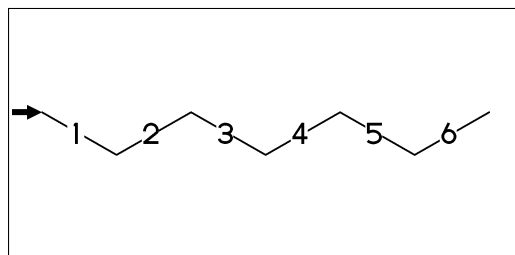


No.1 Chain (1)

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

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

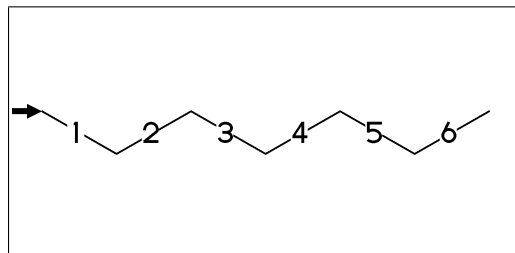


No.2 Chain (2)

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

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

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

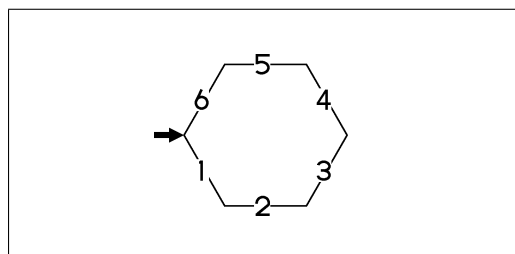


No.3 Ring

six membered ring

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

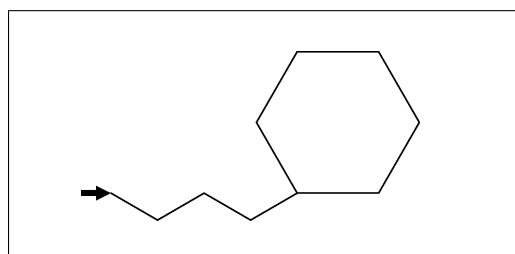
```
** ??6 : ^^ -120,60,60,60,60,60,&(-5)  
?6 : {,??6,}
```



No.4 Rotate current angle

^^angle:rotate current angle

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

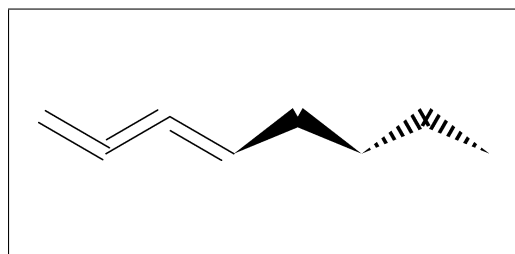


No.5 Change bond type (1)

~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
```

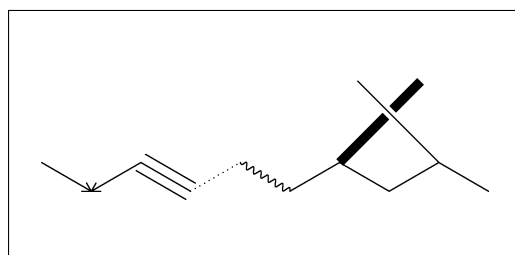


No.6 Change bond type (2)

Bn=bond type : \$(Bn)bond type (change bond type at Bn)

```
vf:vector forward, vb:vector backward,  
tm:triple, wv:waved, bd:broad single,  
ov:over line
```

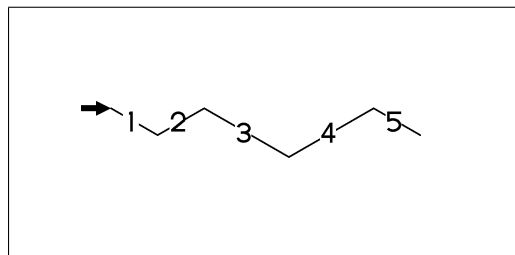
```
^^30,!9,1=vf,2=vb,3=tm,4=dt,5=wv,  
@(7~bd~-45'2,9~ov~45'2)/Me
```



No.7 Change bond length (1)

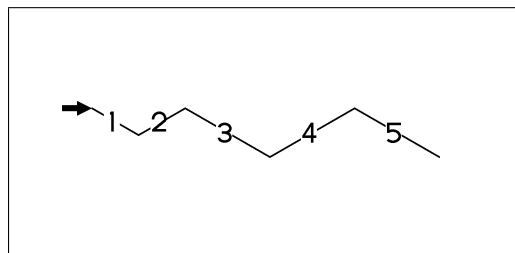
Bn'length : change bond length at Bn

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

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

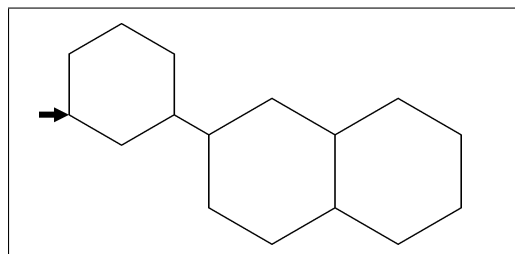
''length : change all bond length after

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

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

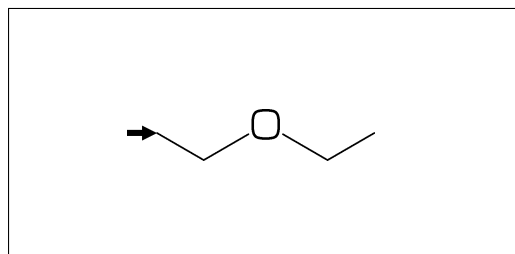
?n'length : change ring length

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

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

Insert hetero atom

