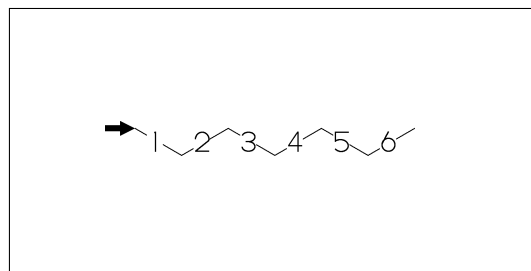


No.1 Chain (1)

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

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

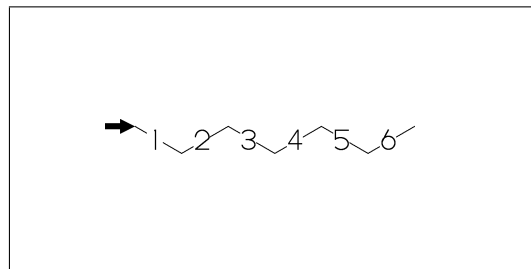
**No.2 Chain (2)**

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

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

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

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

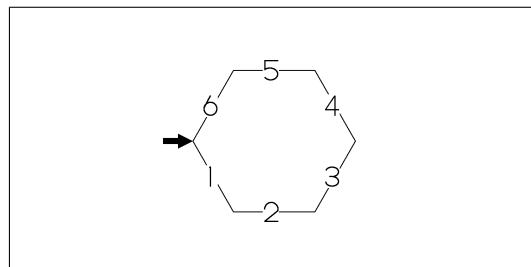
**No.3 Ring**

six membered ring

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

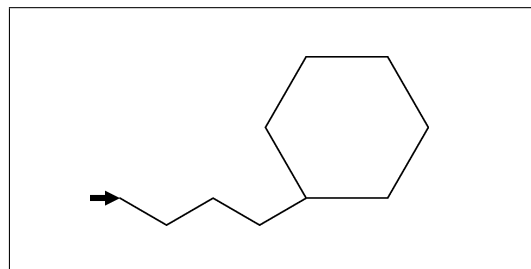
```
** ??6 : ^^ -120,60,60,60,60,60,&(-5)  

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

**No.4 Rotate**

^^angle:rotate current angle

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

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

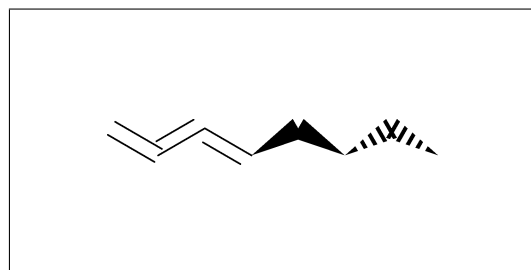
~bond change bond

```
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

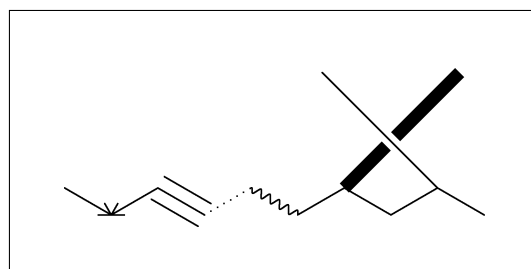
```
vf:vector forward, vb:vector backward,  

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

ov:over line
```

