

Molecular Coding Format manual

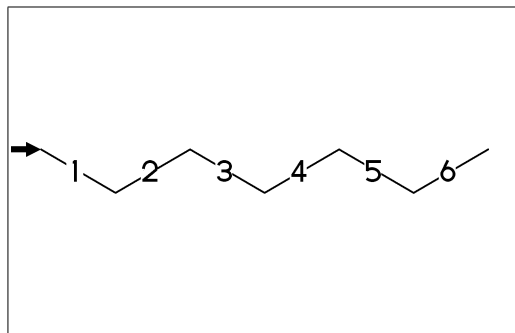
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Located at : <http://www.ctan.org/pkg/mcf2graph>

Molecular Coding Format(MCF) is new linear notation represent chemical structure diagram.
This 'Coding' is named from coding(programing) technique like adresssing,grouping,macro,etc.
There are no Meta language commands in MCF. mcf2graph.mf(metapost/metafont macro)
convert MCF file to graphics file pk font,PNG,SVG,EPS or MDL MOL file(V2000).

No.1 Chain

plus(+):anticlockwise,minus(-):clockwise
! : take value depend on
 current angle and enviroment

<30,-60,60,-60,60,-60,60
<30,!,,!,!,!,!,!

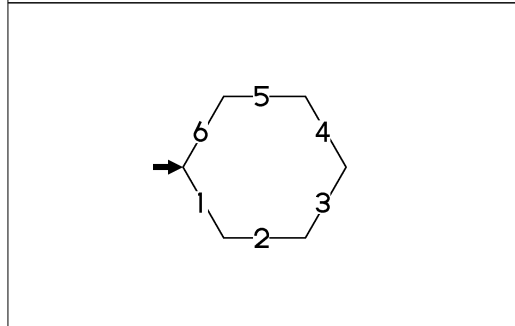


No.2 Ring

six membered ring

?6

** ?6 : <-120,60,60,60,60,60,&1
** &1 : make bond connect to A1

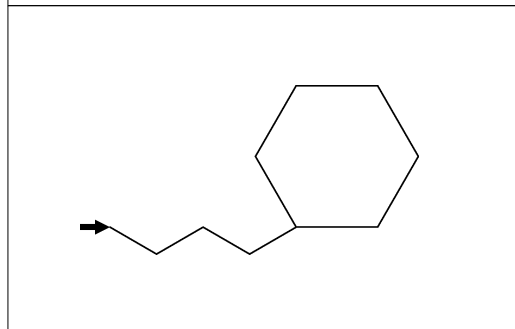


No.3 Rotate current angle

<angle : rotate current angle

<30,!4,<30,?6

** !4: !,,!,!,!
** bold arrow is default angle and position

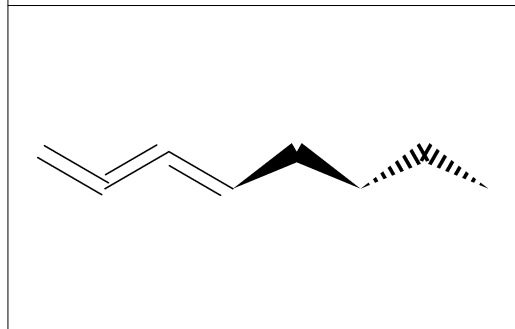


No.4 Change bond type (1)

~bond : change bond

dm:double,dl:double left,dr:double right,
wf:wedge forward,wb:wedge backward,
zf:wedge dotted,zb:wedge dotted backward

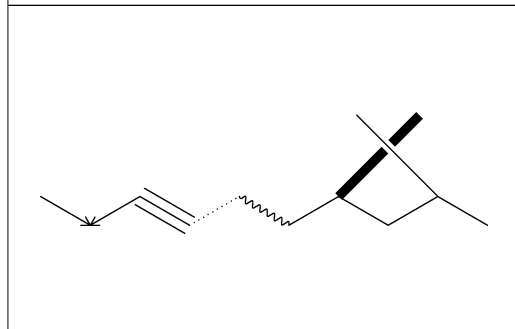
<30,!~dm,!~dl,!~dr,!~wf,!~wb,!~zf,!~zb



No.5 Change bond type (2)

Bn=bond type : change bond type at Bn
vf:vector forward, vb:vector backward,
tm:triple, wv:waved, bd:broad single,
ov:over line

