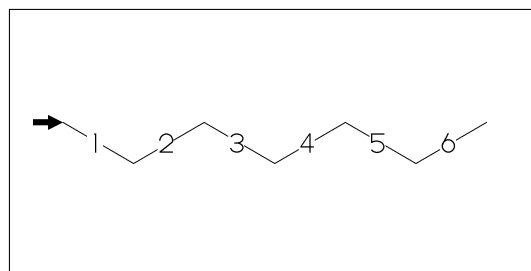


No.1 Chain (1)

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

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

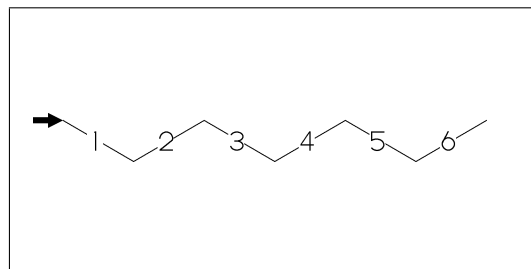
**No.2** Chain (2)

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

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

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

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

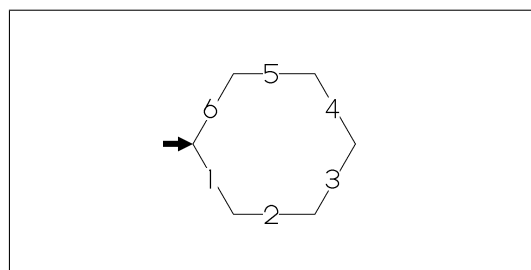
**No.3** Ring

six membered ring

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

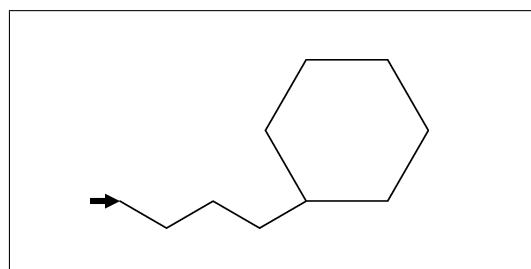
```
** ??6 : ^^ -120,60,60,60,60,60,&(-5)  

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

**No.4** rotate

^^angle:rotate current angle

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

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

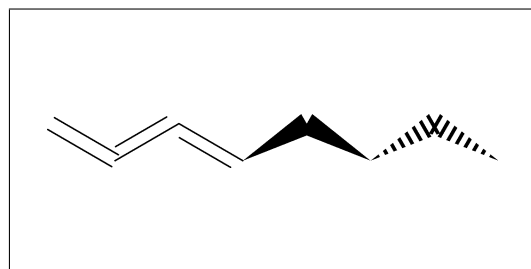
~bond change bond

```
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

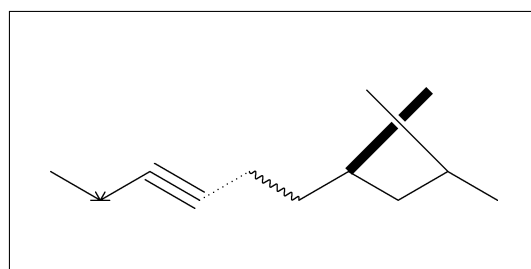
```
dm:double,dl:double(left),dr:double(right),  

wf:wedge forward,wb:wedge backward,  

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

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

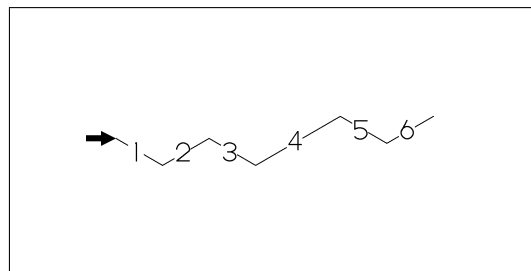
@(7~bd~-45'2,9~ov~45'2)/Me
```



No.7 Change bond length (1)

