

Molecular Coding Format manual

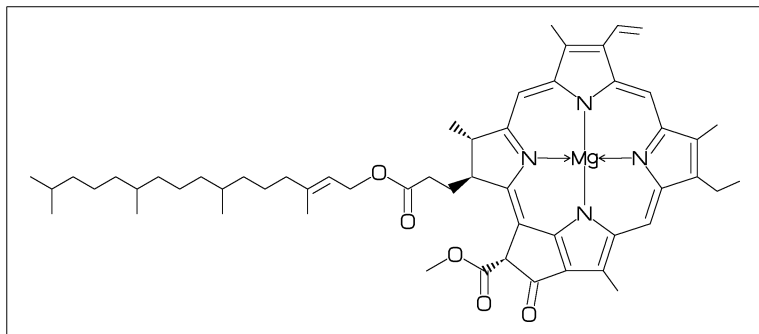
Author : Akira Yamaji Date : April 2, 2016
Located at : <http://www.ctan.org/pkg/mcf2graph>

Molecular Coding Format(MCF) is new linear notation represent chemical structure diagrams. 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).

(Molecular definition file)

```
%-----
input mcf2graph.mf;                                % input macro
%-----
sw_auxout:=1;          % aux(information) file output on > Gloval setting
sw_numberA:=0;         % numbering atom off              >
sw_numberB:=0;         % numbering bond off              >
sw_expand:=0;          % substituent expand mode off     >
sw_start_vector:=0;    % start vector output off         >
sw_font_frame:=0;      % font frame off                  >
font_wd#:=60mm#;       % font width                    >
font_ht#:=40mm#;       % font height                    >
var3:="calc_weight";  tag3:="MWc";                     > AUX file table
var4:="calc_formula"; tag4:="FMc";                     >
outputformat:="png";  hppp:=vppp:=0.1;                 > PNG output
outputtemplate:="%j-%3c.png";                          >
%-----
beginfont("N0:1","EN:Chlorophyll a","MW:893.49") % begin font(information)
  sw_font_frame:=1;    % font frame on                  >
  font_wd#:=120mm#;    % font width set                  > Local setting
  font_ht#:=80mm#;     % font height set                 >
%-----
Mcf(                                                    % begin MCF
  <54,{, '1,?5,$(2,5)d,4:N,3\,54~d1,                  %
  |,?5,$(2,4)d,5:N,                                     %
  -2\,54~d1,|,?5,2=d,5:N,-2\~d1,54,                   %
  |,?5,5=d,5:N,-2\~d1,&#5,                             %
  -1*,24,/*COOMe~15,72,//0,&#1,},                     %
  4\ '1.48,Mg,&17,-1*,&11~vb,-1*,&23~vb,               %
  @ (2,9,15,20~zf)/Me,8:/Et,14\,!~dr,                 %
  21*,-6~wf,!2,//0,!0,!2,!~d1,                        %
  |,!13,@(1,5,9,13)/Me,                                %
)                                                         % end MCF
endfont                                                  % end font
%-----
bye
```

(Molecular structure diagram output)



(Molecular information output)

F:mcf_man_soc ,C:0 ,MWc:893.48962 ,FMc:C55H72MgN4O5
 ,NO:1 ,EN:Chlorophyll a ,MW:893.49

'filename'-info.aux : for use in T_EX, it takes over filename, char number, molecular information,etc.
F:filename C:char number,MWc:molecular weight calculated, FMc:molecular formula calculated
NO:serial number, EN:english name, MW:molecular weight from literature data

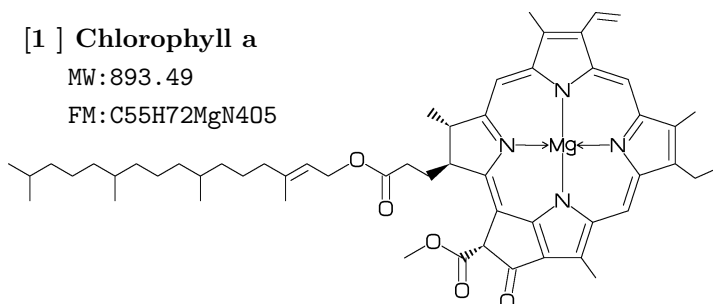
(LaTeX file example)

```
%-----  
\documentclass[a4paper]{article}  
\usepackage{graphicx}  
\pagestyle{empty}  
\makeatletter%  
%-----  
\def\mol@sel#1{%  
\if#1\empty\relax\else%  
  \edef\@fst{\expandafter\@fst@param#1;}%  
  \edef\@sec{\expandafter\@sec@param#1;}%  
  \ifx\@fst\F\edef\MOLfile{\@sec}\fi%  
  \ifx\@fst\C\edef\MOLchar{\@sec}\fi%  
  \ifx\@fst\EN\edef\MOLnameE{\@sec}\fi%  
  \ifx\@fst\NO\edef\MOLnum{\@sec}\fi%  
  \ifx\@fst\MW\edef\MOLmw{\@sec}\fi%  
  \ifx\@fst\FMc\edef\CALfm{\@sec}\fi%  
\fi}%  
\def\F{F}\def\C{C}\def\EN{EN}\def\NO{NO}\def\MW{MW}\def\FMc{FMc}%  
\def\@fst@param#1:#2;{#1}%  
\def\@sec@param#1:#2;{#2}%  
\def\put@char{%  
  \begin{picture}(120,45)%  
    \put(10,35){\bf [\MOLnum] \MOLnameE}%  
    \put(16,30){\sf MW:\MOLmw}%  
    \put(16,25){\sf FM:\CALfm}%  
    \put(0,0){\font\@strufont=\MOLfile\relax%  
      \hbox{\@strufont\char\MOLchar}}%  
  \end{picture}%  
}  
%-----  
\def\INFO#1{\@for\@temp:=#1\do{\mol@sel\@temp}\put@char}%  
\makeatother  
%-----  
\begin{document}  
\unitlength=1mm%  
\INFO{F:mcf_man_soc ,C:0 ,MWc:893.48962 ,FMc:C55H72MgN4O5%  
  ,NO:1 ,EN:Chlorophyll a ,MW:893.49}%  
\end{document}  
%-----
```