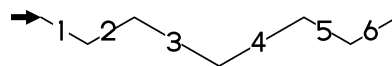
<30,!9,1=vf,2=vb,3=tm,4=dt,5=wv,
@(7~bd~-45'2,9~ov~45'2)/Me



No.6 Change bond length (1)

Bn'length : change bond length at Bn

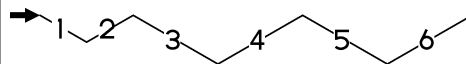
<30,!2,!2'1.2,!2



No.7 Change bond length (2)

'length : change all bond length after

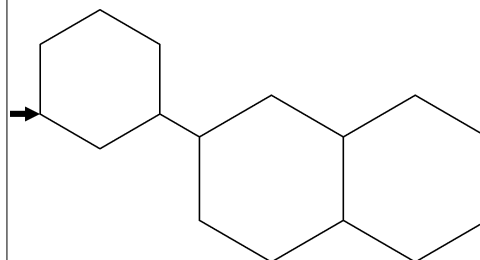
<30,!2,'1.2,!4



No.8 Change chain length (3)

?n'length : change ring length

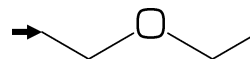
<30,!6,3\,|,!6'1.2,4=?6



No.9 Change atom (1)

Insert hetero atom

<30,!2,0,!2



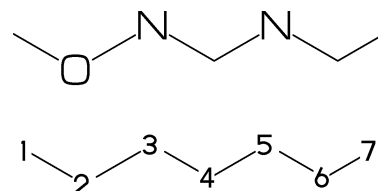
No.10 Change atom (2)

2:0 : change A2 C to O

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

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

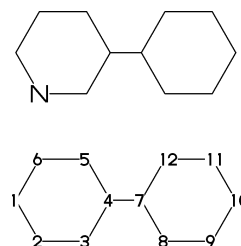
An(n:numeric): atom number



No.11 Change atom (3)

2:N : change A2 C to N

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

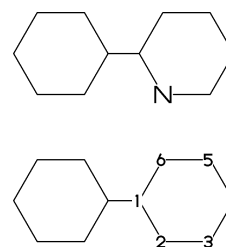


No.12 Change atom (brock address)

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

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

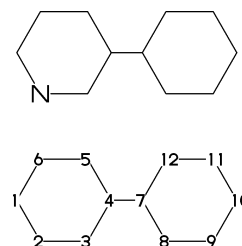
| : divide brock



No.13 Change atoma (absolute address)

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

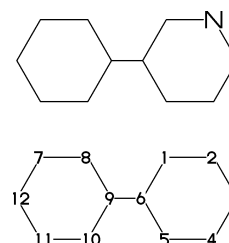
?6,4\,|,?6,#2:N



No.14 Change atom (relative address)

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

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

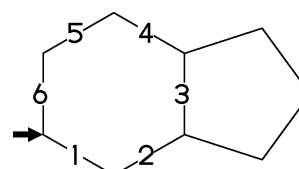


No.15 Fuse ring (attached 1 bond)

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

?6,3=?5

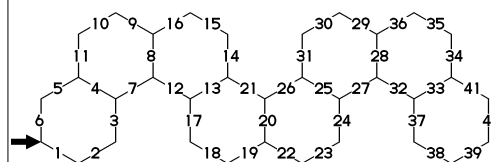
Bn(n:numeric): bond number



No.16 Fuse multi ring (attached 1 bond)

?6,\$(-3,-4,-4,-2,-2,-4,-4)?6

?6,\$(4,8,13,20,25,28,33)?6



No.17 Fuse ring (attached 2 bond)

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

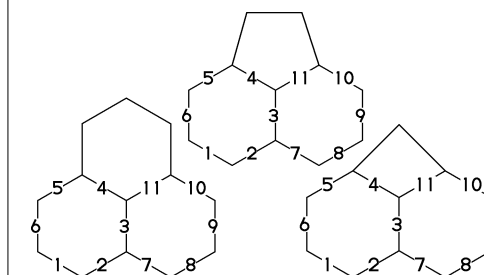
(4,11)=?5[3] : fuse 3/5 ring to B11..B4

(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)(.54,1)(<30,?6,3=?6,(11,4)=?5[3])