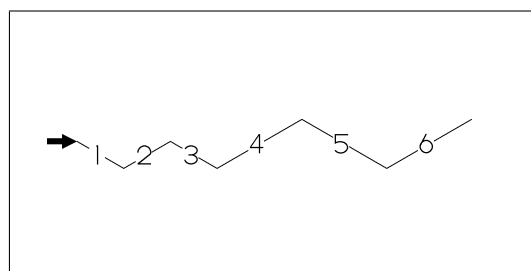
B'length : change bond length of B

^^30,!3,!1.2,!2

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

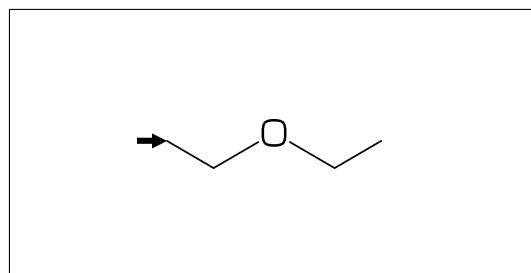
''length : change all bond length after

^^30,!3, ''1.2,!3

**No.9** Change atom (1)

Insert hetero atom

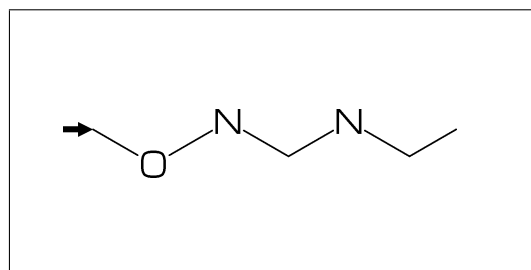
^^30,!2,0,!2

**No.10** Change atom (2)

2:0 : change A2 C to O

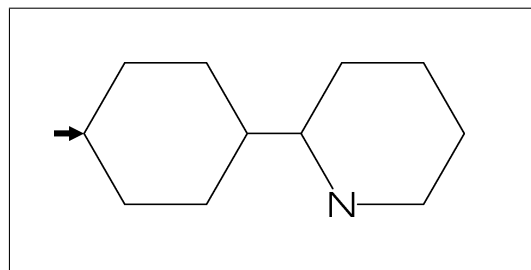
@ (3,5)N : change A3,A5 C to N

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

**No.11** Change atom (3)

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

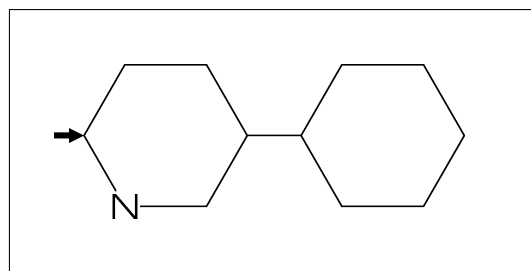
?6,4\,?6,2:N

**No.12** Change atom (4)

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

??6 is not brock

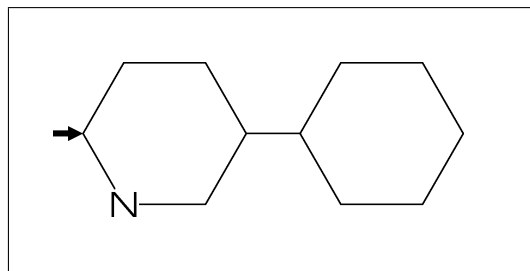
?6,4\,??6,2:N



No.13 Change atom (5)

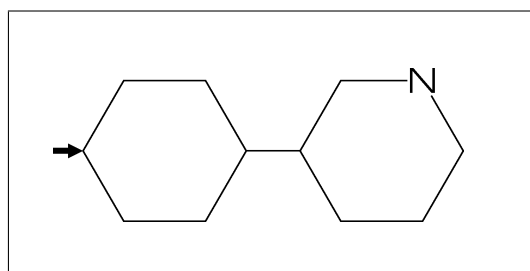
#2:N : change A#2 C to N

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

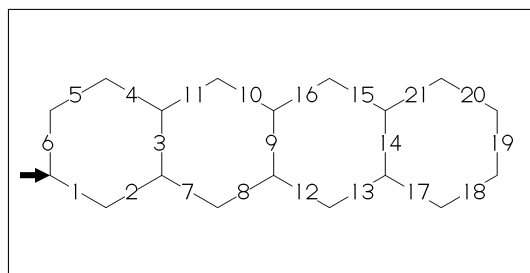
**No.14** Change atom (6)

