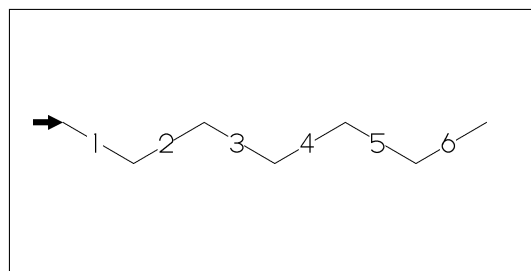


**No.1** Chain (1)

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

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

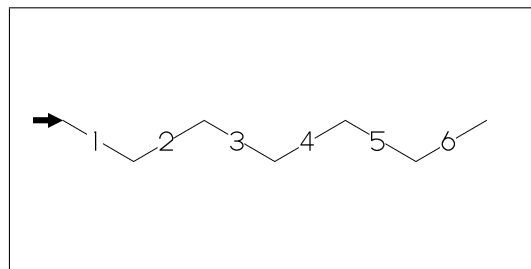
**No.2** Chain (2)

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

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

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

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

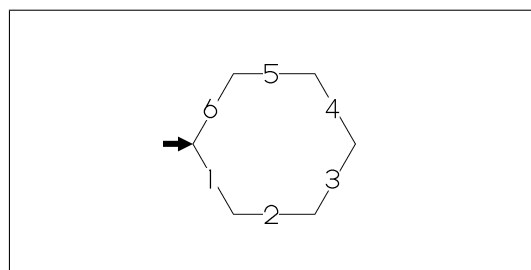
**No.3** Ring

six membered ring

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

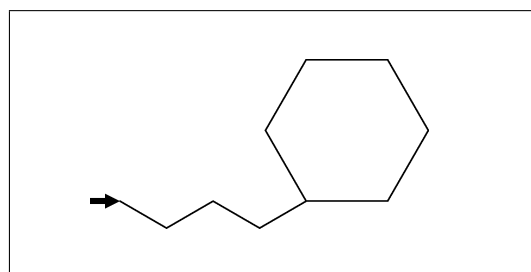
```
** ??6 : ^^ -120,60,60,60,60,60,&(-5)  

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

**No.4** rotate

^^angle:rotate current angle

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

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

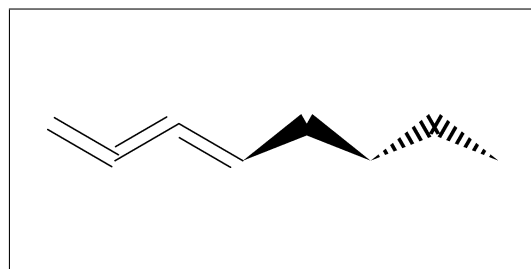
~bond change bond

```
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

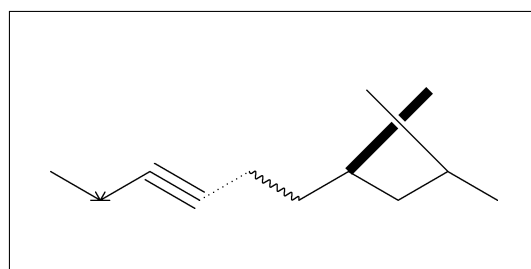
```
vf:vector forward, vb:vector backward,  

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

ov:over line
```