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

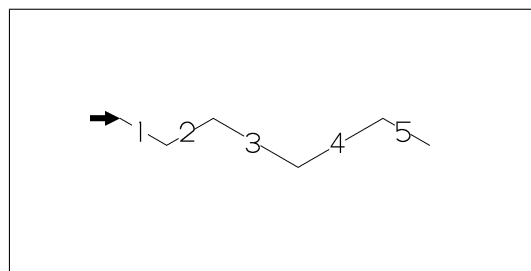
@(7~bd~-45'2,9~ov~45'2)/Me
```



No.7 Change bond length (1)

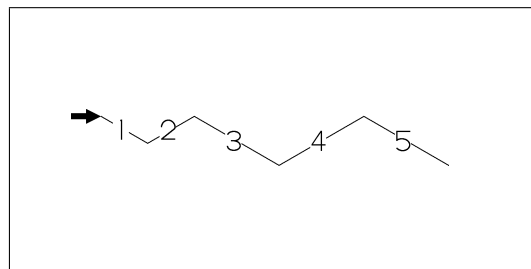
B'length : change bond length of B

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

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

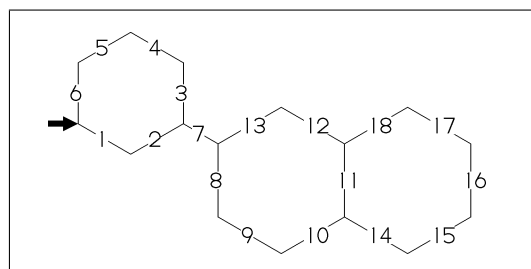
''length : change all bond length after

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

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

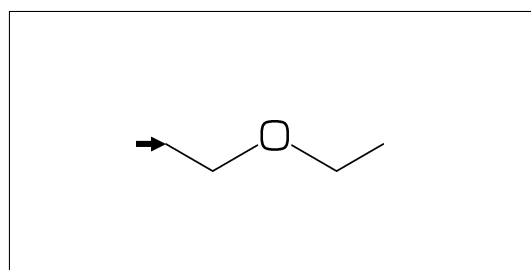
?n'length : change ring length

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

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

Insert hetero atom

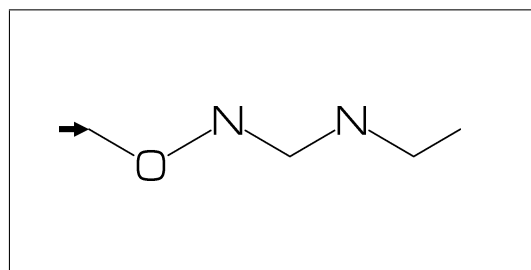
^^30,!2,0,!2

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

2:0 : change A2 C to O

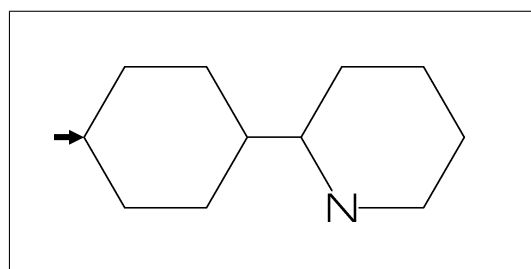
@ (3,5)N : change A3,A5 C to N

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

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

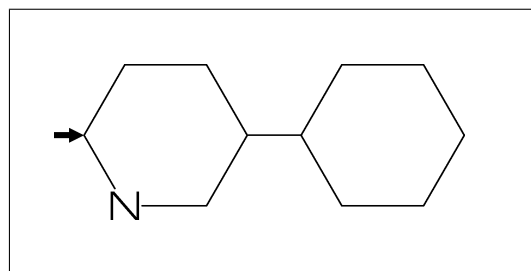
2:N : change A2(brock ahead) C to N

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



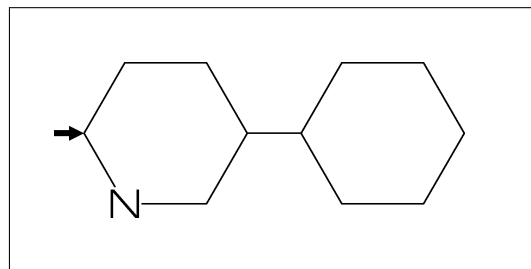
No.13 Change atom (4)

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



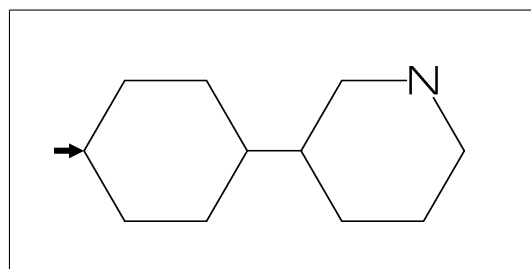
No.14 Change atom (5)

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



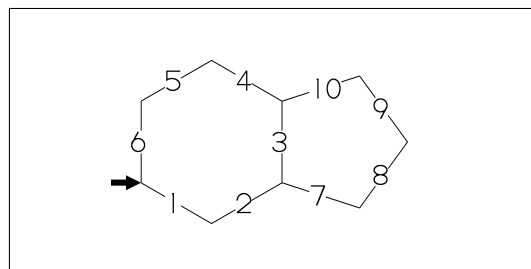
No.15 Change atom (6)

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



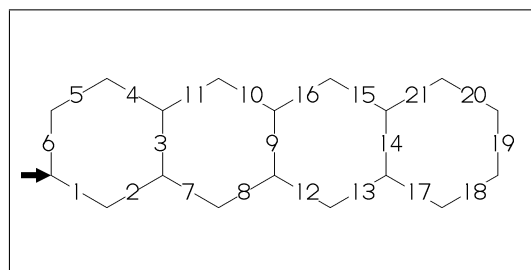
No.16 Fused ring (1)

?6,3=?5 : fuse ?5 at B3
?6,3=?5



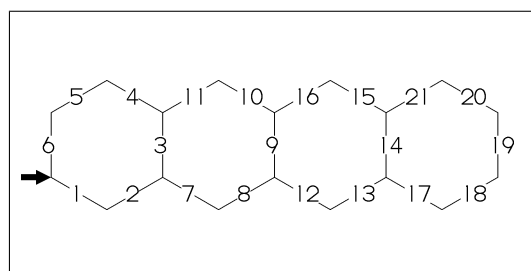
No.17 Fused ring (2)

?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)

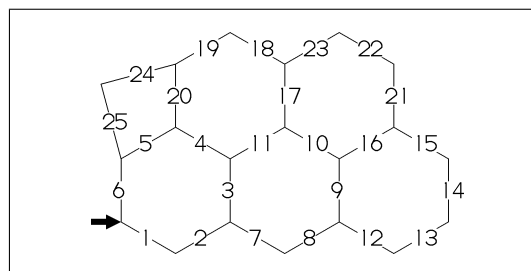
?6,\$(3,3,3)?6 OK
?6,\$(3,9,14)?6 NG
?6,\$(-4,-3,-3)?6 OK
?6,\$(#3,#9,#14)?6 OK



No.19 Fused ring (4)

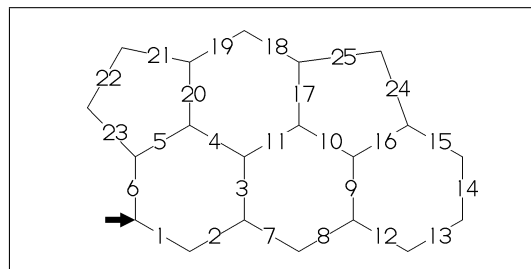
(4,11)=??6[4] : fuse 4/6 ring to B4 ..B11
 (16,17)=??6[3] : fuse 3/6 ring to B16..B17
 (20,5)=??4[2] : fuse 2/4 ring to B20.. B5