[1] Chlorophyll a

MW: 893.49

FM: C55H72MgN4O5

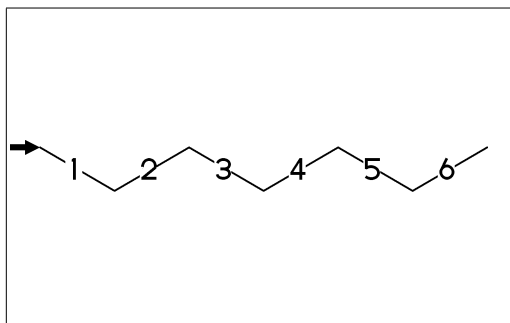


No.1 Chain(1)

plus(+):anticlockwise,minus(-):clockwise

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

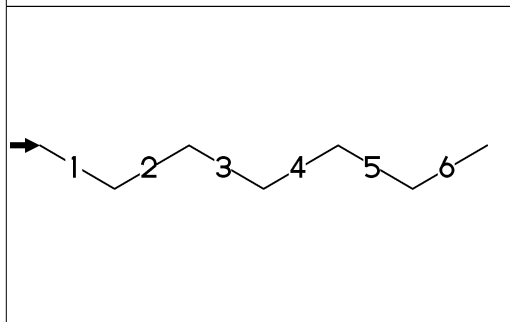
** bold arrow is default angle and position



No.2 Chain(2)

! : take value(60 or -60) depend on
current angle and enviroment

<30,!,,!,!,!,!,!

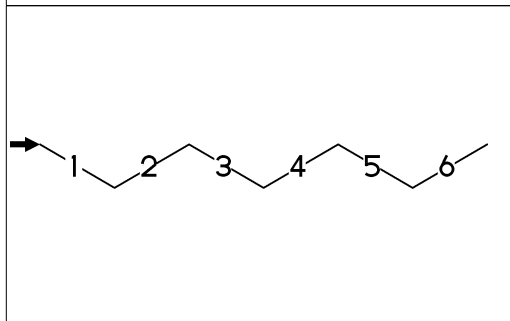


No.3 Chain(3)

!6 : !,!,!,!,!,!,!

<30,!6

** !n(0<=n<=20)

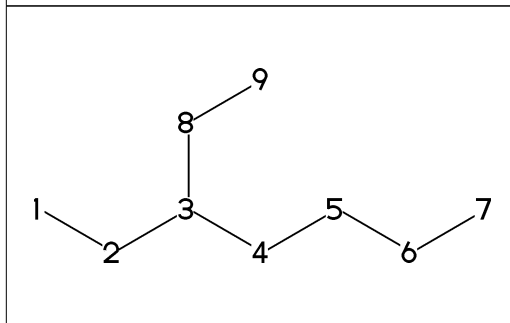


No.4 Jump to atom

3* : Jump to A3

<30,!6,3*,0,!

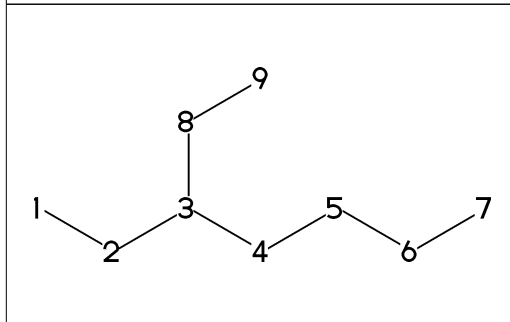
** An(-999<=n<=4095): atom number



No.5 Jump to atom and branch bond

3\ : 3*,0

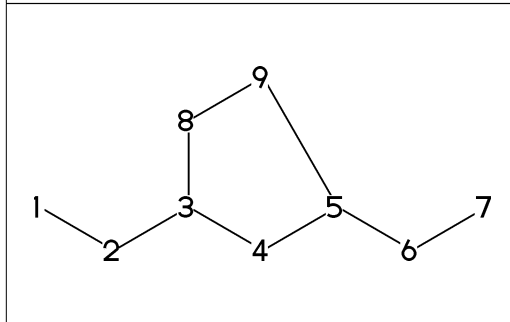
<30,!6,3\,!



No.6 Connect bond

&5 : Connect to A5

<30,!6,3\,-60,&5

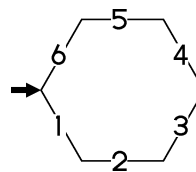


No.7 Ring

six membered ring

?6

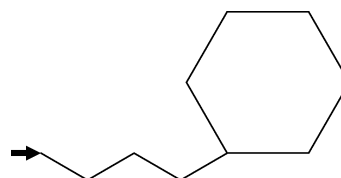
```
** ?6 : <-120,60,60,60,60,60,&1
** ?n(3<=n<=20)
```



No.8 Rotate current angle

<angle : rotate current angle

<30,!4,<30,?6



No.9 Change bond type (1)

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

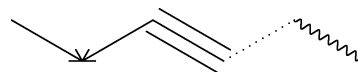
<30,!~dm,!~dl,!~dr,!~wf,!~wb,!~zf,!~zb



No.10 Change bond type (2)