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

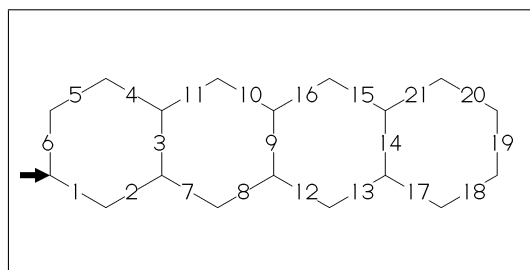
?6,4\,?6,-2:N

**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
```

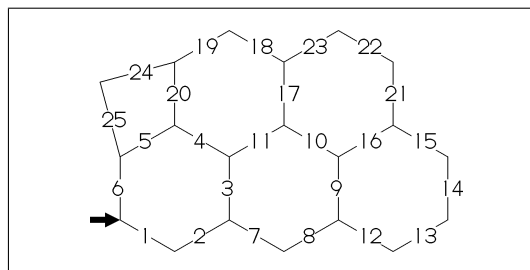
**No.16** Fused ring (2)

```
?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)

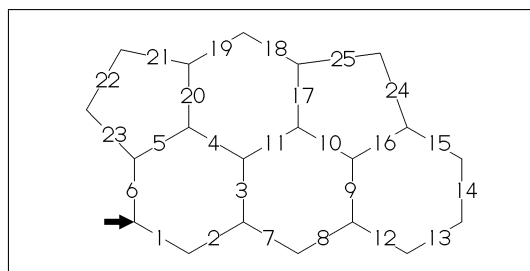
```
(4,11)=??6[4] : fuse 4/6 ring to B4 ..B11
(16,17)=??6[3] : fuse 3/6 ring to B16..B17
(20,5)=??4[2] : fuse 2/4 ring to B20.. B5
```

```
^^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
```

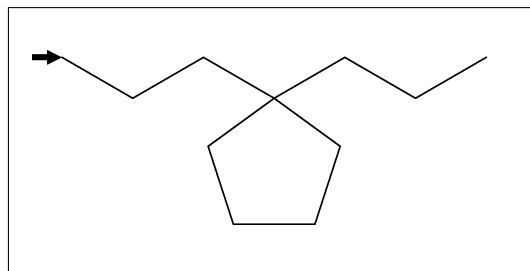
```
^^30,?6,$(3,9)?6,(4,11)=??6[4],
      (20,5)=??5[3],(16,17)=??5[2]
```