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

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

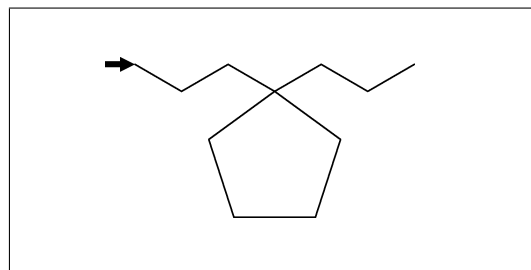
(20,5)=??5[3] : fuse 3/5 ring to B20..B5
 (16,17)=??5[2] : fuse 2/5 ring to B16..B17

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

**No.21 Spiro ring**

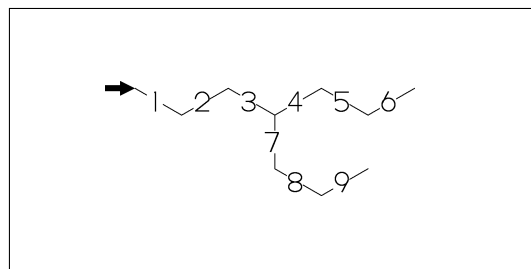
4*,?5 : add ?5(5 membered ring) to A4

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

**No.22 Branch (1)**

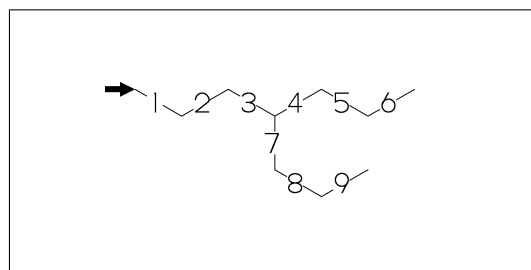
/ : branch bond(make at last)

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

**No.23 Branch (2)**

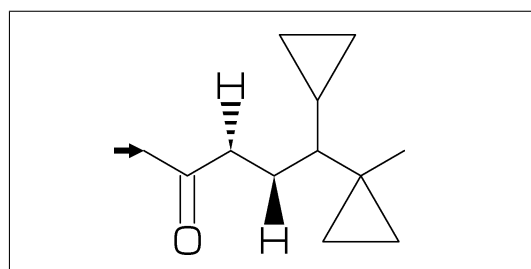
4\ : branch bond at A4

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

**No.24 Substituent (1)**

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

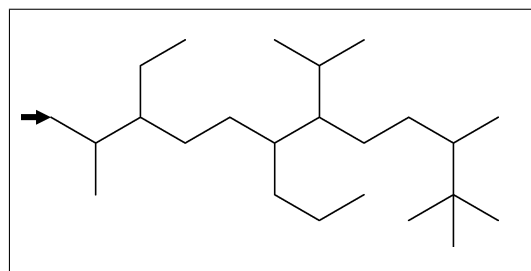
```
^^30,!,//0,!/*H,!/*H,!/?3,!,**?3,!
```



No.25 Substituent (2)

Insert substituent

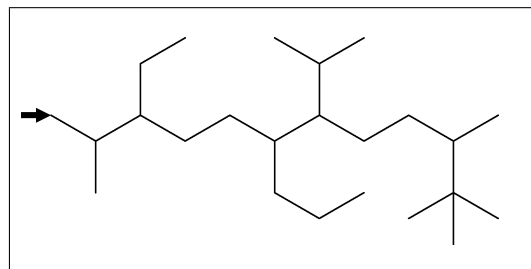
```
^^30,!/,Me,!/,Et,!3,/Pr,!/,iPr,!3,/tBu,!
```



No.26 Substituent (3)

Add substituent

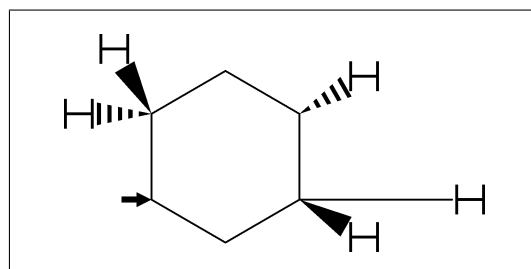
```
^^30,!10,2:/Me,3:/Et,6:/Pr,7:/iPr,10:/tBu
```



No.27 Substituent (4)

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

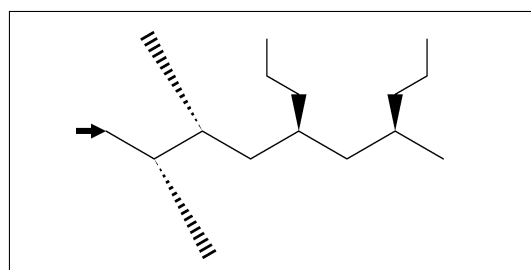
```
^^30,?6,  
@(3^2^30,3~wf,4~zf,6~wf^~30,6~zf^30)/H
```



No.28 Substituent (5)

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

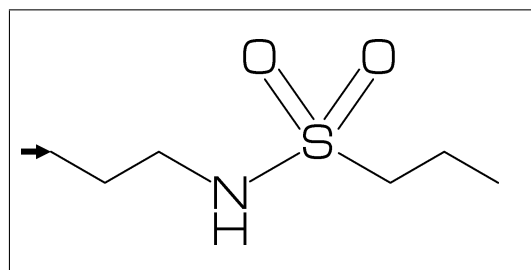
```
^^30,!7^1,  
@(2,3)/*Me^2^30,5:*/Pr>lr,7:*/Pr>r1
```



No.29 Change atom and Substituent

NH,S00 : inset hetero atom and substituent simultaneously

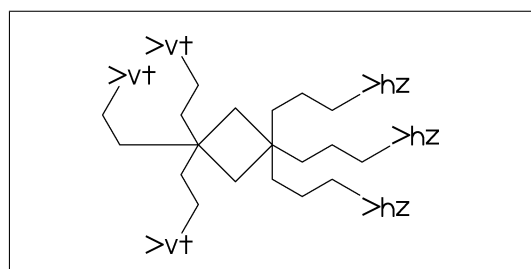
```
^^30,!3,NH,!/,S00,!3
```



No.30 Chain stretch direction environment (1)

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

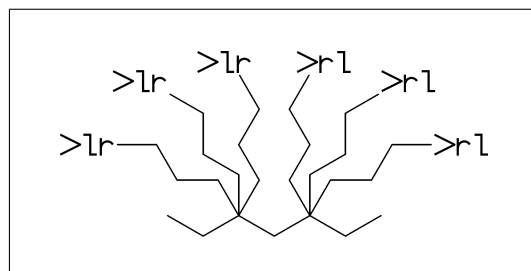
```
?4,  
@(3^~90,3^~30,3^90)/'(!3,"{>hz}")>hz,  
@(1^~60,1^1.5,1^60)/'(!2,"{>vt}")>vt
```



No.31 Chain stretch direction environment (2)

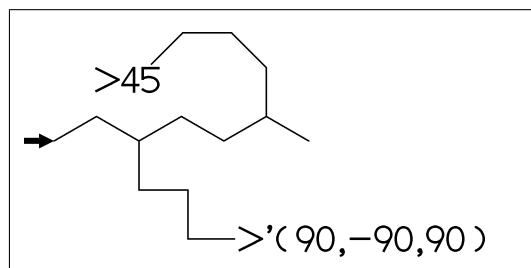
>lr : left-right enviroment
 >rl : right-left enviroment