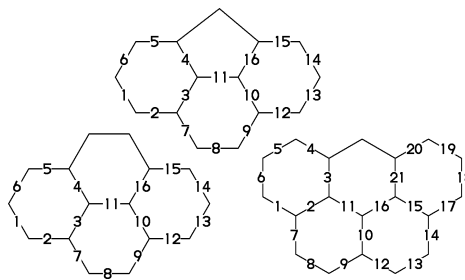
MCd(1,.6)(1,0)(<30,?6,3=?6,(11,4)=?4[2])



No.18 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

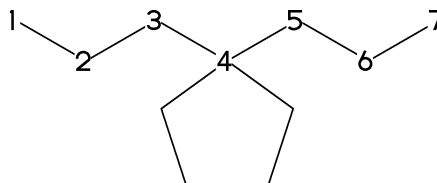
MCd(1,.55)(0, 0)(?6,\$(3,10)?6,(16,4)=?6[3])
 MCd(1,.55)(.43,1)(?6,\$(3,10)?6,(16,4)=?5[2])
 MCd(1,.53)(1,0)(<30,?6,\$(2,10,15)?6,(21,3)=?6[2])

**No.19 Spiro ring**

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

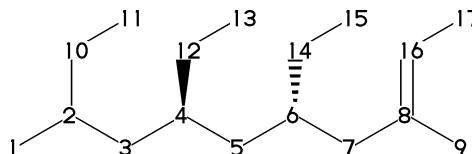
<30,!6,4*,?5

An* : jump to An

**No.20 Branch bond (1)**

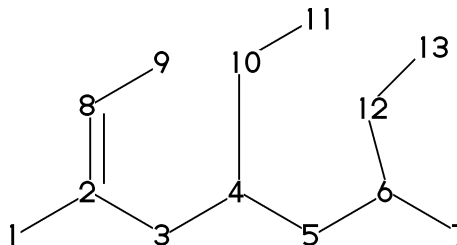
2\ : 2*,0 4*\ : 4*,0~wf
 6* : 6*,0~zf 8\\ : 8*,0~dm

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

**No.21 Branch bond (2)**

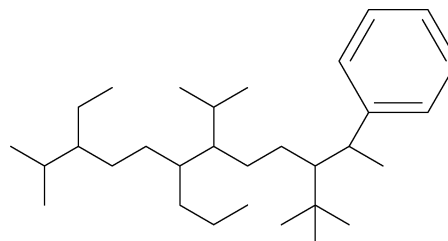
2\~dr : 2*,0~dr
 4\'1.5 : 4*,0\'1.5
 6\^15 : 6*,0^15

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

**No.22 Insert substituent(1)**

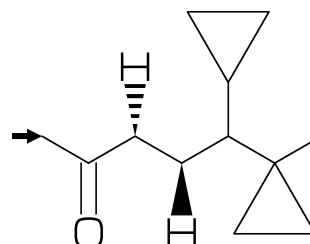
MCf(<30,
 !,/Me,!,/Et,!3,/Pr,!/iPr,!3,/tBu,!/Ph^-30,!)

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

**No.23 Insert substituent(2)**

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

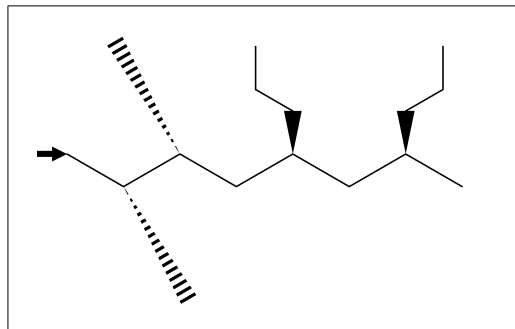
MCf(<30,!//0,!/*H,!*/H,!/?3,!,**?3,!)



No.24 Insert substituent(3)

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

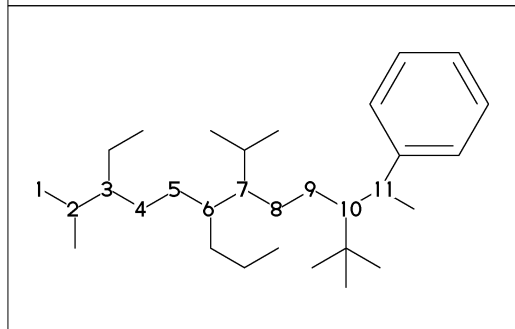
```
MCf(<30,!^1,/Me~zf^2^30,!^1,/Me~zf^2^30,
    !2^1,*/Pr>lr,!2^1,*/Pr>rl,!^1)
```