No.19 Spiro ring

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

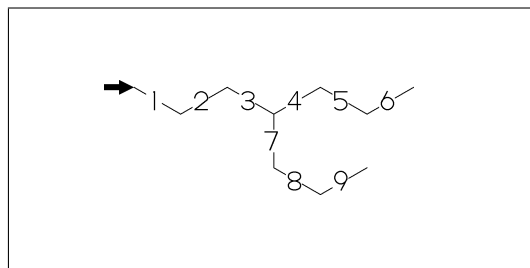
^^30,!6,4*,?5

**No.20** Branch (1)

/ : branch bond

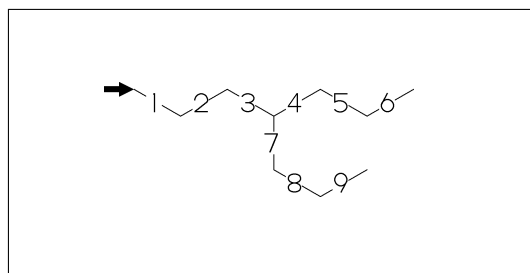
/ : process at last

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

**No.21** Branch (2)

4\ : branch bond at A4

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

**No.22** Substituent (1)

/ : single

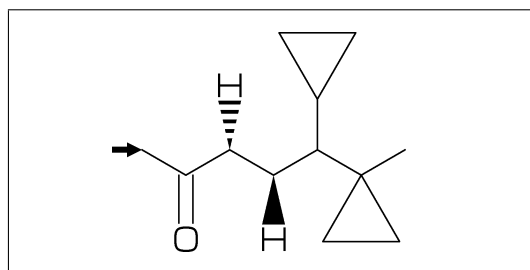
// : double

*/ : wedge forward

/* : wedge backward

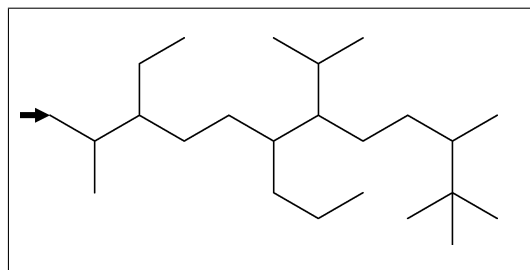
** : direct

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

**No.23** Substituent (2)

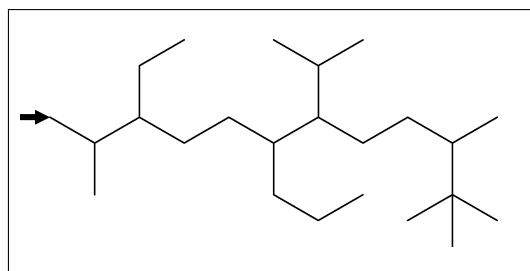
Insert substituent

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

**No.24** Substituent (3)

Add substituent

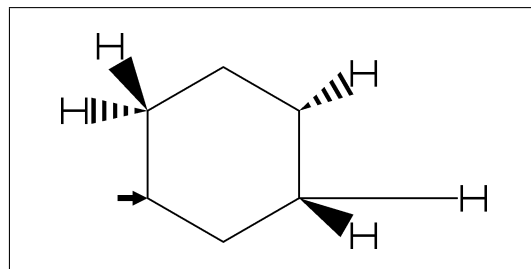
^^30,!10,2:/Me,3:/Et,6:/Pr,7:/iPr,10:/tBu



No.25 Substituent (4)

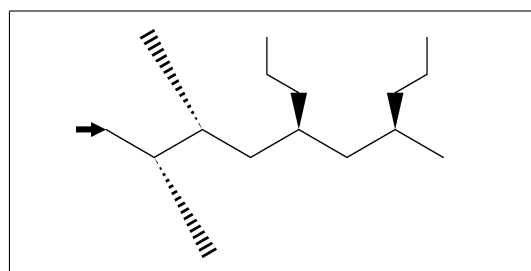
~,^,','> : change type,angle,length,enviroment
of substituent

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

**No.26** Substituent (5)

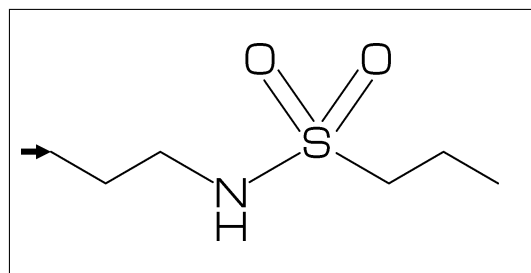
~,^,','> : change type,angle,length,enviroment
of substituent

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

**No.27** Change atom and Substituent

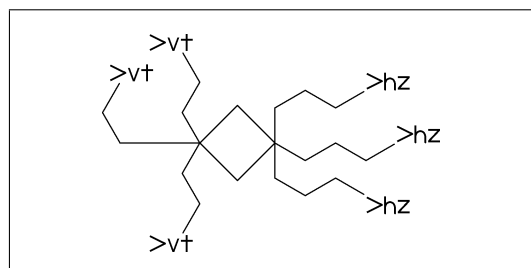
NH,S00 : inset hetero atom and substituent
simultaneously