```
^^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)**

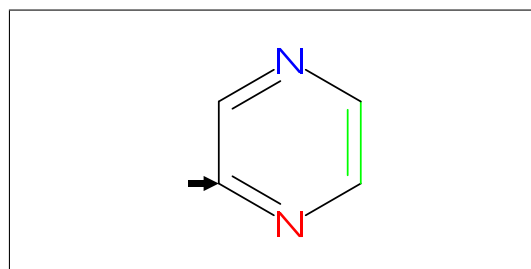
>45 : fixed angle enviroment
 >'(-90,90,-90) : multi angle enviroment

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

**No.33 Change color**

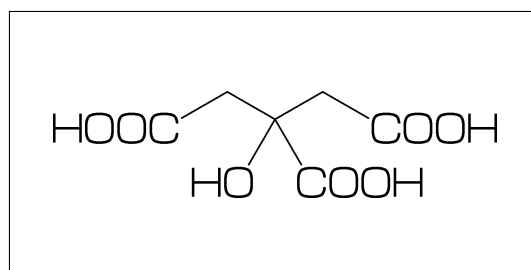
@(5)green : change color of A5 green
 \$(3)red : change color of B3 red

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

**No.34 Chain start multiple characters**

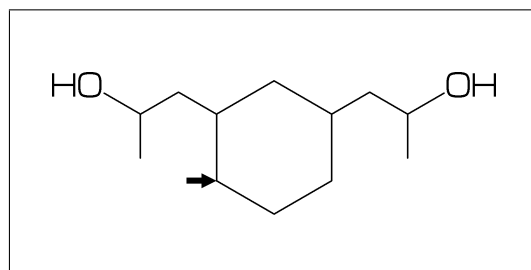
Use !0 instead of !,
 if begin with multi charactor string

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

**No.35 User definition**

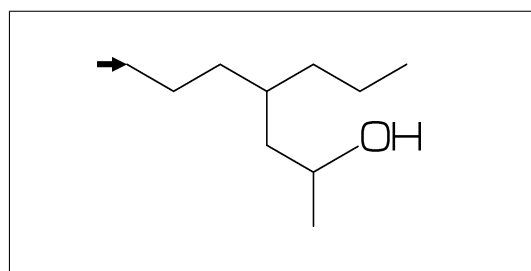
iBuOH : user defined substructure

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

**No.36 Inline definition**

Insert user defined substructure

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

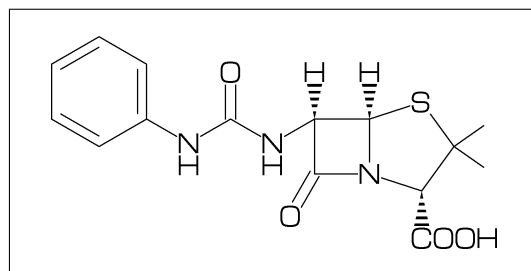


No.37 Example(1) Ampicillin

```

^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

```

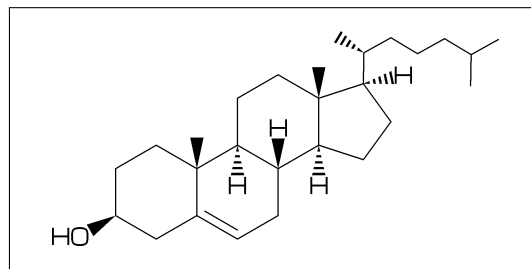


No.38 Example(2) Cholesterol

```

^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,! ,

```

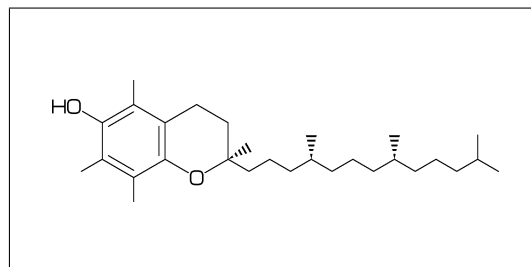


No.39 Example(3) alfa-Tocopherol

```

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

```

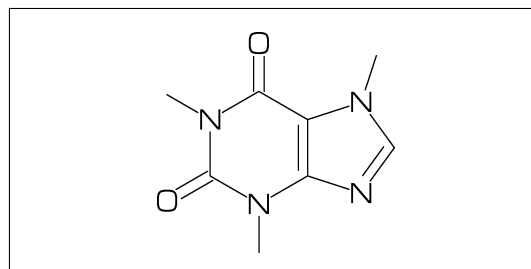


No.40 Example(4) Caffeine

```

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