No.25 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)
```

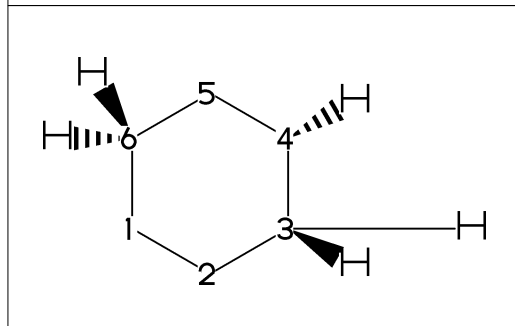
** _skeletonA_end :
end number of molecular skeleton atom



No.26 Add substituent(2)

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

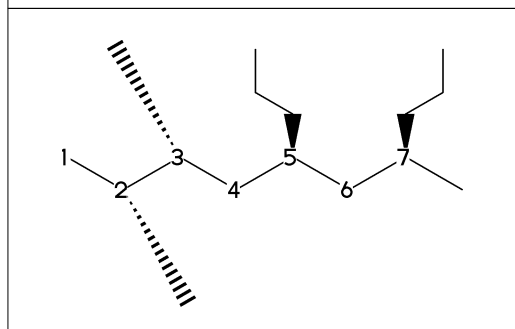
```
MCf(<30,?6,
    @(3^2^30,3~wf,4~zf,6~wf^-30,6~zf^30)/H)
```



No.27 Add substituent(3)

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

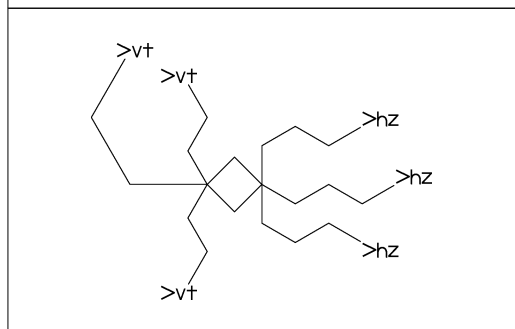
```
MCF(<30,!7^1,
    @(2,3)/Me^2^30,5:*/Pr>lr,7:*/Pr>rl)
```



No.28 Chain stretch direction environment (1)

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

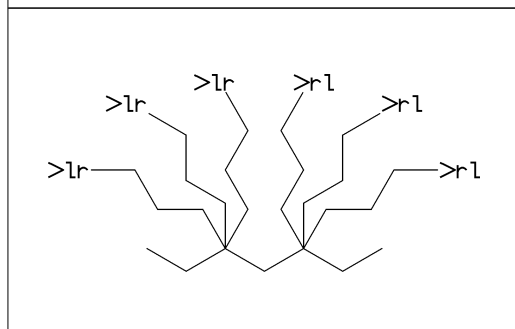
```
?4,
    @(3^-90,3^-30,3^90)/'(!3,"{>hz}")>hz,
    @(1^-60,1^2,1^60)/'(!2,"{>vt}")>vt
```



No.29 Chain stretch direction environment (2)

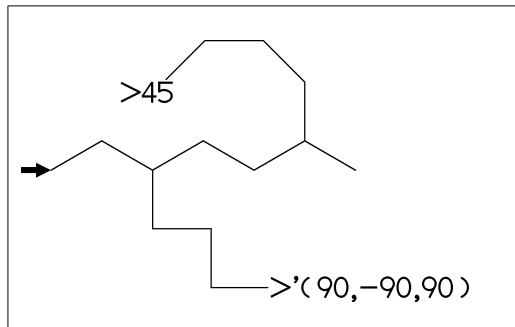
>lr : left-right enviroment
>rl : right-left enviroment

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



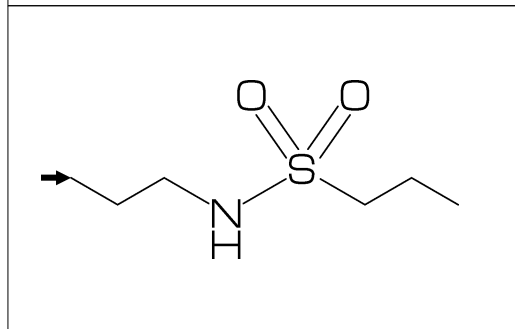
No.30 Chain stretch direction environment (3)

>45 : fixed angle environment
 >'(-90,90,-90) : multi angle environment
 <-30,!6,@(2>45)/'(!3,"{>45}"),
 @(>'(-90,90,-90))/'(!3,"{>(-90,90,-90)}")

**No.31 Change atom and Substituent**

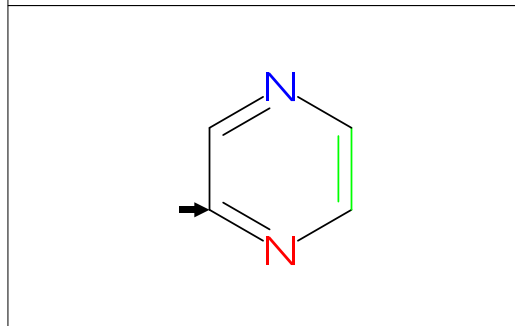
NH,S00 : inset hetero atom and substituent simultaneously

<30,!3,NH,! ,S00,!3