```
^^30,!2,0,!2
```

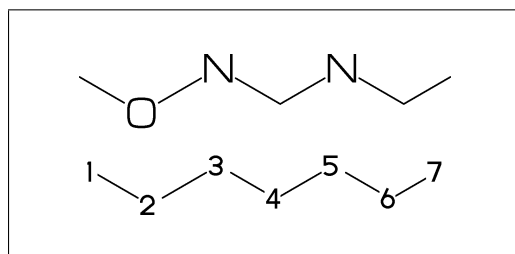
**No.11 Change atom (2)**

2:0 : change A2 C to O

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

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

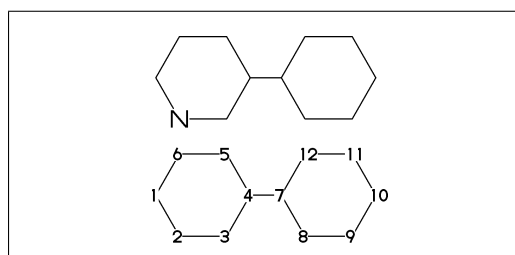
An(n:numeric): atom number

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

2:N : change A2 C to N

??6 do not make brock

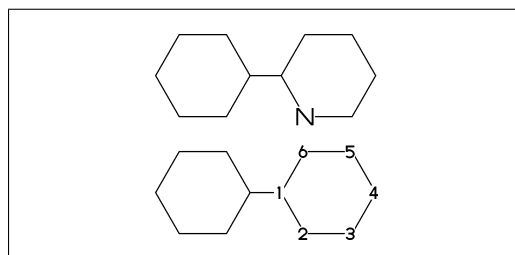
```
?6,4\,??6,2:N
```



No.13 Change atom (brock address)

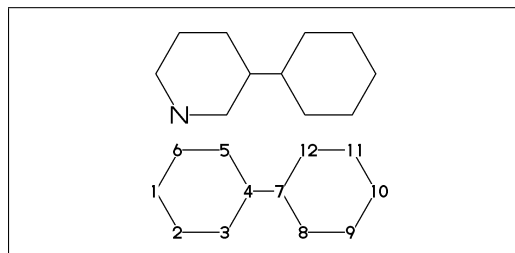
2:N : change A2(brock address) C to N

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

**No.14 Change atoma (absolute address)**

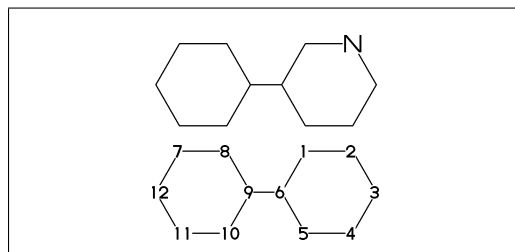
#2:N : change A#2 C to N

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

**No.15 Change atom (relative address)**

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

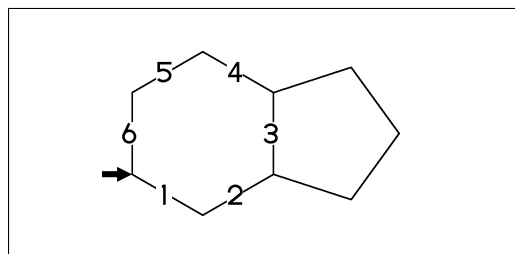
?6,4\,?6,-2:N

**No.16 Fuse ring (attached 1 bond)**

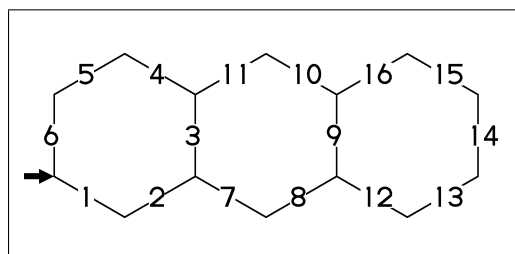
?6,3=?5 : fuse ?5 at B3

?6,3=?5

Bn(n:numeric): bond number

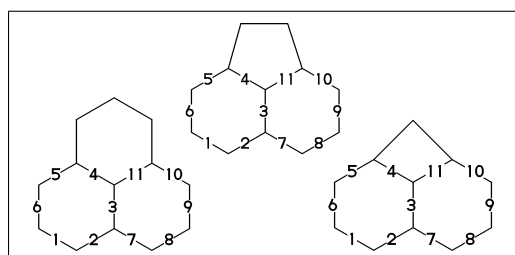
**No.17 Fuse multi ring (attached 1 bond)**

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

**No.18 Fuse ring (attached 2 bond)**

(4,11)=??6[4] : fuse 4/6 ring to B11..B4
 (4,11)=??5[3] : fuse 3/5 ring to B11..B4
 (4,11)=??4[2] : fuse 2/4 ring to B11..B4

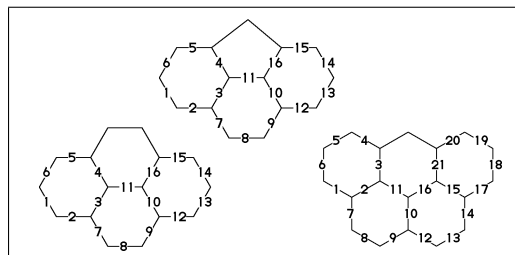
MCd(1,.7)(0,0)(^30,?6,\$(3)??6,(11,4)=??6[4])
 MCd(1,.6)(.5,1)(^30,?6,\$(3)??6,(11,4)=??5[3])
 MCd(1,.6)(1,0)(^30,?6,\$(3)??6,(11,4)=??4[2])



No.19 Fuse ring (attached 3,4 bond)

(16,4)=??6[3] : fuse 3/6 ring to B16..B4
 (16,4)=??5[2] : fuse 2/5 ring to B16..B4
 (21,3)=??6[2] : fuse 2/6 ring to B21..B3

MCd(1,.55)(0,0)(?6,\$(3,10)?6,(16,4)=??6[3])
 MCd(1,.55)(.43,1)(?6,\$(3,10)?6,(16,4)=??5[2])
 MCd(1,.53)(1,0)(^30,?6,\$(2,10,15)?6,(21,3)=??6[2])

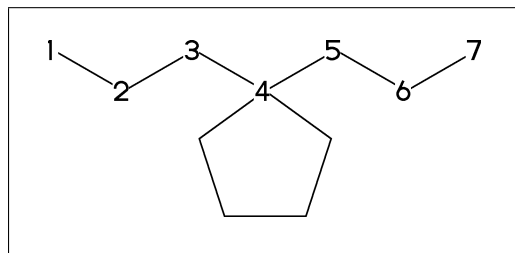


No.20 Spiro ring

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

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

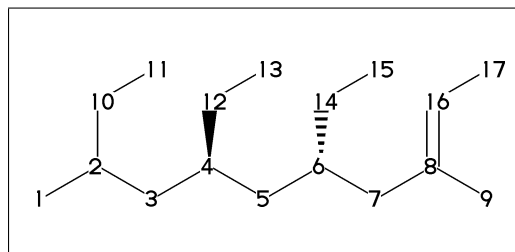
An* : jump to An



No.21 Branch bond (1)

2\ : 2*,0 4*\ : 4*,0~wf
 6* : 6*,0~zf 8\\ : 8*,0~dm

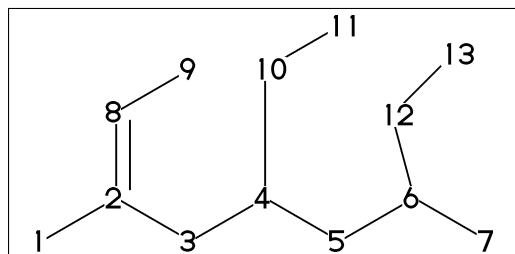
MCf(^^30,!8,2\,! ,4*\,! ,6*,! ,8\\,!)



No.22 Branch bond (2)

2\~dr : 2*,0~dr
 4\'1.5 : 4*,0\'1.5
 6\^15 : 6*,0^15

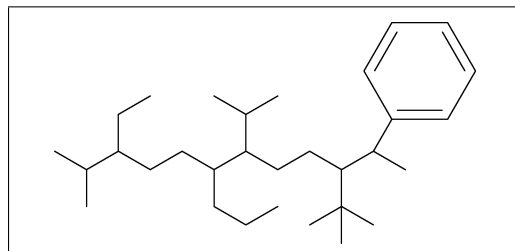
MCf(^^-30,!6,2\~dr,! ,4\'1.5,! ,6\^15,-60)



No.23 Insert substituent(1)

^^30,
 !,/Me,! ,/Et,!3,/Pr,! ,/iPr,!3,/tBu,! ,/Ph^-30,!)

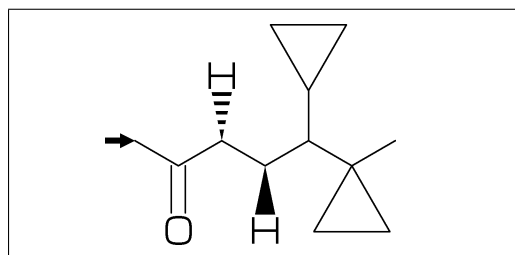
** Me:methyl Et:ethyl Pr:propyl iPr:isopropyl
 tBu:tertial buthyl Ph:phenyl



No.24 Insert substituent(2)

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

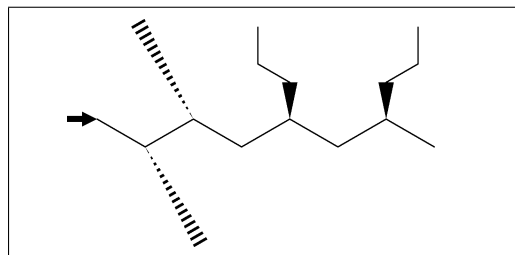
^^30,! ,//0,! ,/*H,! ,*/H,! ,/?3,! ,**?3,!)



No.25 Insert substituent(3)

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

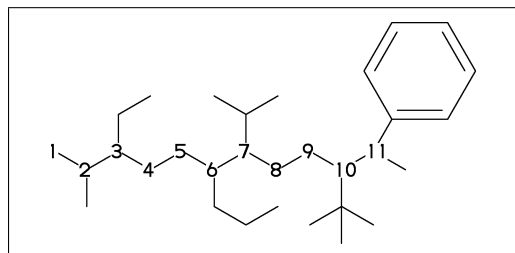
```
MCf(^~30,!^1,/Me~zf^2^30,!^1,/Me~zf^2^30,
    !2^1,*/Pr>lr,!2^1,*/Pr>rl,!^1)
```



No.26 Add substituent(1)