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

**No.28** Chain stretch direction environment (1)

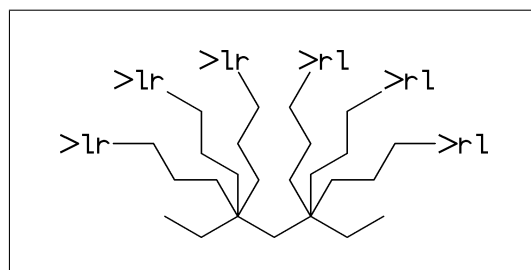
>hz : horizontal enviroment (default)
>vt : vertical enviroment

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

**No.29** Chain stretch direction environment (2)

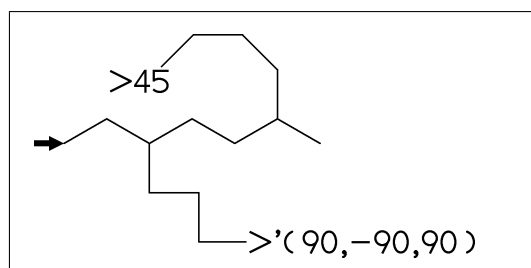
>lr : left-right enviroment
>r1 : right-left enviroment

```
^^30,!6,
@ (3^-30,3,3^30)/' (!3,"{>lr}")>lr,
@ (5^-30,5,5^30)/' (!3,"{>r1}")>r1
```

**No.30** Chain stretch direction environment (3)

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

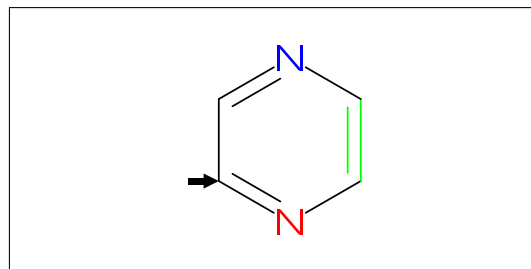
```
^^-30,!6,@ (2>45)/' (!3,"{>45}") ,
@ (6>'(-90,90,-90))/' (!2,"{>'(-90,90,-90)}")
```



No.31 Change color

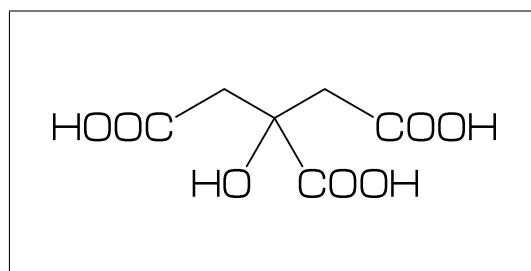
@(5)green : change color of A5 green
 \$(3)red : change color of B3 red

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

**No.32** Chain start multiple characters

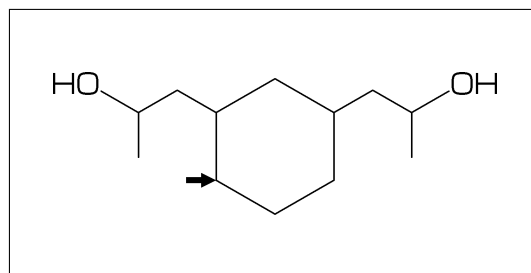
Use !0 instead of !,
 if begin with multi character string