**No.32 Change color**

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

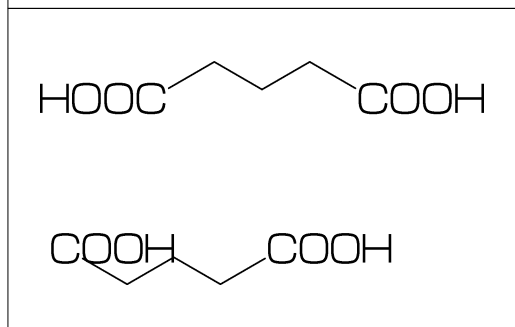
<30,Ph,@(2,5)N,
 2:red,5:blue,3=green

**No.33 Chain start multiple characters**

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

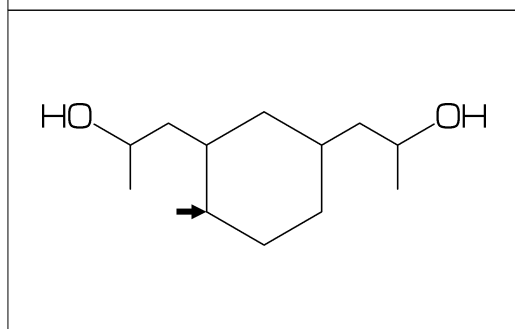
MCd(1,1)(0 ,0.9)(<30,COOH,!0,!3,COOH)

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

**No.34 User definition**

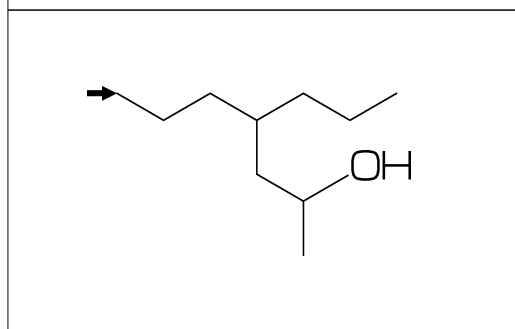
iBuOH : user defined substructure

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

**No.35 Inline definition**

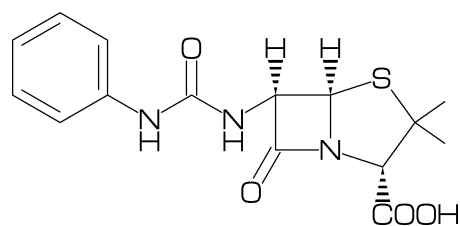
Insert user defined substructure

<30,!3,/'(!,/Me,! ,OH),!3



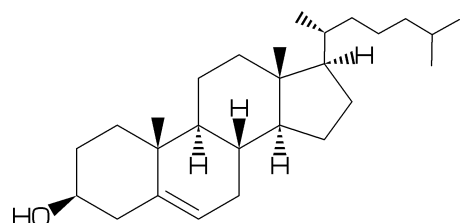
No.36 Example(1) Ampicillin

<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



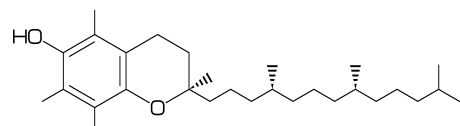
No.37 Example(2) Cholesterol

<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,! ,



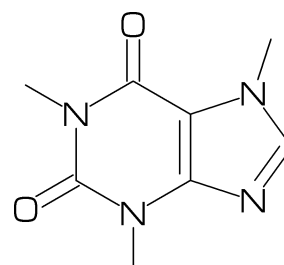
No.38 Example(3) alfa-Tocopherol

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



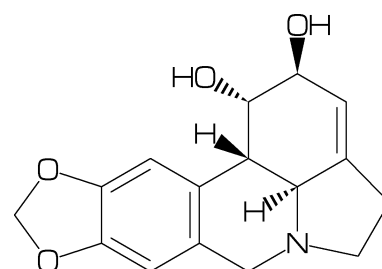
No.39 Example(4) Caffeine

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



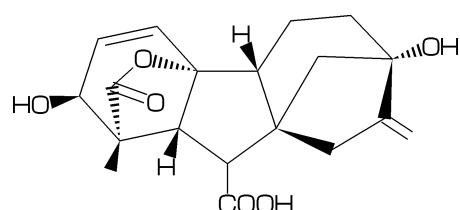
No.40 Example(5) Lycorine

<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.41 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

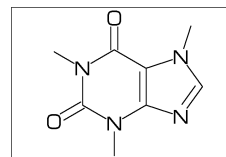


No.42 Font size