```
sw_numberA:=1; numberA_end:=_skeletonA_end;
mcf(^~30,!11,
    2:/Me,3:/Et,6:/Pr,7:/iPr,10:/tBu,11:/Ph^30)
```

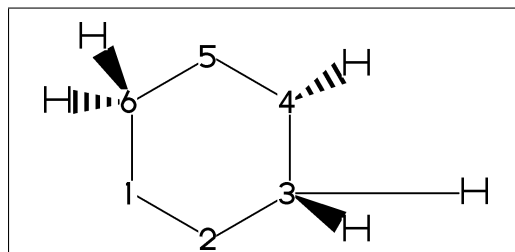
```
** _skeletonA_end :
    end number of molecular skeleton atom
```



No.27 Add substituent(2)

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

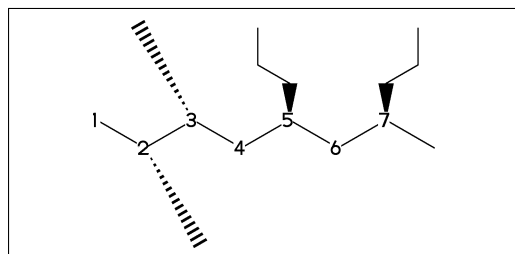
```
sw_numberA:=1; numberA_end:=_skeletonA_end;
Mcf(^~30,?6,
    @(3^2^30,3~wf,4~zf,6~wf^30,6~zf^30)/H)
```



No.28 Add substituent(3)

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

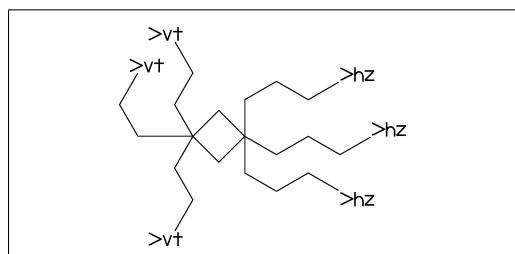
```
sw_numberA:=1; numberA_end:=_skeletonA_end;
MCF(^~30,!7^1,
    @(2,3)/Me^2^30,5:*/Pr>lr,7:*/Pr>rl)
```



No.29 Chain stretch direction environment (1)

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

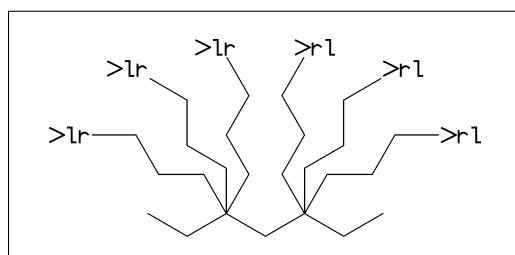
```
?4,
    @(3^-90,3^-30,3^90)/'(!3,"{>hz}")>hz,
    @(1^-60,1^1.5,1^60)/'(!2,"{>vt}")>vt
```



No.30 Chain stretch direction environment (2)

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

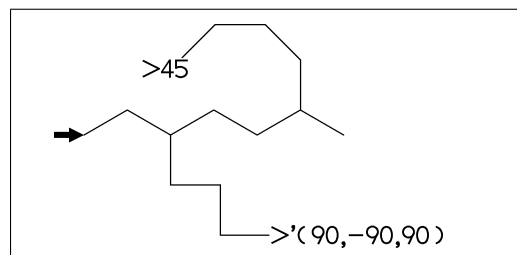
```
^~30,!6,
    @(3^-30,3,3^30)/'(!3,"{>lr}")>lr,
    @(5^-30,5,5^30)/'(!3,"{>rl}")>rl
```



No.31 Chain stretch direction environment (3)

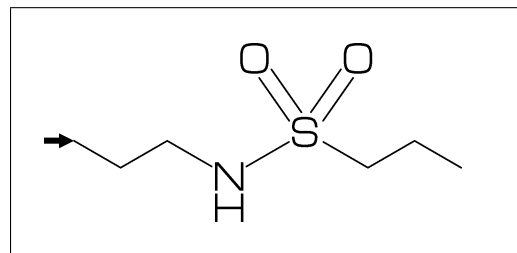
>45 : fixed angle environment
 >'(-90,90,-90) : multi angle environment

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

**No.32 Change atom and Substituent**

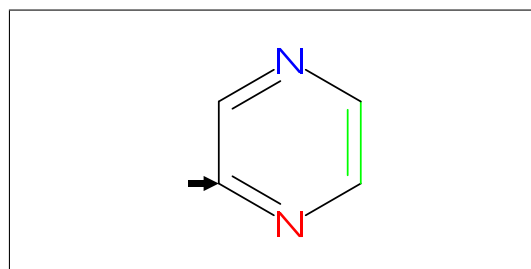
NH,S00 : inset hetero atom and substituent simultaneously

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

**No.33 Change color**

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

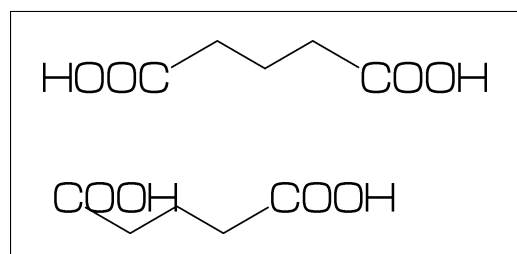
```
^^30,Ph,@(2,5)N,
2:red,5:blue,3=green
```

**No.34 Chain start multiple characters**

if chain start multi character string,
 use !0 instead of !