Bn=bond type : change bond type at Bn
vf : vector forward, vb : vector backward
tm : triple, dt : dotted, ww : wave

<30,!5,1=vf,2=vb,3=tm,4=dt,5=ww

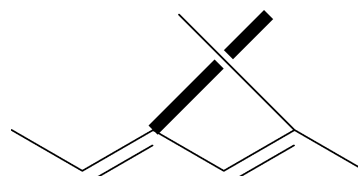


No.11 Change bond type (3)

bd : broad single ov : over line
\$(2,4)dr : 2=dr,4=dr

<30,!5,\$(2,4)dr,
@(3~bd^-45'2,5~ov^45'2)/Me

** 3~bd^-45'2 : ~~bd,^^-45,'2,3

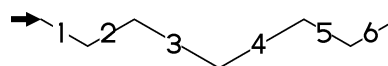


No.12 Change bond length (1)

(!,!n,?n)'length : change length of !,!n,?n

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

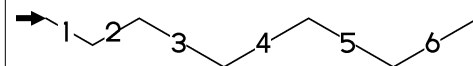
** !2'1.2 : '1.2,!2



No.13 Change bond length (2)

‘length : change all bond length after

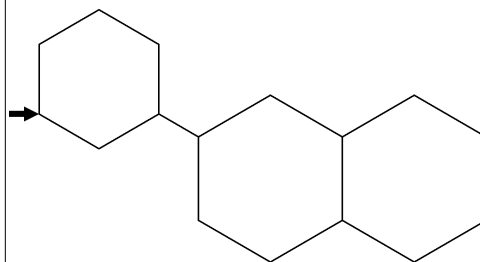
<30,!2,‘1.2,!4



No.14 Change ring length

?n'length : change ring length

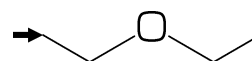
<30,?6,3\,?6'1.2,11=?6



No.15 Change atom (1)

Insert hetero atom

<30,!2,0,!2

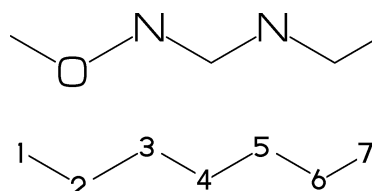


No.16 Change atom (2)

2:0 : change A2 C to O

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

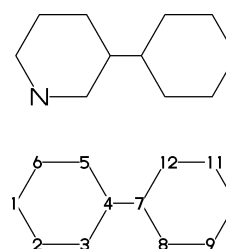
<30,!6,2:0,@(3,5)N



No.17 Change atom (3)

2:N : change A2 C to N

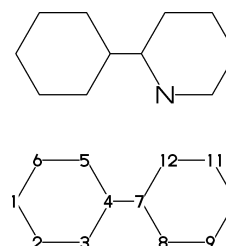
?6,4\,?6,2:N



No.18 Change atom (brock address 1)

| : divide brock

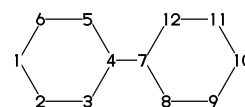
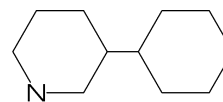
?6,4\,|,?6,2:N,



No.19 Change atom (brock address 2)

|| : reset brock address

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

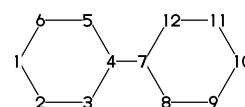
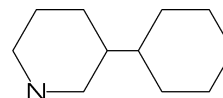


No.20 Change atom (absolute address)

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

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

** #n : (1<=n<=3095)

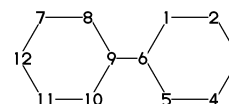
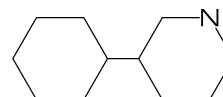


No.21 Change atom (relative address)

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

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

** -n : (1<=n<=999)

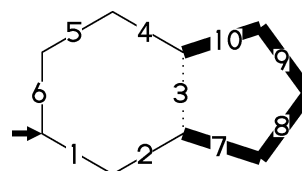


No.22 Fuse ring (attached 1 bond)

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

?6,3=?5

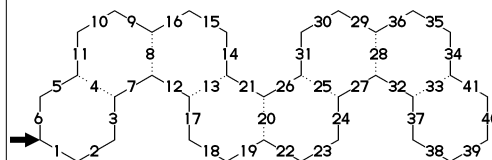
** Bn(n:-999<=n<=4095): bond number



No.23 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.24 Fuse ring (attached 2 bond)

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

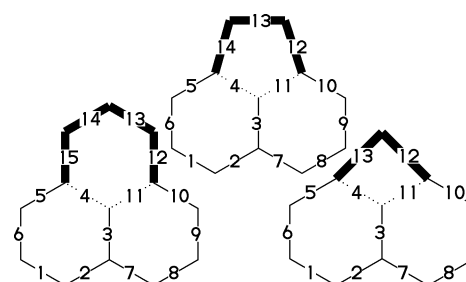
(4,11)=?5[3] : fuse 3/5 ring to B11..B4

(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])

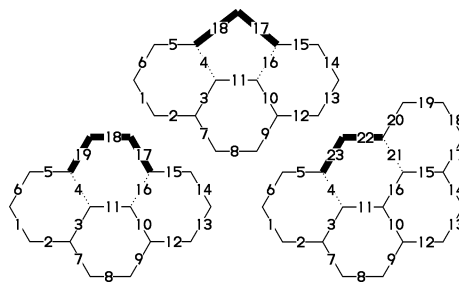
MCd(1,.6)(1,0)(<30,?6,3=?6,(11,4)=?4[2])