```

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

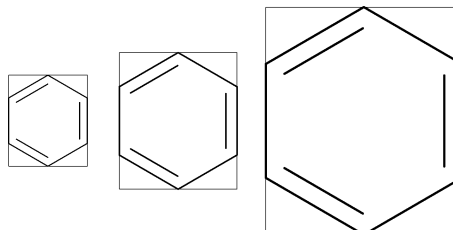
```

**No.43 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:=0.25;
MCd(1,1)( 1, .5)(<30,Ph)

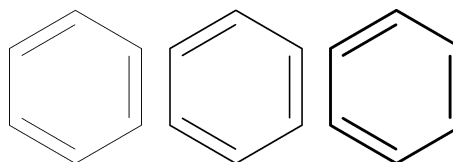
```

**No.44 Ratio thickness/bond length**

```

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

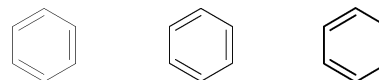
```

**No.45 Offset thickness of bond**

```

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

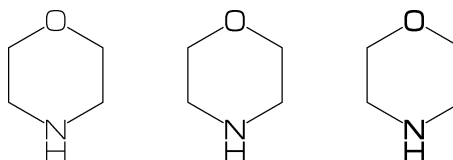
```

**No.46 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; %<==
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)

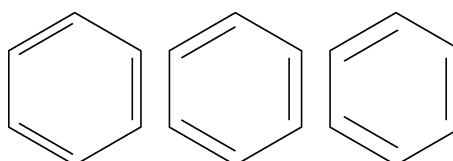
```

**No.47 Ratio bondgap/bond length**

```

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

```



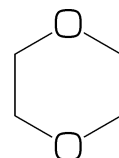
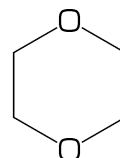
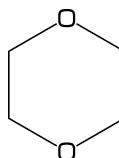
No.48 Offset of doublebond gap

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



No.49 Ratio atom/bond length

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



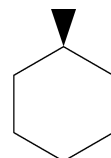
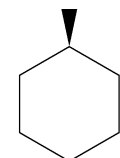
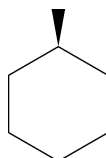
No.50 Offset of atom width

```
beginfont() offset_atom#:=0.0pt#;  
MCd(1,.3)(0, .5)(<30,Ph,@(2,4,6)N) endfont  
beginfont() offset_atom#:=0.8pt#; %<==  
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.51 Ratio wedge/bond length

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



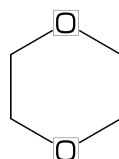
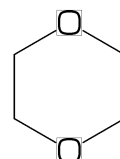
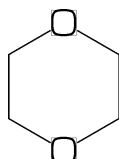
No.52 Offset of wedge width