```
MCd( 1,1)(0 ,0.9)(^^30,COOH,!0,!3,COOH)
```

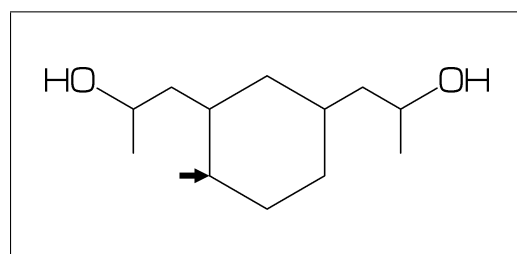
```
MCd(.8,1)(0.3,0.1)(^^30,COOH,!4,COOH)
```

**No.35 User definition**

iBuOH : user defined substructure

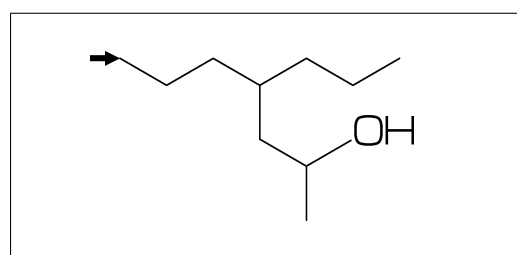
```
iBuOH:= '(!,/Me,! ,OH)
```