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

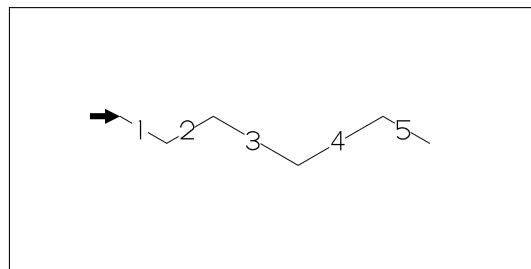
@(7~bd~-45'2,9~ov~45'2)/Me
```



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

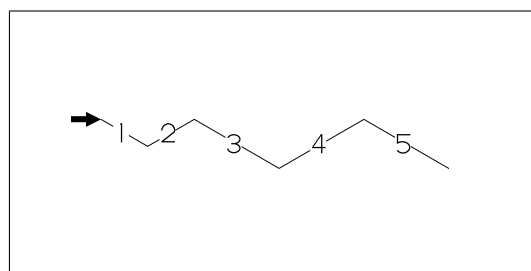
B'length : change bond length of B

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

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

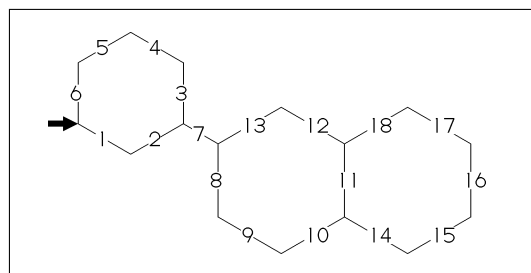
''length : change all bond length after

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

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

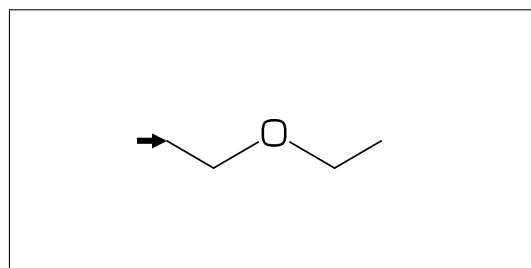
?n'length : change ring length

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

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

Insert hetero atom

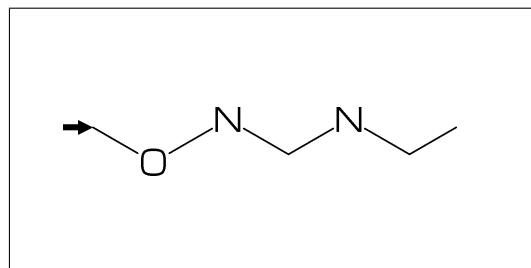
^^30,!2,0,!2

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

2:0 : change A2 C to O

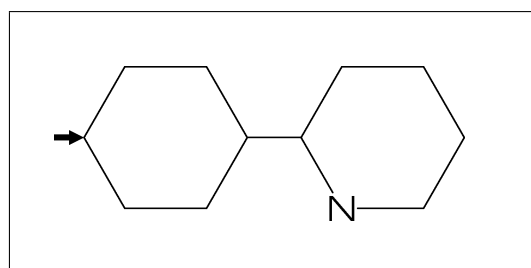
@ (3,5)N : change A3,A5 C to N

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

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

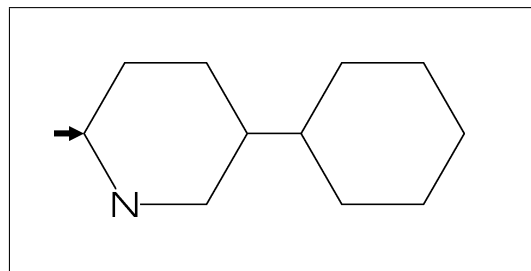
2:N : change A2(brock ahead) C to N

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



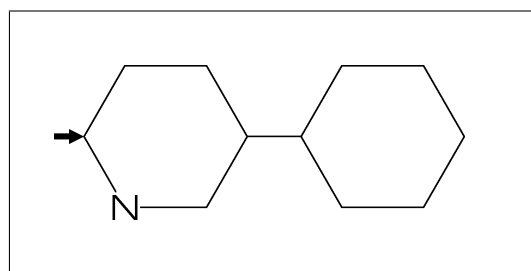