No.25 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
 (21,4)=?6[2] : fuse 2/6 ring to B21..B4

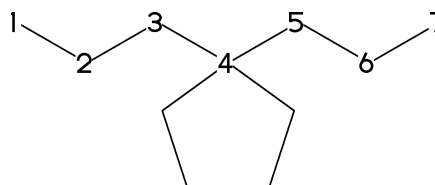
MCd(1,.55)(0,0)(?6,\$(3,10)?6,(16,4)=?6[3])
 MCd(1,.55)(.5,1)(?6,\$(3,10)?6,(16,4)=?5[2])
 MCd(1,.68)(1, 0)(?6,\$(3,10,15)?6,(21,4)=?6[2])

**No.26 Spiro ring**

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

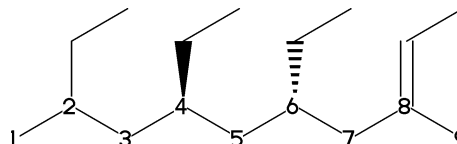
<30,!6,4*,?5

An* : jump to An

**No.27 Branch bond (1)**

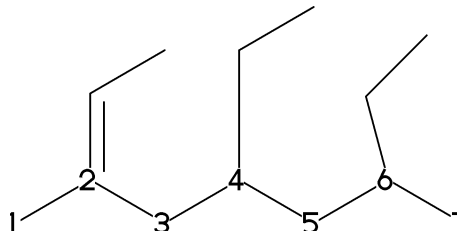
2\ : 2*,0 4*\ : 4*,0~wf
 6* : 6*,0~zf 8\\ : 8*,0~dm

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

**No.28 Branch bond (2)**

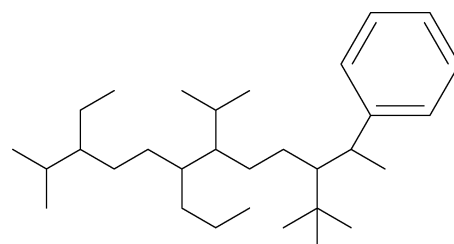
2~dr : 2*,0~dr
 4\'1.5 : 4*,0\'1.5
 6^15 : 6*,0^15

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

**No.29 Insert substituent(1)**

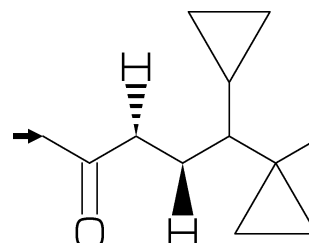
MCf(<30,
 !,/Me,!/Et,!3,/Pr,!/iPr,!3,/tBu,!/Ph^-30,!)

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

**No.30 Insert substituent(2)**

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

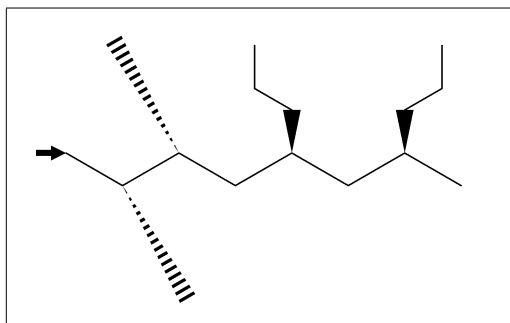
MCf(<30,!//0,!/*H,!/*H,!/?3,!,**?3,!)



No.31 Insert substituent(3)

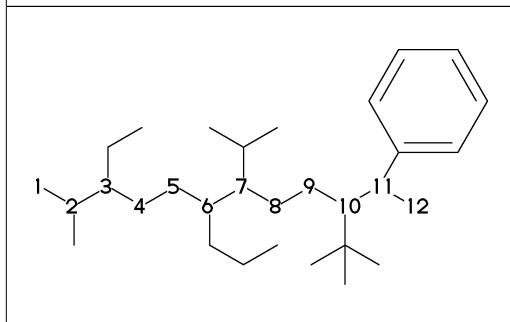
~,^,','> : change type,angle,length,enviroment of substituent

```
MCf(<30,'1,
    !,/Me~zf'2^30,!,/Me~zf'2^30,
    !2,*/Pr>lr,!2,*/Pr>r1,!)
```



No.32 Add substituent(1)

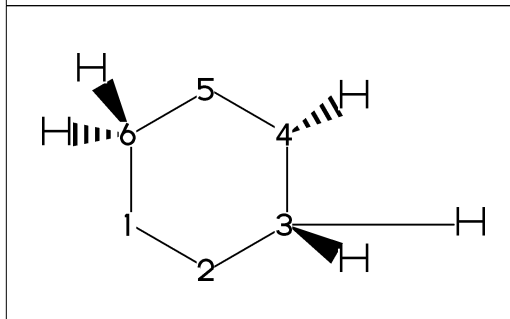
```
sw_numberA:=1; numberA_end:=12;
MCf(<30,!11,
    2:/Me,3:/Et,6:/Pr,7:/iPr,
    10:/tBu,11:/Ph^30)
```



No.33 Add substituent(2)

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

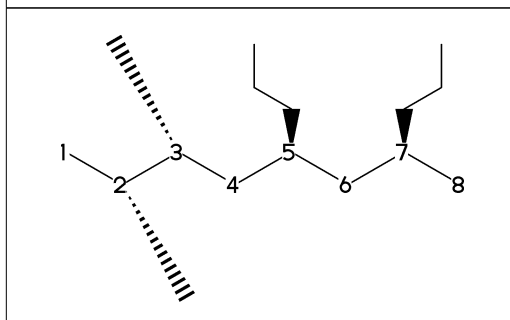
```
MCf(<30,?6,
    @(3'2^30,3~wf,4~zf,6~wf^30,6~zf^30)/H)
```