```

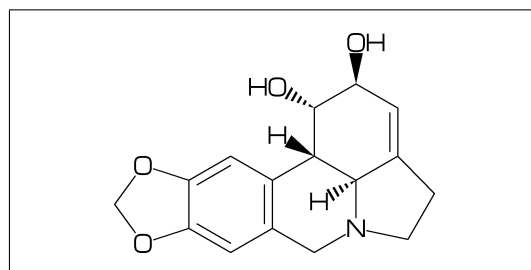


No.41 Example(5) Lycorine

```

^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

```

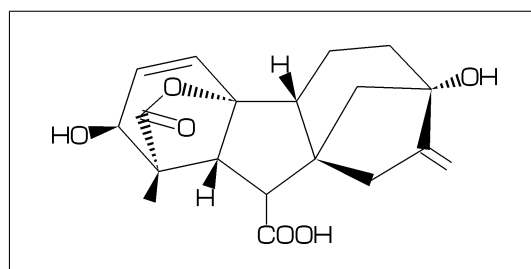


No.42 Example(6) Gibberellin

```

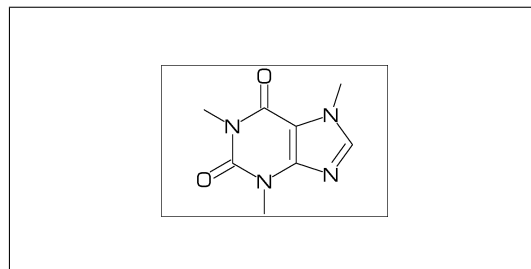
^12,
?6^1.3,3=?5,9=?7,12\^160^1.6,&8,
4\^155~zf^1.2,0,55,//0^180^1,&2^zb,
5=d1,11=wf,13=wb,7:/COOH,11://Me,1:*/OH,
12:*/OH,2:*/Me,@(3^60,9^60)*/H

```

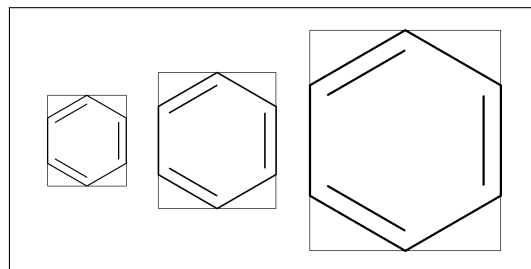


No.43 Font size

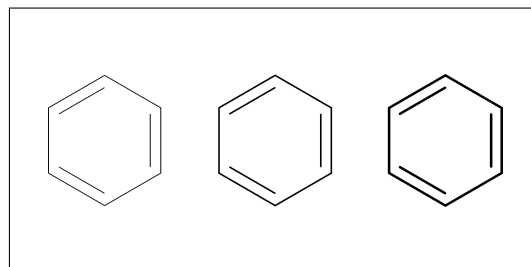
```
font_wd#:=30mm#;
font_ht#:=20mm#;
beginfont("EN:Caffeine")
  sw_font_frame:=1;
  MCf(^30,?6,-4=??5,$(3,8)d1,@(2,6,7,9)N,
    @(2,6,9)/Me,@(1,5)//O)
endfont
```

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

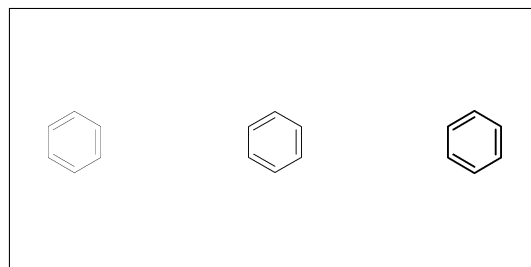
```
max_bond_width:=0.10;
MCd(1,1)(0,.5)(^30,Ph)
max_bond_width:=0.15;          %<== default
MCd(1,1)(.33,.5)(^30,Ph)
max_bond_width:=0.30;
MCd(1,1)(1,.5)(^30,Ph)
```

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

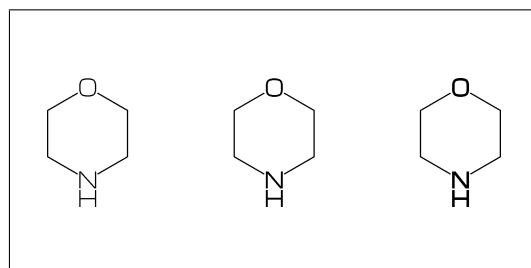
```
ratio_thickness_bond:= 0.005;
MCd(1,.6)(0,.5)(^30,Ph)
ratio_thickness_bond:= 0.015;   %<== default
MCd(1,.6)(.5,.5)(^30,Ph)
ratio_thickness_bond:= 0.030;
MCd(1,.6)(1,.5)(^30,Ph)
```

**No.46 Offset thickness of bond**

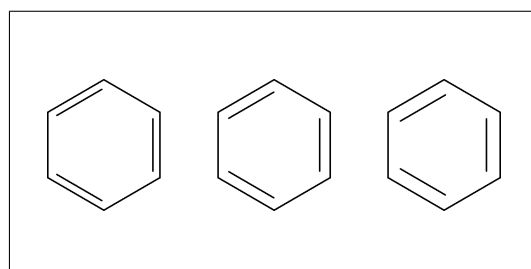
```
beginfont() offset_thickness#:=0pt#;
MCd(1,.3)(0,.5)(^30,Ph) endfont
beginfont() offset_thickness#:=0.2pt#; %<== default
MCd(1,.3)(.5,.5)(^30,Ph) endfont
beginfont() offset_thickness#:=0.5pt#;
MCd(1,.3)(1,.5)(^30,Ph) endfont
```