**No.13** Change atom (4)

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



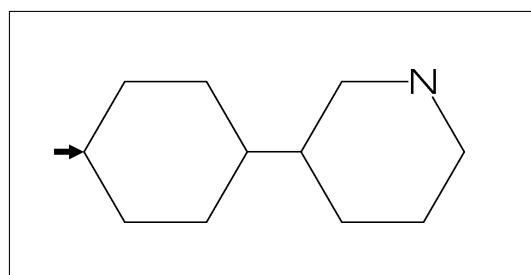
**No.14** Change atom (5)

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



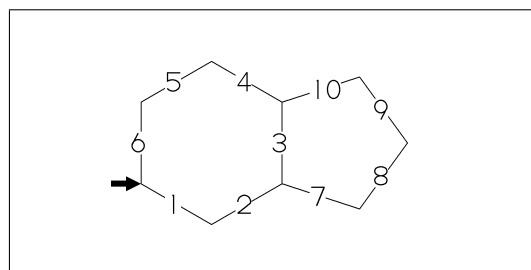
**No.15** Change atom (6)

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



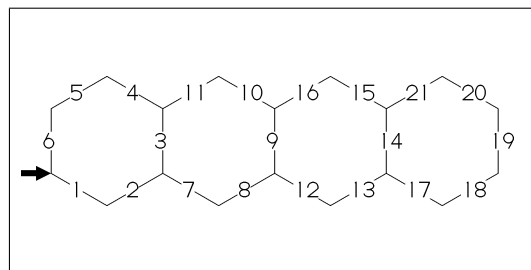
**No.16** Fused ring (1)

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



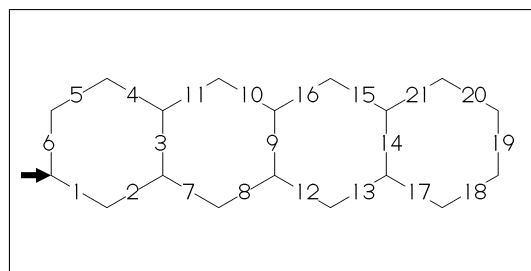
**No.17** Fused ring (2)

?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)

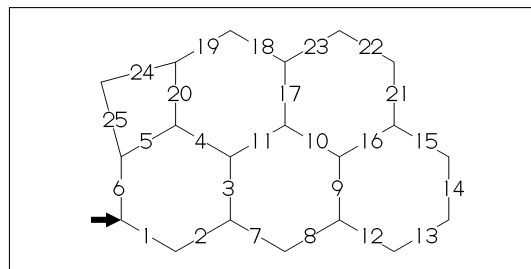
?6,\$(3,3,3)?6 OK  
?6,\$(3,9,14)?6 NG  
?6,\$(-4,-3,-3)?6 OK  
?6,\$(#3,#9,#14)?6 OK



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

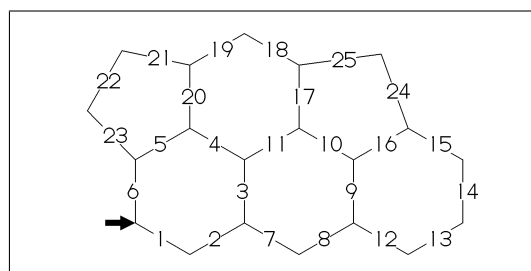
(4,11)=??6[4] : fuse 4/6 ring to B4 ..B11  
 (16,17)=??6[3] : fuse 3/6 ring to B16..B17  
 (20,5)=??4[2] : fuse 2/4 ring to B20.. B5

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

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

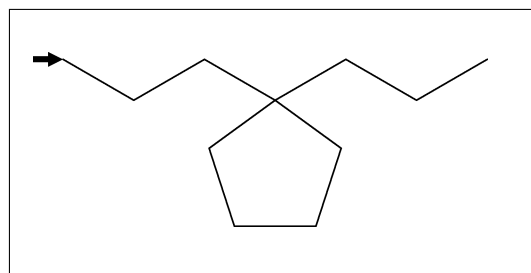
(20,5)=??5[3] : fuse 3/5 ring to B20..B5  
 (16,17)=??5[2] : fuse 2/5 ring to B16..B17

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

