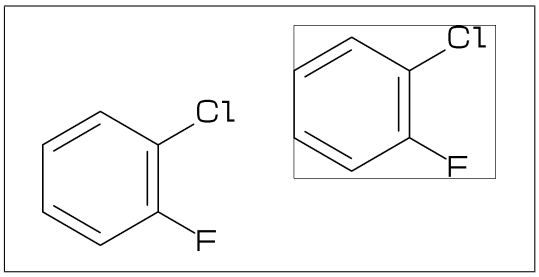
No.37 Switch NumberingB

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



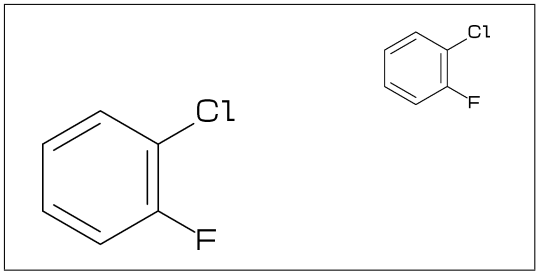
No.38 Switch Frame

```
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)
```



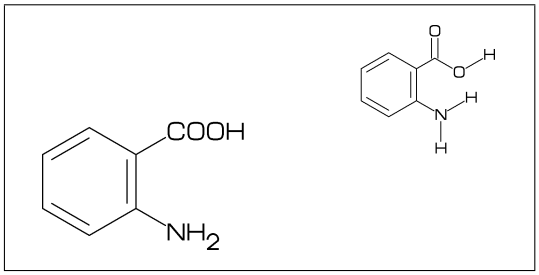
No.39 Switch Solid ratio

```
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)
```



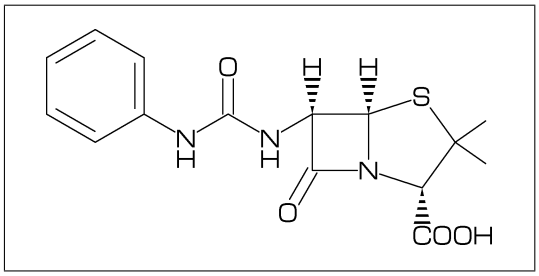
No.40 Switch Expand

```
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.41 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.42 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,!,
```