No.34 Add substituent(3)

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

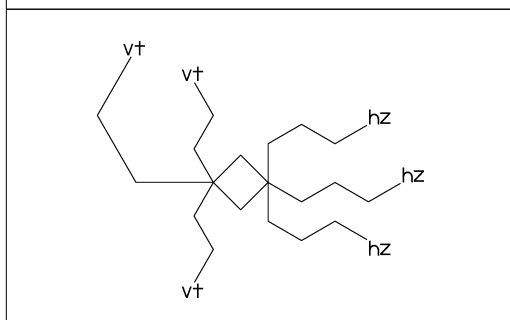
```
MCF(<30,!7'1,
    @(2,3)/Me'2^30,5:*/Pr>lr,7:*/Pr>r1)
```



No.35 Chain stretch direction environment (1)

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

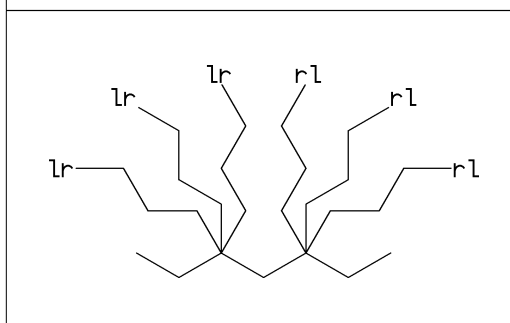
```
?4,
    @(3^-90,3^-30,3^90)/'(!3,"{hz}")>hz,
    @(1^-60,1'2,1^60)/'(!2,"{vt}")>vt
```



No.36 Chain stretch direction environment (2)

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

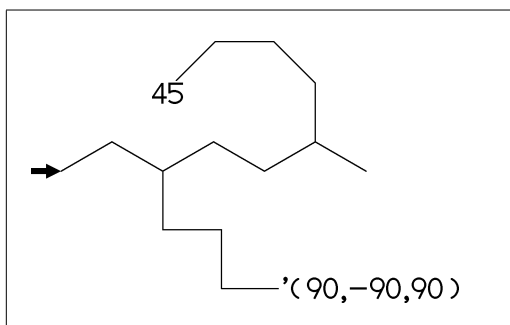
```
<30,!6,
    @(3^-30,3,3^30)/'(!3,"{lr}")>lr,
    @(5^-30,5,5^30)/'(!3,"{r1}")>r1
```



No.37 Chain stretch direction environment (3)

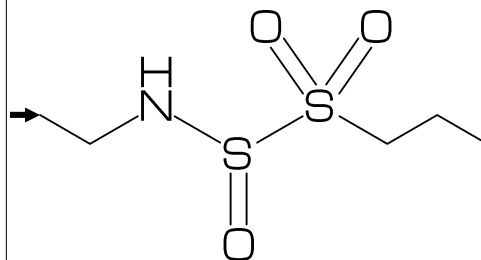
>45 : fixed angle environment
 >'(-90,90,-90) : multi angle environment

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

**No.38 Change atom and Substituent**

NH,S0,S00 : inset hetero atom and substituent simultaneously

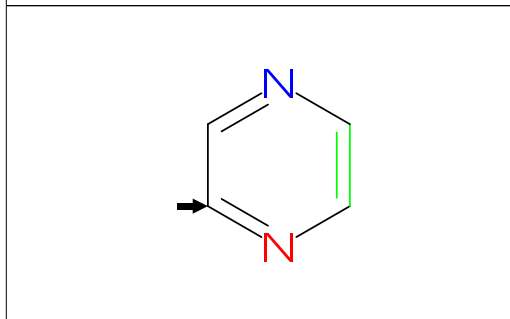
<30,!2,NH,! ,S0,! ,S00,!3

**No.39 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

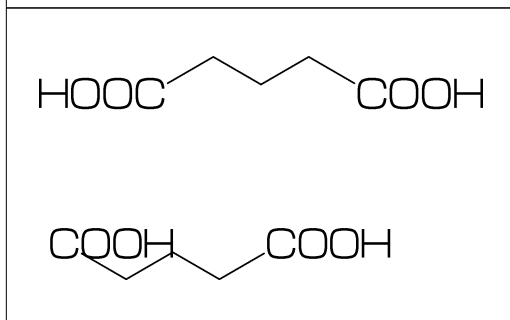
** METAFONT ignore color command

**No.40 Chain start multiple characters**

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

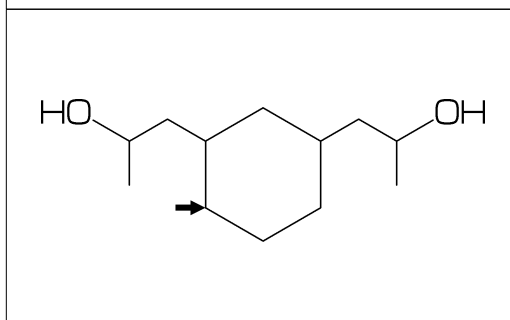
MCd(1,1)(0 ,0.9)(<30,COOH,!0,!3,COOH)