```
MCf(^^30,?6,@(4,6)/iBuOH)
```

**No.36 Inline definition**

Insert user defined substructure

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

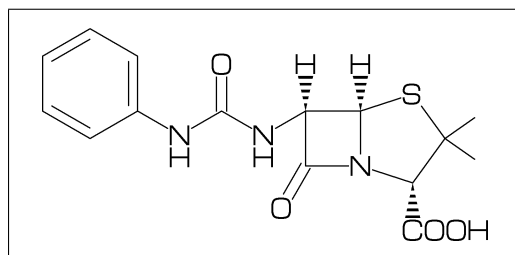


No.37 Example(1) Ampicillin

```

^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

```

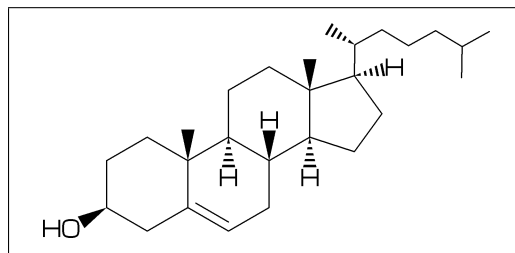


No.38 Example(2) Cholesterol

```

^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,! ,

```

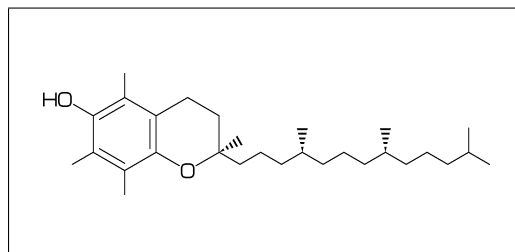


No.39 Example(3) alpha-Tocopherol

```

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

```

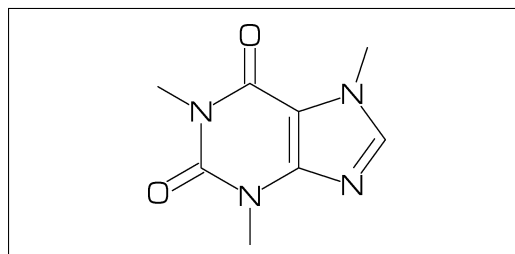


No.40 Example(4) Caffeine

```

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

```

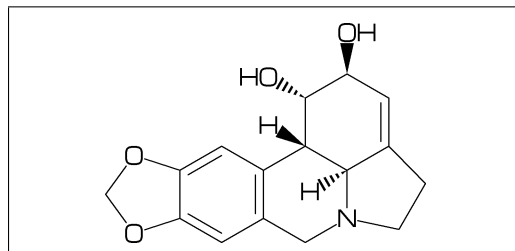


No.41 Example(5) Lycorine

```

^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

```

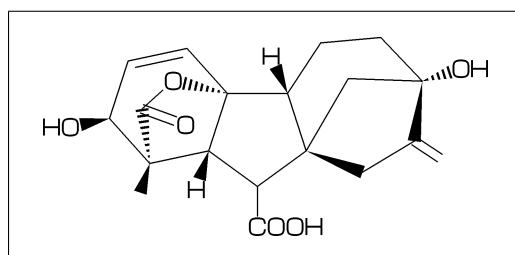


No.42 Example(6) Gibberellin

```

^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

```

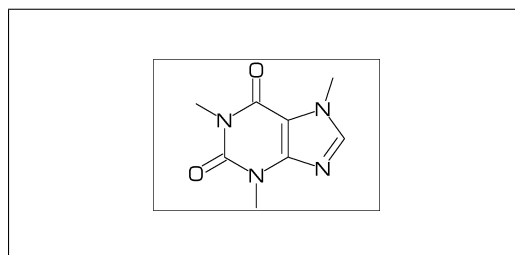


No.43 Font size

```

beginfont("EN:Caffeine")
font_wd#:=30mm#; %<==font width
font_ht#:=20mm#; %<==font height
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

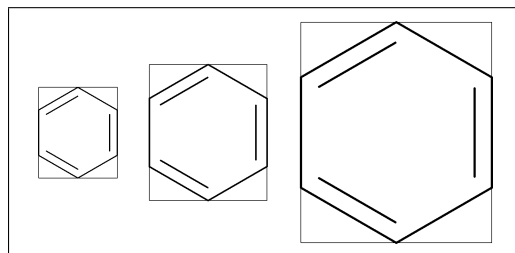
```

**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)

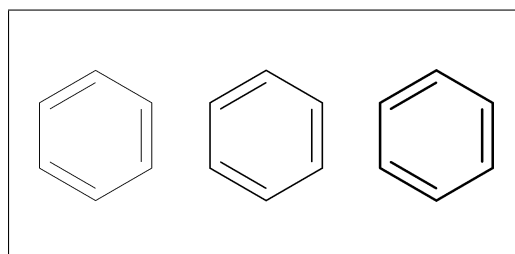
```