**No.21** Spiro ring

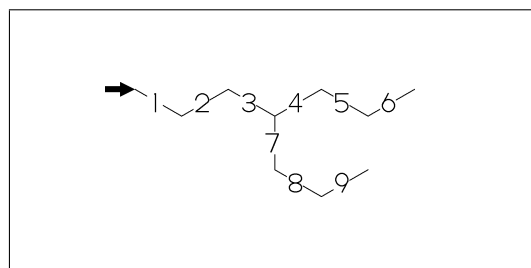
4\*,?5 : add ?5(5 membered ring) to A4

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

**No.22** Branch (1)

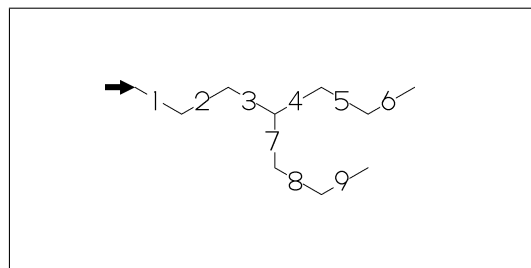
/ : branch bond  
 / : process at last

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

**No.23** Branch (2)

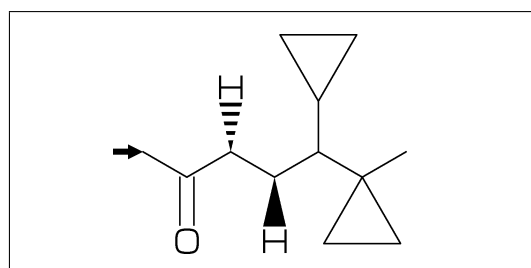
4\ : branch bond at A4

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

**No.24** Substituent (1)

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

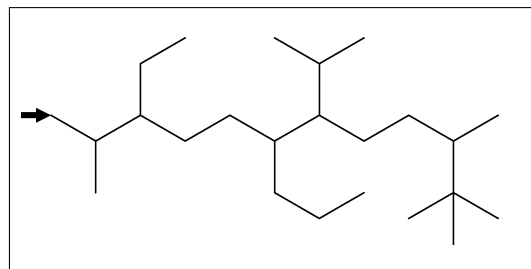
```
^^30,! ,//0,! ,/*H,! ,*/H,! ,/?3,! ,**?3,!
```



**No.25** Substituent (2)

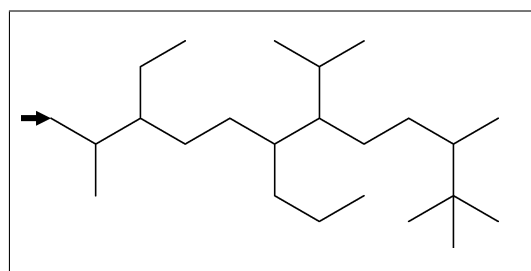
Insert substituent

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

**No.26** Substituent (3)

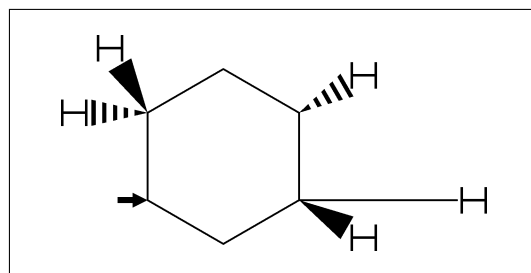
Add substituent

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

**No.27** Substituent (4)

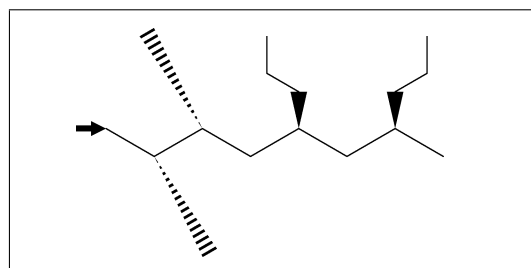
~,^,^,> : change type,angle,length,enviroment  
of substituent

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

**No.28** Substituent (5)

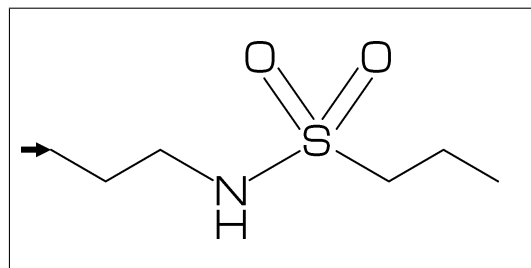
~,^,^,> : change type,angle,length,enviroment  
of substituent