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



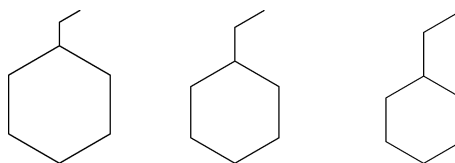
No.53 Ratio font atom gap/atom length

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

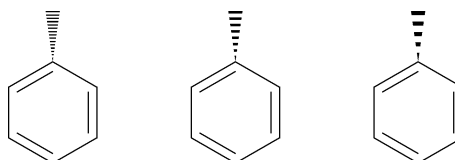


No.54 Ratio chain/ring length

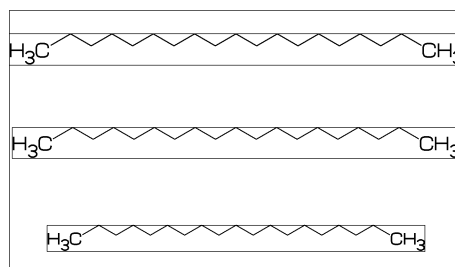
```
ratio_chain_ring:= 0.4;
MCd(1,.6)(0, .5)(<30,?6,5:/Et)
ratio_chain_ring:= 0.66; %<==
MCd(1,.6)(.5,.5)(<30,?6,5:/Et)
ratio_chain_ring:= 1.0;
MCd(1,.6)(1, .5)(<30,?6,5:/Et)
```

**No.55 Ratio zebra gap/bond length**

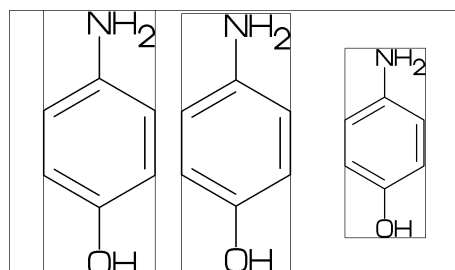
```
ratio_zebragap_bond:=0.06;
MCd(1,.6)(0, .5)(<30,Ph,5:/*Me'1)
ratio_zebragap_bond:=0.12; %<==
MCd(1,.6)(.5,.5)(<30,Ph,5:/*Me'1)
ratio_zebragap_bond:=0.20;
MCd(1,.6)(1, .5)(<30,Ph,5:/*Me'1)
```

**No.56 Margin left and right**

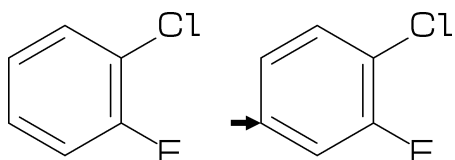
```
margin_left_right:=0mm;
MCd(1,1)(0.5,0.9)(<30,CH3,!0,!17,CH3)
margin_left_right:=0.4mm; %<==
MCd(1,1)(0.5,0.5)(<30,CH3,!0,!17,CH3)
margin_left_right:=5mm;
MCd(1,1)(0.5,0.1)(<30,CH3,!0,!17,CH3)
```

**No.57 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; %<==
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.58 Switch Start Vector**

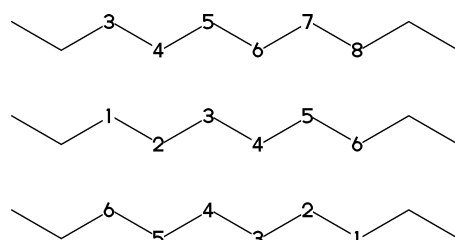
```
MCd(1,.6)( 0,0.5)(<30,Ph,4:/Cl,3:/F)
sw_start_vector:=1;
MCd(1,.6)( 1,0.5)(<30,Ph,4:/Cl,3:/F)
```

**No.59 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.60 Switch Numbering bond

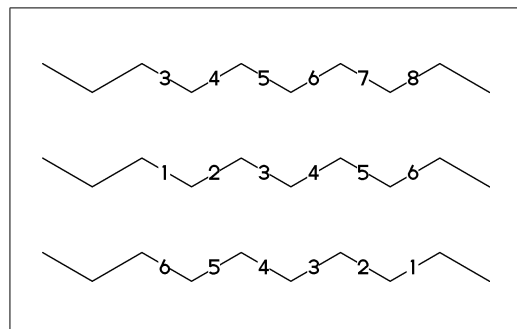
```

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

```

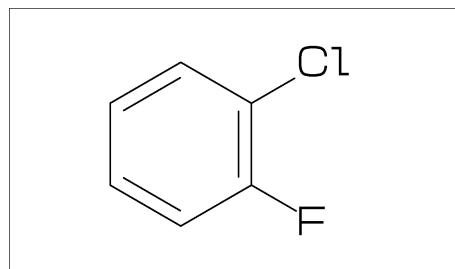
**No.61 Switch font frame**

```

sw_font_frame:=1;

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

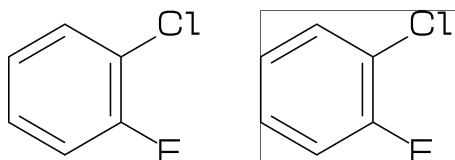
```