**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)

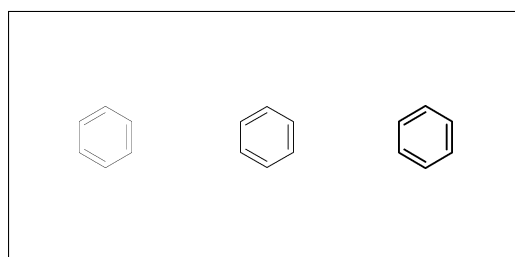
```

**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

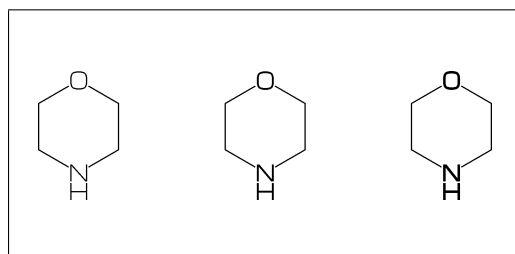
```

**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)

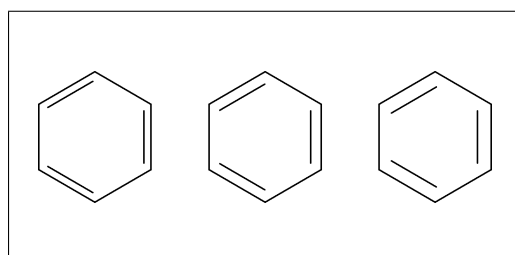
```

**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)

```

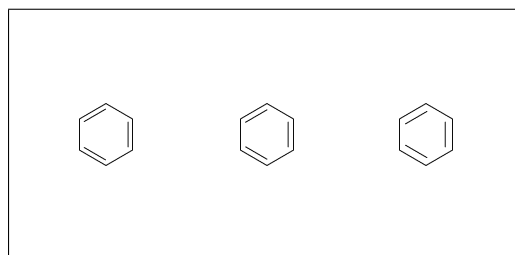


No.49 Offset of doublebond gap

```

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

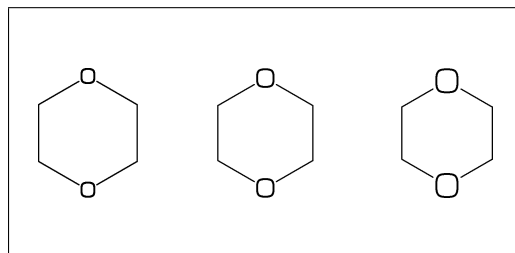
```

**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)

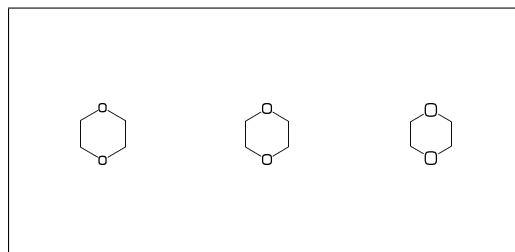
```

**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

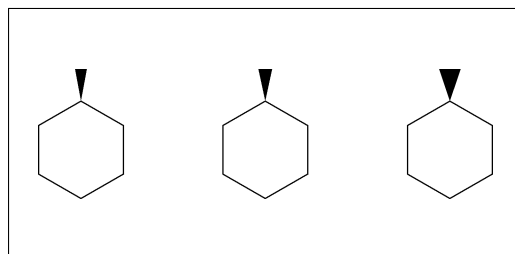
```

**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)

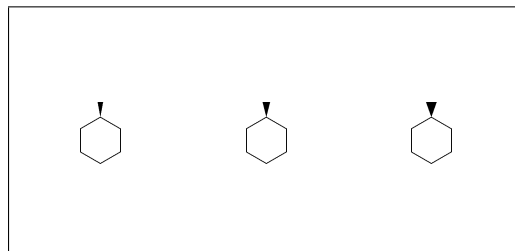
```

**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

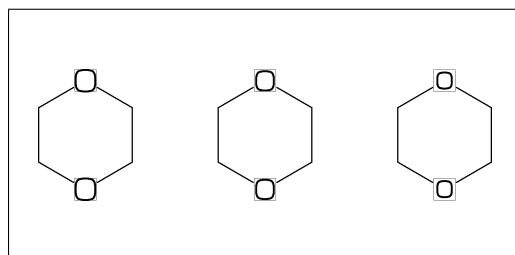
```

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

```

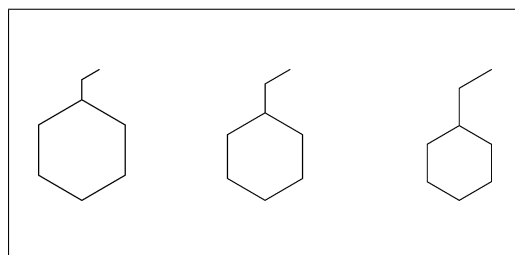
ratio_atomgap_atom:=0.0;
MCd(1,.6)(0, .5)(^^30,?6,@(2,5)O)
ratio_atomgap_atom:=0.050; %<== default
MCd(1,.6)(.5, .5)(^^30,?6,@(2,5)O)
ratio_atomgap_atom:=0.12;
MCd(1,.6)(1, .5)(^^30,?6,@(2,5)O)