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

**No.33** User definition

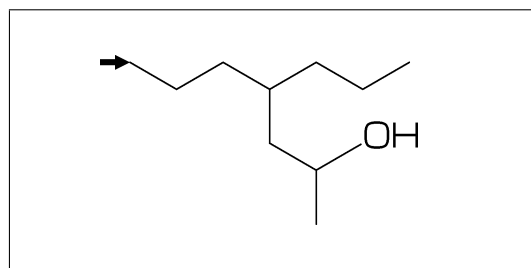
iBuOH : user defined substructure

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

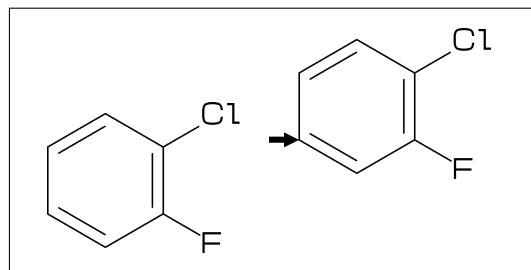
**No.34** Inline definition

Insert user defined substructure

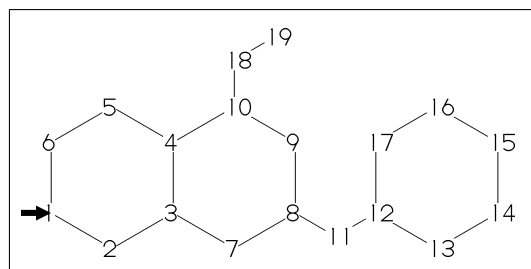
```
^^30,!3,/'(!,/Me,! ,OH),!3
```

**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)
```

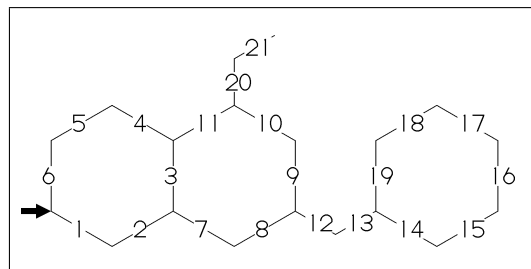
**No.36** Switch NumberingA

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



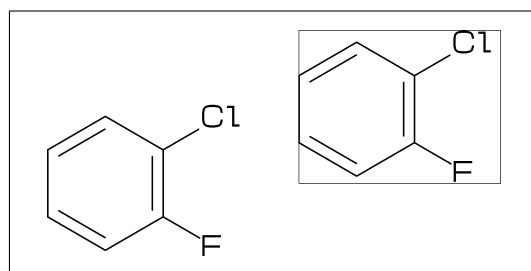
No.37 Switch NumberingB

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



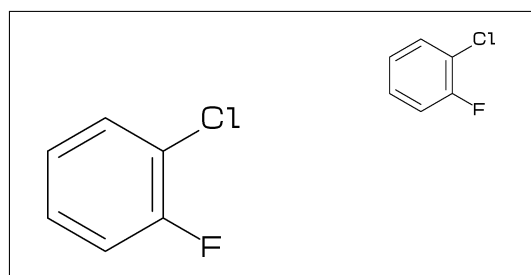
No.38 Switch Frame

```
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)
```



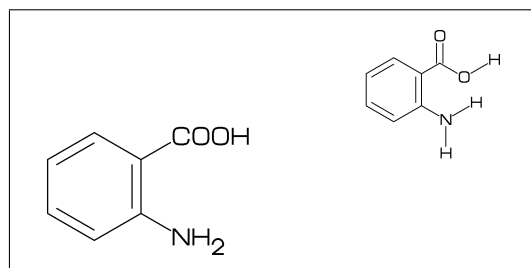
No.39 Switch Solid ratio

```
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)
```



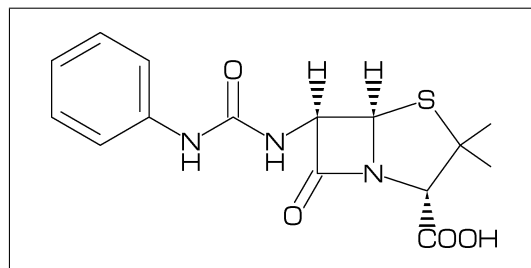
No.40 Switch Expand

```
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://0^15,
5:/*COOH^-18,@ (6^35,6^-35)/Me,
4^75,NH,! ,//0,! ,NH,! ,Ph
```



No.42 Example(2) 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,! ,
```