**No.47 Ratio char/bond thickness**

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

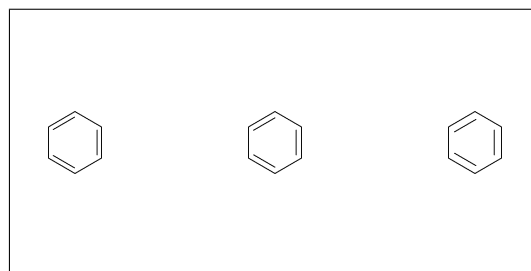
**No.48 Ratio bondgap/bond length**

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

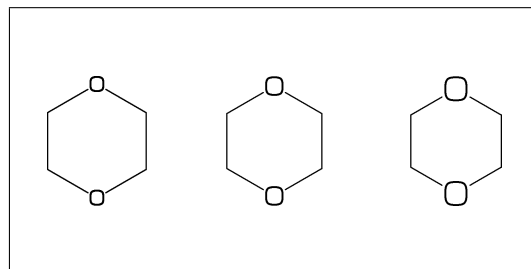


No.49 Offset of doublebond gap

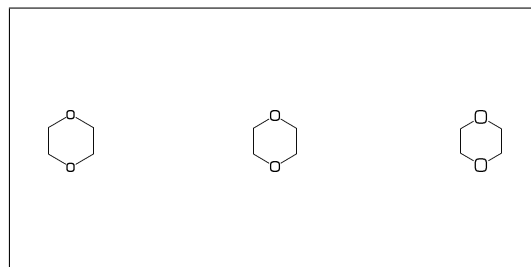
```
beginfont() offset_bond_gap#:=0.0pt#;  
MCd(1,.3)(0, .5)(^^30,Ph) endfont  
beginfont() offset_bond_gap#:=0.3pt#; %<== default  
MCd(1,.3)(.5, .5)(^^30,Ph) endfont  
beginfont() offset_bond_gap#:=1.0pt#;  
MCd(1,.3)(1, .5)(^^30,Ph) endfont
```

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

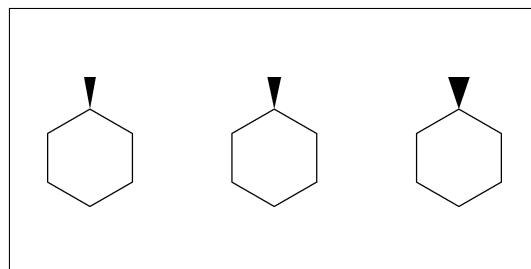
```
ratio_atom_bond:= 0.25;  
MCd(1,.6)(0, .5)(^^30,?6,@(2,5)O)  
ratio_atom_bond:= 0.36; %<== default  
MCd(1,.6)(.5, .5)(^^30,?6,@(2,5)O)  
ratio_atom_bond:= 0.45;  
MCd(1,.6)(1, .5)(^^30,?6,@(2,5)O)
```

**No.51 Offset of atom width**

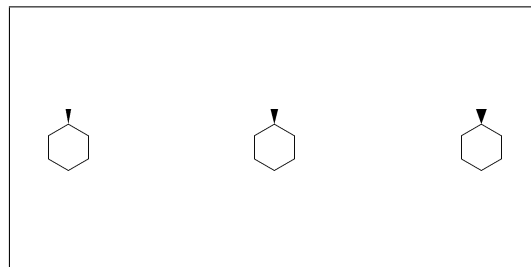
```
beginfont() offset_atom#:=0.0pt#;  
MCd(1,.3)(0, .5)(^^30,Ph,@(2,4,6)N) endfont  
beginfont() offset_atom#:=0.8pt#; %<== default  
MCd(1,.3)(.5, .5)(^^30,Ph,@(2,4,6)N) endfont  
beginfont() offset_atom#:=2.0pt#;  
MCd(1,.3)(1, .5)(^^30,Ph,@(2,4,6)N) endfont
```

**No.52 Ratio wedge/bond length**

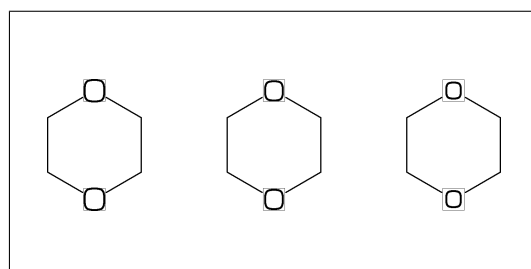
```
ratio_wedge_bond:=0.10;  
MCd(1,.6)(0, .5)(^^30,?6,5:*/Me)  
ratio_wedge_bond:=0.12; %<== default  
MCd(1,.6)(.5, .5)(^^30,?6,5:*/Me)  
ratio_wedge_bond:=0.20;;  
MCd(1,.6)(1, .5)(^^30,?6,5:*/Me)
```

**No.53 Offset of wedge width**

```
beginfont("EN:Offset_wedge")  
offset_wedge#:=0.0pt#;  
MCd(1,.3)(0, .5)(^^30,?6,5:*/Me) endfont  
beginfont() offset_wedge#:=0.4pt#; %<== default  
MCd(1,.3)(.5, .5)(^^30,?6,5:*/Me) endfont  
beginfont() offset_wedge#:=1.0pt#;  
MCd(1,.3)(1, .5)(^^30,?6,5:*/Me) endfont
```

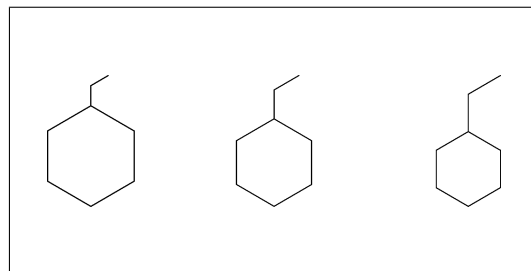
**No.54 Ratio font atom gap/atom length**

```
ratio_atomgap_atom:=0.0;  
MCd(1,.6)(0, .5)(^^30,?6,@(2,5)O)  
ratio_atomgap_atom:=0.050; %<== default  
MCd(1,.6)(.5, .5)(^^30,?6,@(2,5)O)  
ratio_atomgap_atom:=0.12;  
MCd(1,.6)(1, .5)(^^30,?6,@(2,5)O)
```