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

**No.41 User definition**

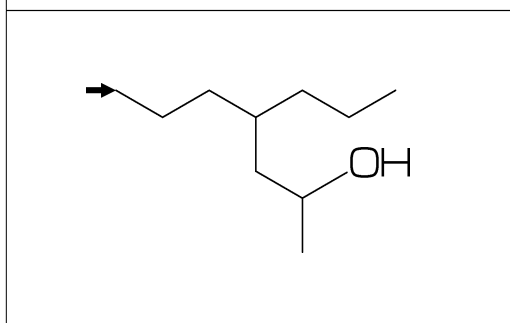
iBuOH : user defined substructure

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

**No.42 Inline definition**

Insert user defined substructure

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

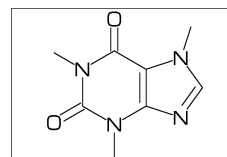


No.43 Font size

```

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

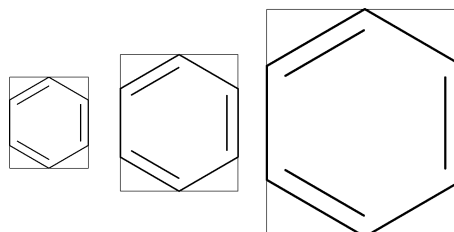
```

**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:=0.25;
MCd(1,1)( 1, .5)(<30,Ph)

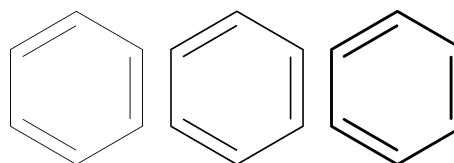
```

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

```

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

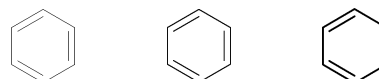
```

**No.46 Offset thickness of bond**

```

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

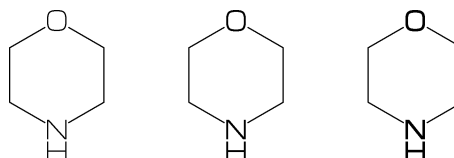
```

**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; %<==
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)

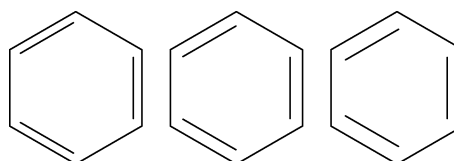
```

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

```

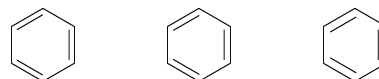
ratio_bondgap_bond:= 0.10;
MCd(1,.6)(0, .5)(<30,Ph)
ratio_bondgap_bond:= 0.15; %<==
MCd(1,.6)(.5,.5)(<30,Ph)
ratio_bondgap_bond:= 0.20;
MCd(1,.6)(1, .5)(<30,Ph)

```

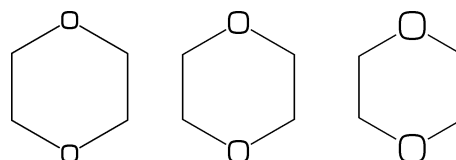


No.49 Offset of doublebond gap

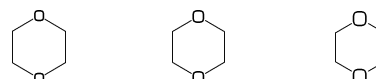
```
beginfont() offset_bond_gap#:=0.0pt#;  
MCd(1,.3)(0, .5)(<30,Ph) endfont  
beginfont() offset_bond_gap#:=0.3pt#; %<==  
MCd(1,.3)(.5,.5)(<30,Ph) endfont  
beginfont() offset_bond_gap#:=1.0pt#;  
MCd(1,.3)(1, .5)(<30,Ph) endfont
```

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

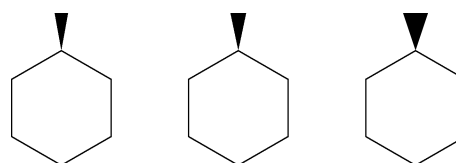
```
ratio_atom_bond:= 0.25;  
MCd(1,.6)(0, .5)(<30,?6,@(2,5)O)  
ratio_atom_bond:= 0.36; %<==  
MCd(1,.6)(.5,.5)(<30,?6,@(2,5)O)  
ratio_atom_bond:= 0.45;  
MCd(1,.6)(1, .5)(<30,?6,@(2,5)O)
```

**No.51 Offset of atom width**

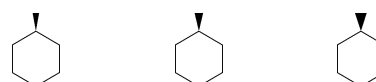
```
beginfont() offset_atom#:=0.0pt#;  
MCd(1,.3)(0, .5)(<30,Ph,@(2,4,6)N) endfont  
beginfont() offset_atom#:=0.8pt#; %<==  
MCd(1,.3)(.5,.5)(<30,Ph,@(2,4,6)N) endfont  
beginfont() offset_atom#:=2.0pt#;  
MCd(1,.3)(1, .5)(<30,Ph,@(2,4,6)N) endfont
```

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

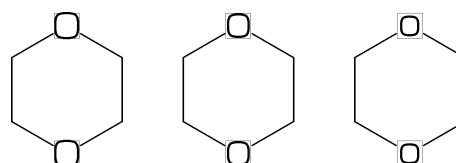
```
ratio_wedge_bond:=0.10;  
MCd(1,.6)(0, .5)(<30,?6,5:*/Me)  
ratio_wedge_bond:=0.12; %<==  
MCd(1,.6)(.5,.5)(<30,?6,5:*/Me)  
ratio_wedge_bond:=0.20;;  
MCd(1,.6)(1, .5)(<30,?6,5:*/Me)
```