```
^^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

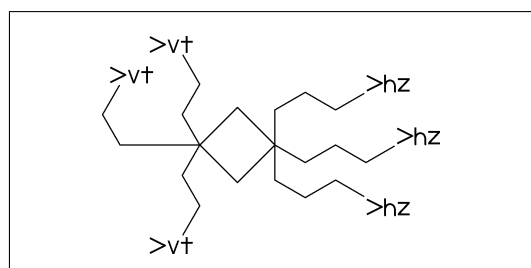
```
^^30,!3,NH,!S00,!3
```

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

>hz : horizontal enviroment (default)

>vt : vertical enviroment

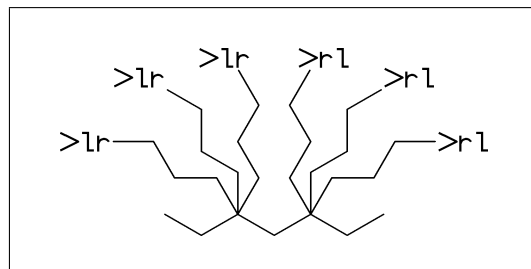
```
?4,  
@(3^-90,3^-30,3^90)/'(!3,"{>hz}")>hz,  
@(1^-60,1'^1.5,1^60)/'(!2,"{>vt}")>vt
```



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

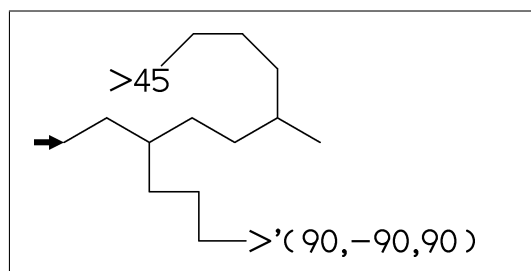
```
>lr : left-right enviroment
>rl : right-left enviroment

^^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)

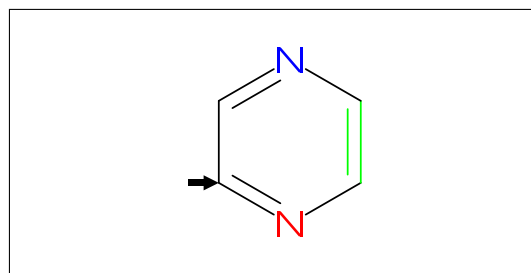
```
>45 : fixed angle enviroment
>'(-90,90,-90) : multi angle enviroment

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

**No.33** Change color

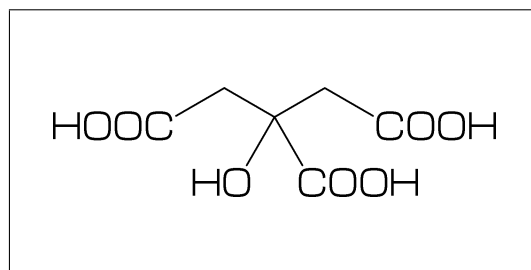
```
@(5)green : change color of A5 green
$(3)red : change color of B3 red

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

**No.34** Chain start multiple characters

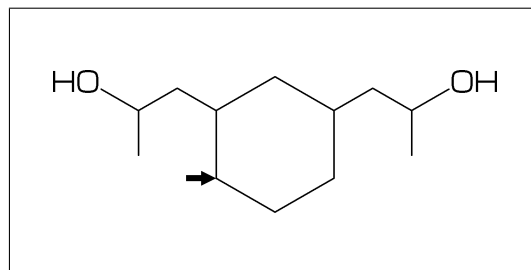
```
Use !0 instead of !,
if begin with multi charactor string