```



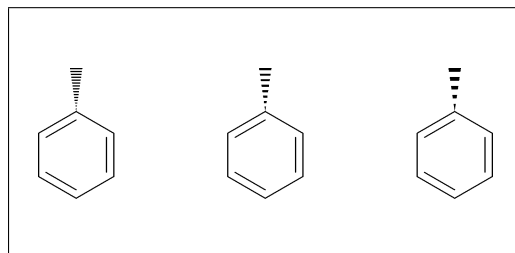
No.55 Ratio chain/ring length

```
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)
```



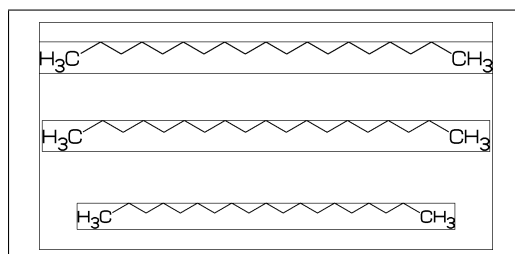
No.56 Ratio zebra gap/bond length

```
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)
```



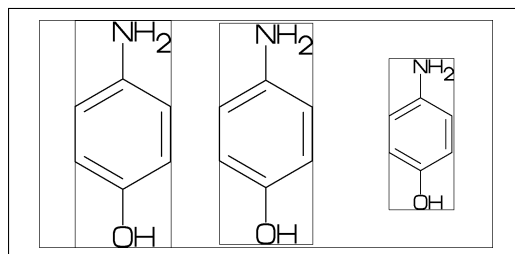
No.57 Margin left and right

```
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:=5mm;
MCd(1,1)(0.5,0.1)(^30,CH3,!0,!17,CH3)
```



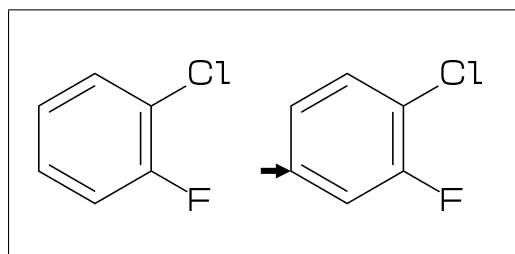
No.58 Margin top and bottom

```
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:=5mm;
MCd(1,1)(0.9,0.5)(^30,Ph,2:/OH,5:/NH2)
```



No.59 Switch Start Vector

```
MCd(1,.8)( 0,0.5)(^30,Ph,4:/Cl,3:/F)
sw_start_vector:=1;
MCd(1,.8)( 1,0.5)(^30,Ph,4:/Cl,3:/F)
```

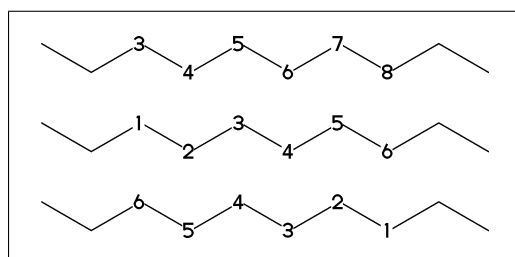


No.60 Switch Numbering atom

```
numberA_start:=3; numberA_end:=8;

sw_numberA:=1; MCd(1,1)(.5,.9)(^30,!9)
sw_numberA:=2; MCd(1,1)(.5,.5)(^30,!9)
sw_numberA:=3; MCd(1,1)(.5,.1)(^30,!9)

** default: numberA_start=1 numberA_end=4095
```



No.61 Switch Numbering bond

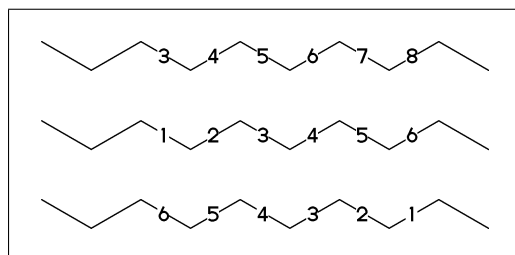
```

numberB_start:=3; numberB_end:=8;

sw_numberB:=1; MCd(1,1)(.5,.9)(^^30,!9)
sw_numberB:=2; MCd(1,1)(.5,.5)(^^30,!9)
sw_numberB:=3; MCd(1,1)(.5,.1)(^^30,!9)

** default: numberB_start=1 numberB_end=4095

```

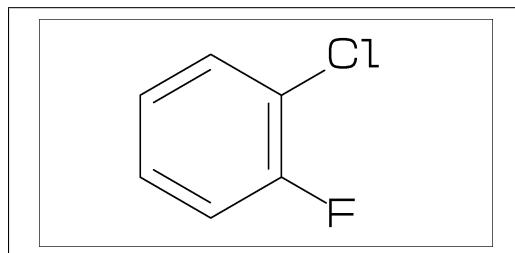
**No.62 Switch font frame**

```

sw_font_frame:=1;

MCf(^^30,Ph,4:/Cl,3:/F)

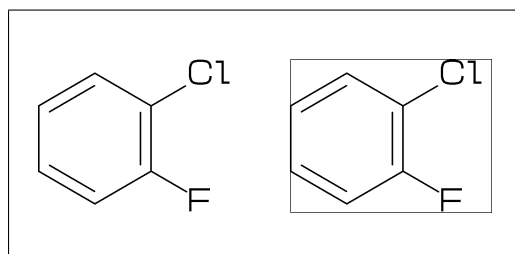
```

**No.63 Switch molecular frame**

```

MCd(1,.8)(0,0.5)(^^30,Ph,4:/Cl,3:/F)
sw_mol_frame:=1;
MCd(1,.8)(1,0.5)(^^30,Ph,4:/Cl,3:/F)