**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#; %<==  
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
```

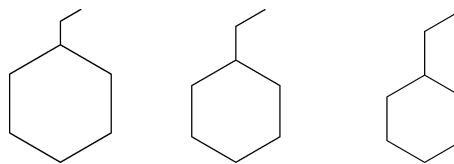
**No.54 Ratio font atom gap/atom length**

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



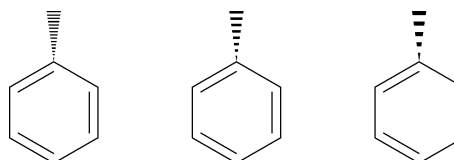
No.55 Ratio chain/ring length

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



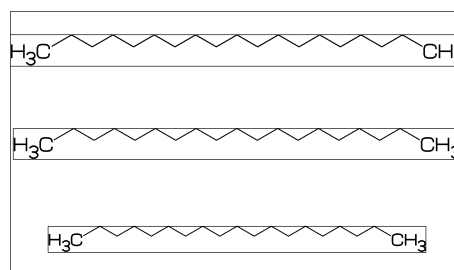
No.56 Ratio zebra gap/bond length

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



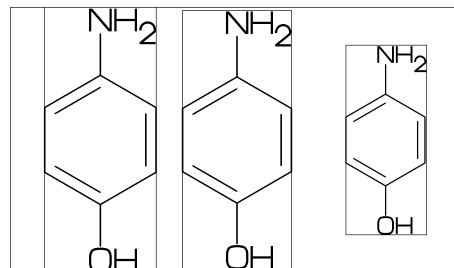
No.57 Margin left and right

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

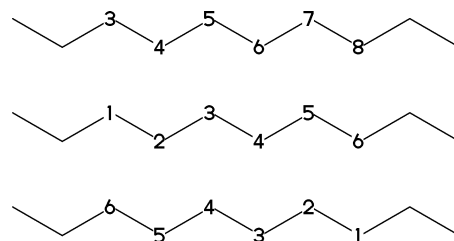


No.59 Switch numbering atom

```
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
```

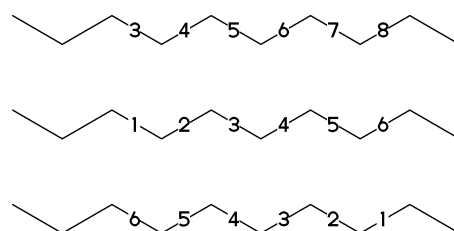


No.60 Switch numbering bond

```
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)

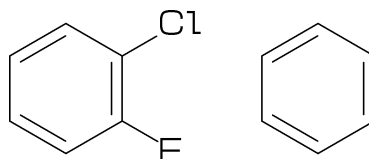
** default: numberB start=1 numberB_end=4095
```



No.61 Switch substituent off

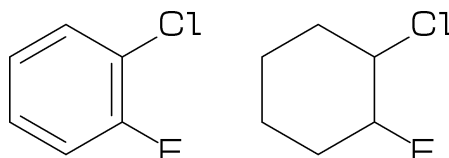
```
MCd(1,.6)( 0,0.5)(<30,Ph,4:/Cl,3:/F)
sw_subst_off:=1;
MCd(1,.6)( 1,0.5)(<30,Ph,4:/Cl,3:/F)
```

```
** default: sw_subst_off=0
```

**No.62 Switch all bond single**

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

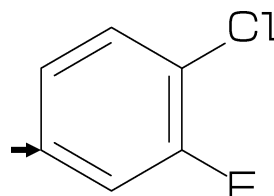
```
** default: sw_bond_single=0
```

**No.63 Switch start vector**

```
sw_start_vector:=1;
```

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

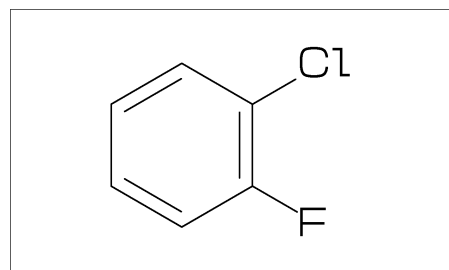
```
** default: sw_start_vector=0
```

**No.64 Switch font frame**

```
sw_font_frame:=1;
```

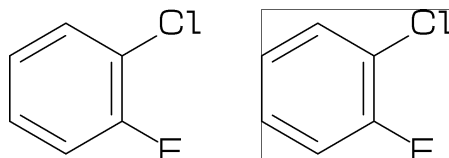
```
MCf(<30,Ph,4:/Cl,3:/F)
```

```
** default: sw_font_frame=0
```

**No.65 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)
```

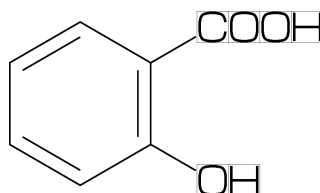
```
** default: sw_mol_frame=0
```

**No.66 Switch atom frame**

```
sw_atom_frame:=1;
```

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

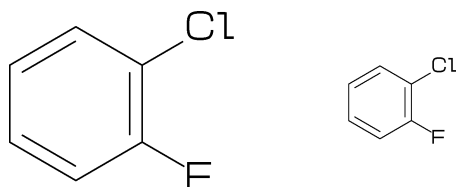
```
** default: sw_atom_frame=0
```



No.67 Switch solid mode

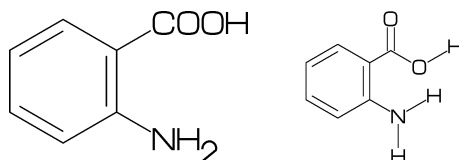
```
MCd(1,.8)( 0,0.5)(<30,Ph,4:/Cl,3:/F)
sw_solid:=1; ratio_bond_width:=0.08;
MCd(1,.8)( 1,0.5)(<30,Ph,4:/Cl,3:/F)
```

```
** default: sw_solid=0
```