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

**No.35** User definition

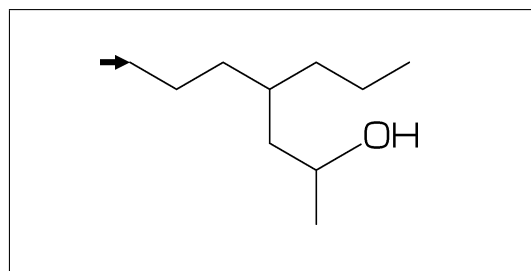
```
iBuOH : user defined substructure

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

**No.36** Inline definition

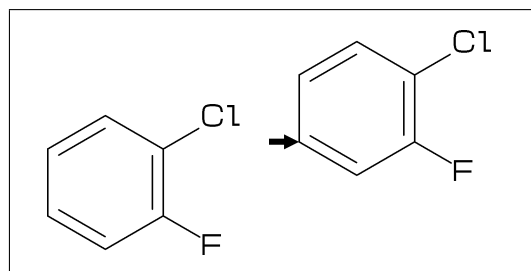
```
Insert user defined substructure

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

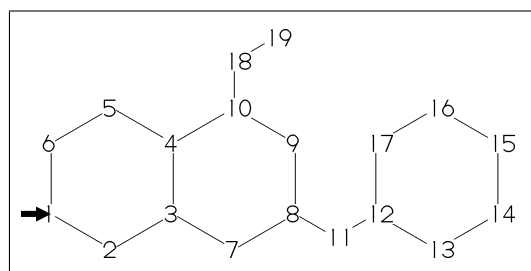


**No.37** Switch Start Vector

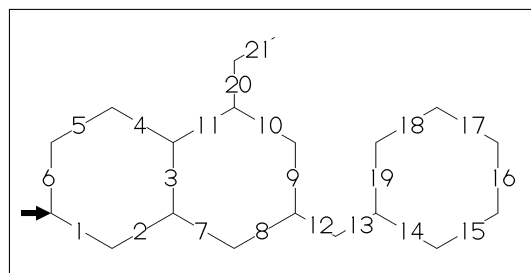
```
MCd(.8,.8)( 0, 0)(^^30,Ph,4:/Cl,3:/F)
sw_start_vector:=1;
MCd(.8,.8)( 1, 1)(^^30,Ph,4:/Cl,3:/F)
```

**No.38** Switch NumberingA

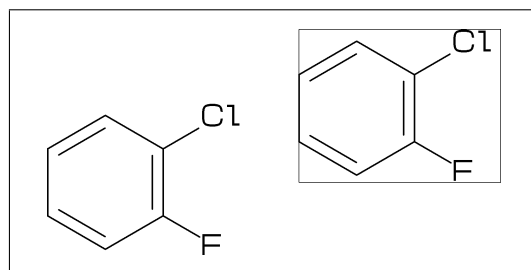
```
sw_numberA:=1;
MCf(^^30,
    Ph,-4=Ph1,-3\,! ,Ph,10:/Et)
```

**No.39** Switch NumberingB

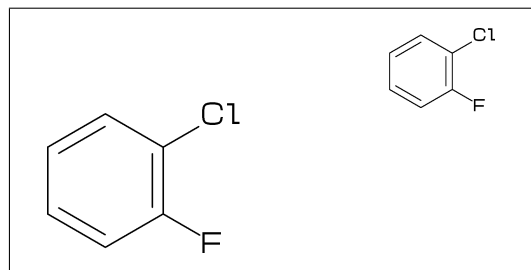
```
sw_numberB:=1;
MCf(^^30,
    Ph,-4=Ph1,-3\,! ,Ph,10:/Et)
```