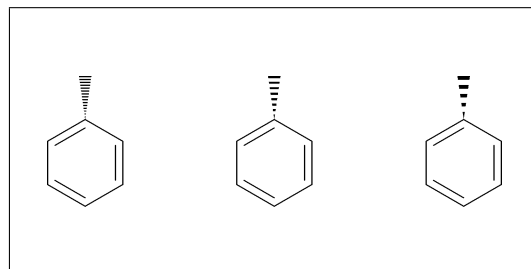
No.55 Ratio chain/ring length

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



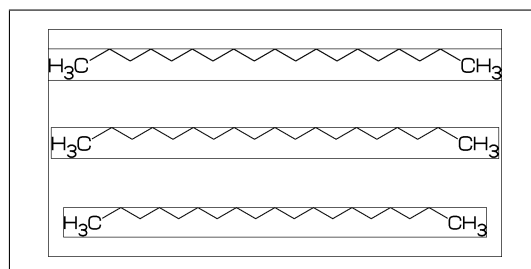
No.56 Ratio zebra gap/bond length

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



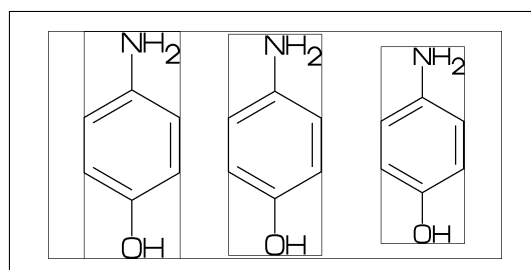
No.57 Margin left and right

```
margin_left_right:=0mm;
MCd(1,1)(0.5,0.9)(^30,CH3,!0,!17,CH3)
margin_left_right:=0.4mm;      %<== default
MCd(1,1)(0.5,0.5)(^30,CH3,!0,!17,CH3)
margin_left_right:=2mm;
MCd(1,1)(0.5,0.1)(^30,CH3,!0,!17,CH3)
```



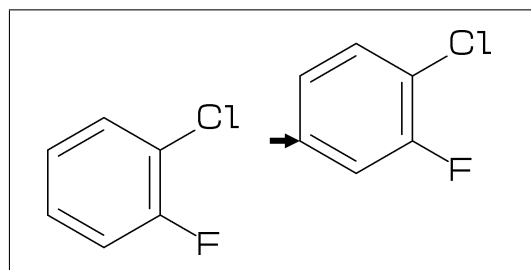
No.58 Margin top and bottom

```
margin_top_bottom:=0mm;
MCd(1,1)(0.1,0.5)(^30,Ph,2:/OH,5:/NH2)
margin_top_bottom:=0.4mm;      %<== default
MCd(1,1)(0.5,0.5)(^30,Ph,2:/OH,5:/NH2)
margin_top_bottom:=2mm;
MCd(1,1)(0.9,0.5)(^30,Ph,2:/OH,5:/NH2)
```



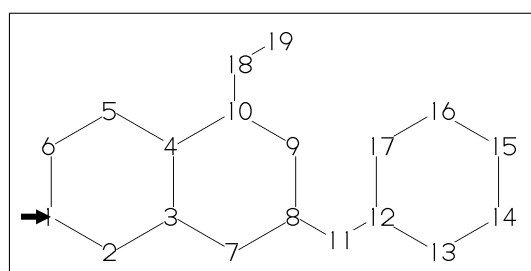
No.59 Switch Start Vector

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



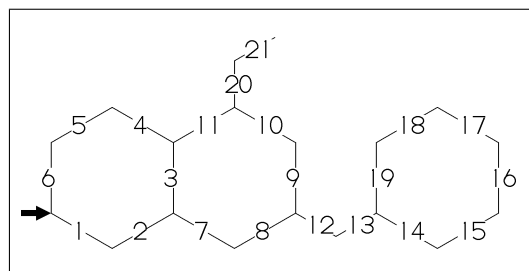
No.60 Switch NumberingA

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



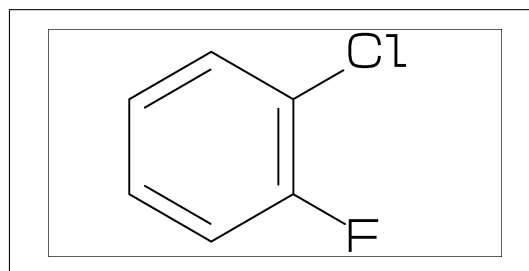
No.61 Switch NumberingB

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



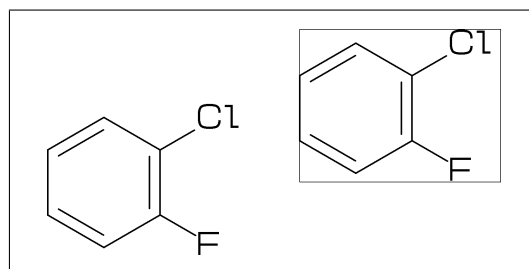
No.62 Switch font frame

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



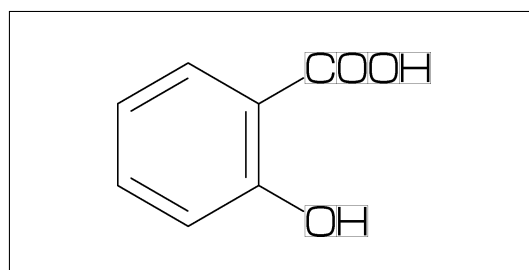
No.63 Switch molecular frame

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



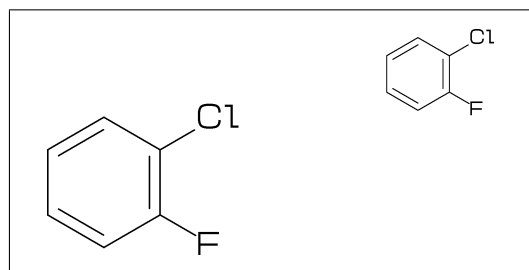
No.64 Switch atom frame

```
sw_atom_frame:=1;
MCf(^^30,Ph,4:/COOH,3:/OH)
```