```

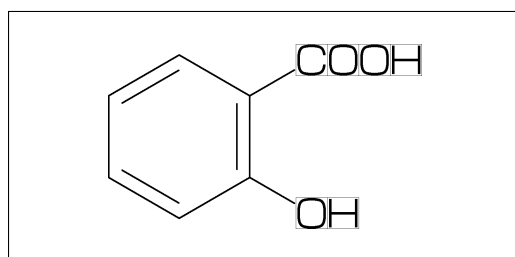
**No.64 Switch atom frame**

```

sw_atom_frame:=1;

MCf(^^30,Ph,4:/COOH,3:/OH)

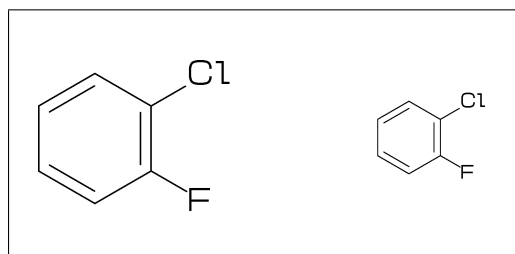
```

**No.65 Switch solid mode**

```

MCd(1,.8)( 0,0.5)(^^30,Ph,4:/Cl,3:/F)
sw_solid:=1; ratio_bond_width:=0.08;
MCd(1,.8)( 1,0.5)(^^30,Ph,4:/Cl,3:/F)

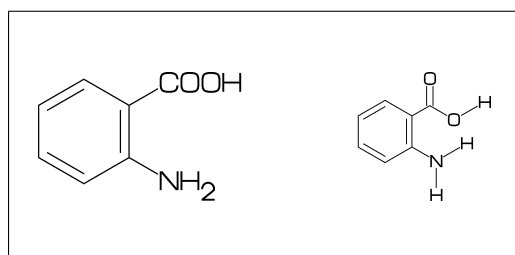
```

**No.66 Switch Expand**

```

MCd(1,.6)(0,0.5)(^^30,Ph,4:/COOH,3:/NH2)
sw_expand:=1;
MCd(1,.6)(1,0.5)(^^30,Ph,4:/COOH,3:/NH2)

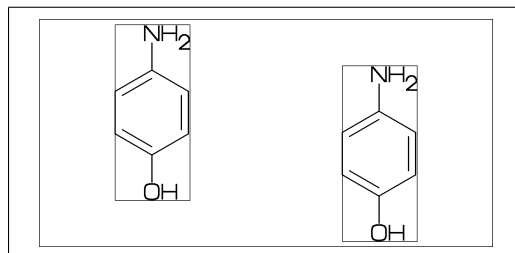
```



No.67 Function MCd (draw)

```
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

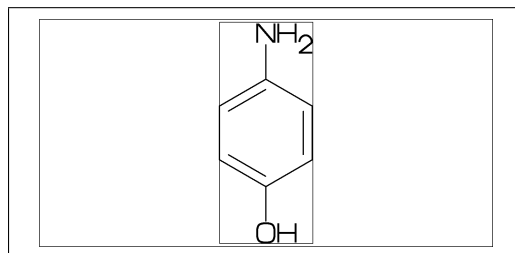
MCd(1,0.8)(0.2,0.9)(^30,Ph,2:/OH,5:/NH2)
MCd(1,0.8)(0.8,0.1)(^30,Ph,2:/OH,5:/NH2)
```

**No.68 Function MCf (fit draw)**

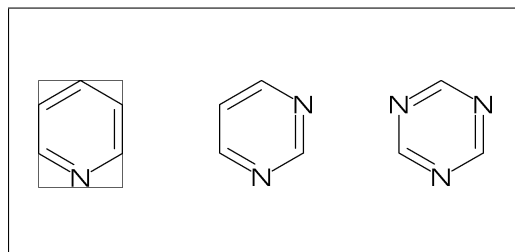
```
MCf(...) : MCd(1,1)(0.5,0.5)(...)

sw_font_frame:=1;  sw_mol_frame:=1;

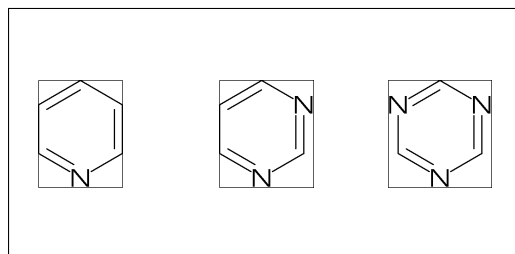
MCf(^30,Ph,2:/OH,5:/NH2)
```

**No.69 Local setting**

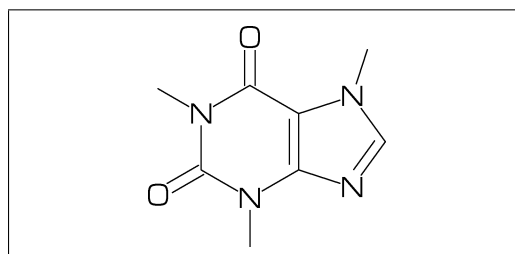
```
beginfont("N0:1")
  sw_mol_frame:=1; % <== Local setting
  MCd(1,.5)(0.0,0.5)(^30,Ph,@(2)N) endfont
beginfont("N0:2")
  MCd(1,.5)(0.5,0.5)(^30,Ph,@(2,4)N) endfont
beginfont("N0:3")
  MCd(1,.5)(1.0,0.5)(^30,Ph,@(2,4,6)N) endfont
```

**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:58-08-2}}%
*F:filename *C:char number EN:molecular name
CAS:CAS number *:default output
```