**No.40** Switch Frame

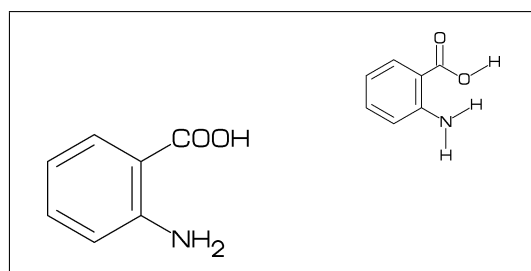
```
MCd(.8,.8)(0,0)(^^30,Ph,4:/Cl,3:/F)
sw_frame:=1;
MCd(.8,.8)(1,1)(^^30,Ph,4:/Cl,3:/F)
```

**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)
```

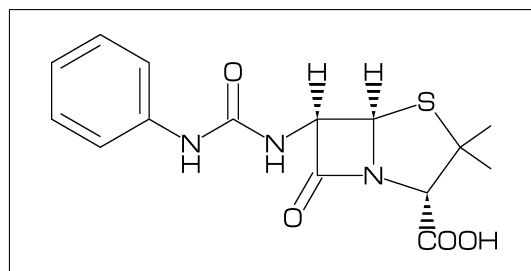
**No.42** Switch Expand

```
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)
```



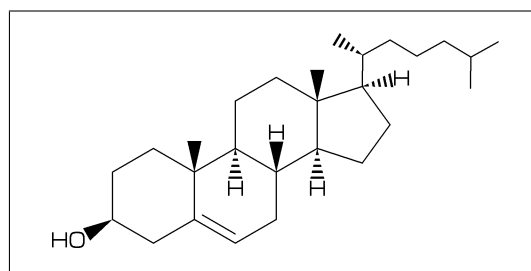
**No.43** Example(1) Ampicillin

^45,  
74,2:N,2=?5,-1:S,  
@ (3^45,4^-45)/H,1://0^15,  
5:/\*COOH^-18,@ (6^35,6^-35)/Me,  
4^75,NH,! ,//0,! ,NH,! ,Ph



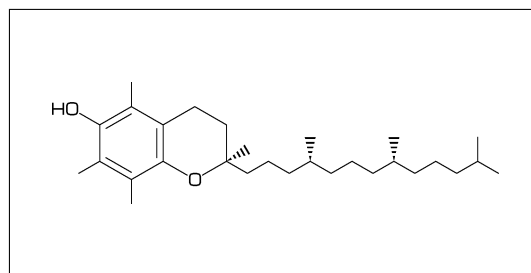
**No.44** Example(2) Cholesterol

^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,  
-1^17,/\*Me,!4,/Me,! ,



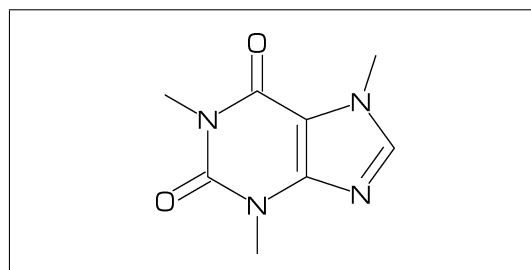
**No.45** Example(3) alfa-Tocopherol

^30,  
Ph,3=?6,  
7:0,@ (1,2,5)/Me,8:/\*Me^60,6:\*/OH,  
8\,!12,@ (4,8)\*/Me,12:/Me



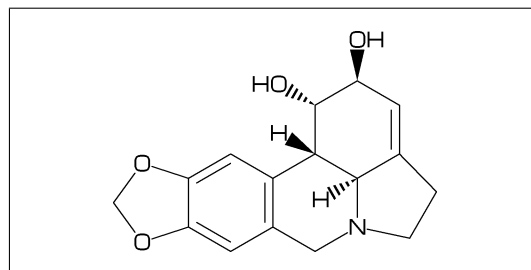
**No.46** Example(4) Caffeine

^30,  
76,-4=?5,\$ (3,8)d1,@ (2,6,7,9)N,  
@ (2,6,9)/Me,@ (1,5)//0



**No.47** Example(5) 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.48** Example(6) Gibberellin

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