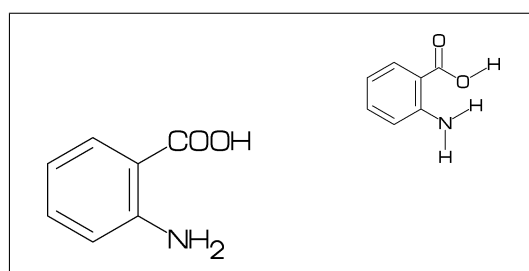
No.65 Switch solid mode

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



No.66 Switch Expand

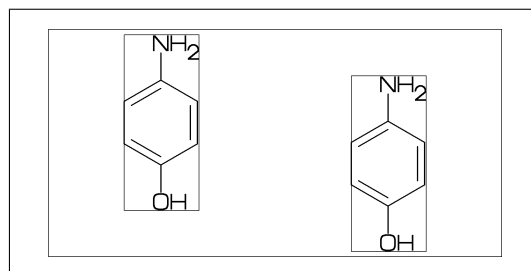
```
MCd(1,.6)(0,0)(^^30,Ph,4:/COOH,3:/NH2)
sw_expand:=1;
MCd(1,.6)(1,1)(^^30,Ph,4:/COOH,3:/NH2)
```



No.67 Function MCd

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

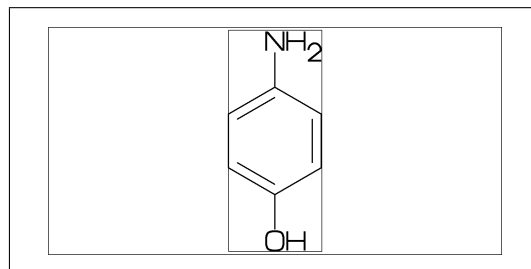
MCd(1,0.8)(0.2,0.9)(^30,Ph,2:/OH,5:/NH2)
MCd(1,0.8)(0.8,0.1)(^30,Ph,2:/OH,5:/NH2)
```

**No.68 Function MCf**

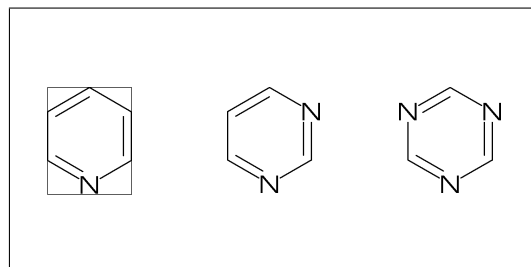
```
MCf(...) : MCd(1,1)(0.5,0.5)(...)

sw_font_frame:=1;  sw_mol_frame:=1;

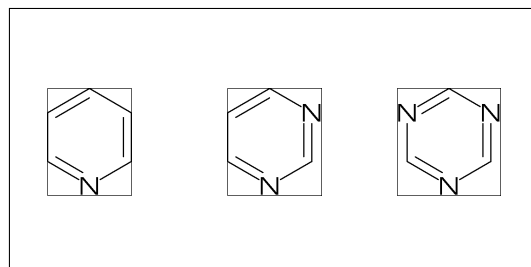
MCf(^30,Ph,2:/OH,5:/NH2)
```

**No.69 Local setting**

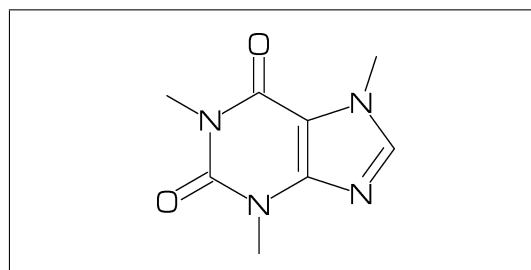
```
beginfont("N0:1")
  sw_mol_frame:=1; % <== Local setting
  MCd(1,.5)(0.0,0.5)(^30,Ph,@(2)N) endfont
beginfont("N0:2")
  MCd(1,.5)(0.5,0.5)(^30,Ph,@(2,4)N) endfont
beginfont("N0:3")
  MCd(1,.5)(1.0,0.5)(^30,Ph,@(2,4,6)N) endfont
```

**No.70 Global setting**

```
sw_mol_frame:=1; % <== Global setting
beginfont("N0:1")
  MCd(1,.5)(0.0,0.5)(^30,Ph,@(2)N) endfont
beginfont("N0:2")
  MCd(1,.5)(0.5,0.5)(^30,Ph,@(2,4)N) endfont
beginfont("N0:3")
  MCd(1,.5)(1.0,0.5)(^30,Ph,@(2,4,6)N) endfont
```

**No.71 Output molecular infomation**

```
beginfont() sw_info_weight:=sw_info_formula:=1;
MCf(...) endfont
%% Output to mcf_man_soc_info.aux %%
\INFO{{F:mcf_man_soc}{C:82}{MWc:194.19174}
      {FMc:C8H10N4O2}}%
MWc:calculated molecular weight
FMc:calculated molecular formula
```

**No.72 Output additional infomation**

```
beginfont("EN:Caffeine","CAS:58-08-2")
MCf(...) endfont
%% Output to mcf_man_soc_info.aux %%
\INFO{{F:mcf_man_soc}{C:83}{EN:Caffeine}
      {CAS:111-111-111}}%
*F:filename *C:char number EN:molecular name
CAS:CAS number *:default output
```