**No.62 Switch molecular frame**

```

MCd(1,.6)(0,0.5)(<30,Ph,4:/Cl,3:/F)
sw_mol_frame:=1;
MCd(1,.6)(1,0.5)(<30,Ph,4:/Cl,3:/F)

```

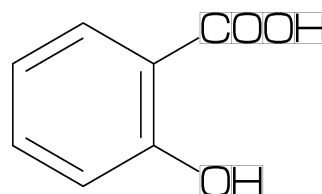
**No.63 Switch atom frame**

```

sw_atom_frame:=1;

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

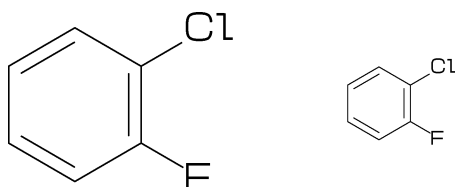
```

**No.64 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)

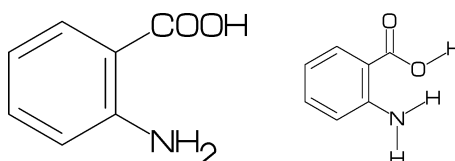
```

**No.65 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)

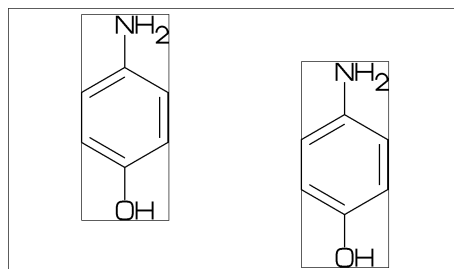
```



No.66 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

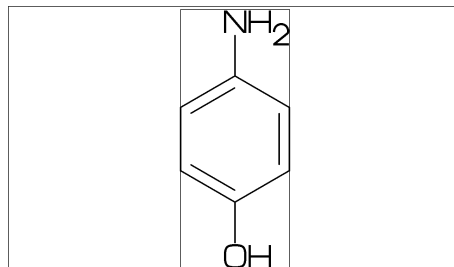
MCd(1,0.8)(0.2,0.9)(<30,Ph,2:/OH,5:/NH2)
MCd(1,0.8)(0.8,0.1)(<30,Ph,2:/OH,5:/NH2)
```

**No.67 Function MCf (fit draw)**

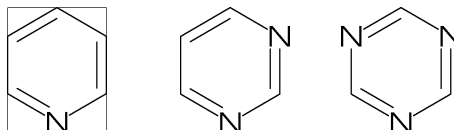
```
MCf(...) : MCd(1,1)(0.5,0.5)(...)

sw_font_frame:=1;  sw_mol_frame:=1;

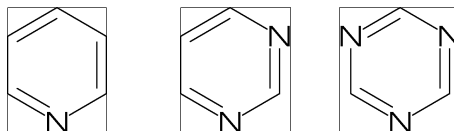
MCf(<30,Ph,2:/OH,5:/NH2)
```

**No.68 Local setting**

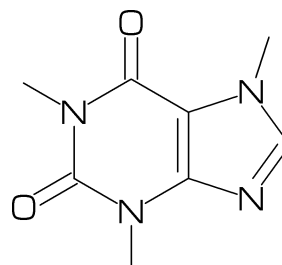
```
beginfont("NO:1")
  sw_mol_frame:=1; % <== Local setting
  MCd(1,.5)(0.0,0.5)(<30,Ph,@(2)N) endfont
beginfont("NO:2")
  MCd(1,.5)(0.5,0.5)(<30,Ph,@(2,4)N) endfont
beginfont("NO:3")
  MCd(1,.5)(1.0,0.5)(<30,Ph,@(2,4,6)N) endfont
```

**No.69 Global setting**

```
sw_mol_frame:=1; % <== Global setting
beginfont("NO:1")
  MCd(1,.5)(0.0,0.5)(<30,Ph,@(2)N) endfont
beginfont("NO:2")
  MCd(1,.5)(0.5,0.5)(<30,Ph,@(2,4)N) endfont
beginfont("NO:3")
  MCd(1,.5)(1.0,0.5)(<30,Ph,@(2,4,6)N) endfont
```

**No.70 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.71 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
```