**No.68 Switch Expand**

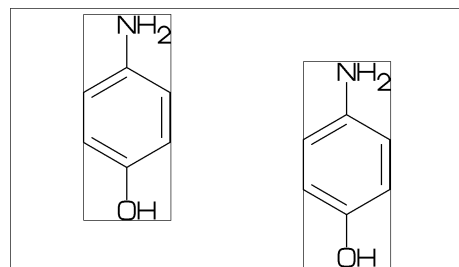
```
MCd(1,.6)(0,0.5)(<30,Ph,4:/COOH,3:/NH2)
sw_expand:=1;
MCd(1,.6)(1,0.5)(<30,Ph,4:/COOH,3:/NH2)
```

```
** default: sw_expand=0
```

**No.69 Function MCd (draw)**

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

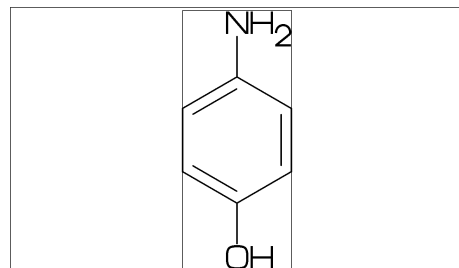
```
MCd(1,0.8)(0.2,0.9)(<30,Ph,2:/OH,5:/NH2)
MCd(1,0.8)(0.8,0.1)(<30,Ph,2:/OH,5:/NH2)
```

**No.70 Function MCf (fit draw)**

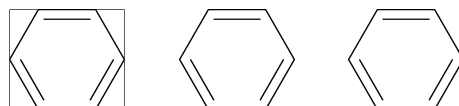
```
MCf(...) : MCd(1,1)(0.5,0.5)(...)
```

```
sw_font_frame:=1; sw_mol_frame:=1;
```

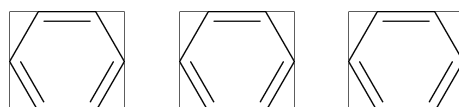
```
MCf(<30,Ph,2:/OH,5:/NH2)
```

**No.71 Local setting**

```
beginfont()
sw_mol_frame:=1; % <== Local setting
MCd(1,.4)( 0,.5)(Ph)
endfont
beginfont() MCd(1,.4)(.5,.5)(Ph) endfont
beginfont() MCd(1,.4)( 1,.5)(Ph) endfont
```

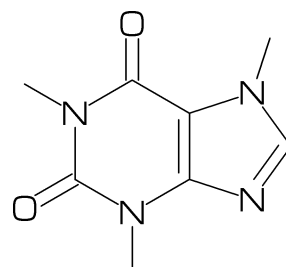
**No.72 Global setting**

```
sw_mol_frame:=1; % <== Global setting
beginfont() MCd(1,.4)( 0,.5)(Ph) endfont
beginfont() MCd(1,.4)(.5,.5)(Ph) endfont
beginfont() MCd(1,.4)( 1,.5)(Ph) endfont
```

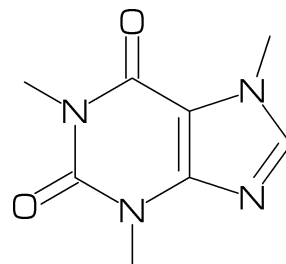


No.73 Output molecular information

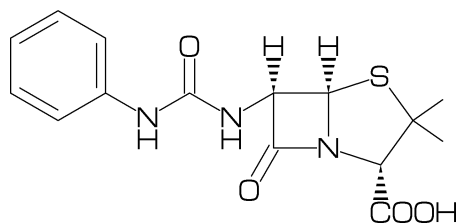
```
var3:="calc_weight"; tag3:="MWc";
var4:="calc_formula"; tag4:="FMc";
%% Output to mcf_man_soc-info.aux %%
F:mcf_man_soc,C:82,MWc:194.19174,FMc:C8H10N4O2
MWc:calculated molecular weight
FMc:calculated molecular formula
```

**No.74 Output additional information**

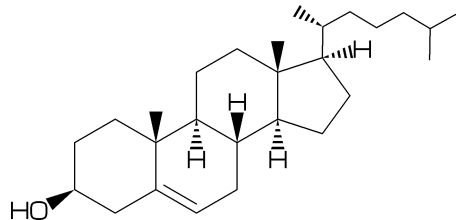
```
beginfont("EN:Caffeine","CAS:58-08-2")
MCf(...) endfont
%% Output to mcf_man_soc-info.aux %%
F:mcf_man_soc ,C:83 ,EN:Caffeine ,CAS:58-08-2
*F:filename *C:char number EN:molecular name
CAS:CAS number *:default output
```

**No.75 Example(1) Ampicillin**

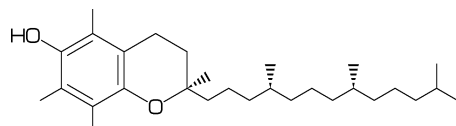
```
<45,?4,2:N,2=?5,-1:S,
@(3^45,4^-45)/*H,1://0^15,
5:/*COOH^-18,@(6^35,6^-35)/Me,
4\^75,NH,!://0,! ,NH,! ,Ph
```

**No.76 Example(2) Cholesterol**

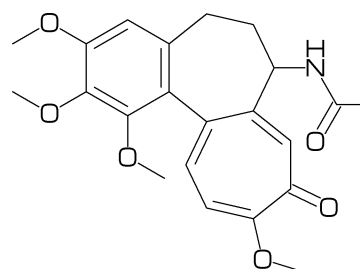
```
<30,?6,$(-4,-2)?6,-4=?5,7=d1,
1:*/OH,@(4,12)*/Me^60,9:*/H^60,
10:*/H^180,@(11,-1)*/H^-60,
-1\^17,/*Me,!4,/Me,! ,
```

**No.77 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
```

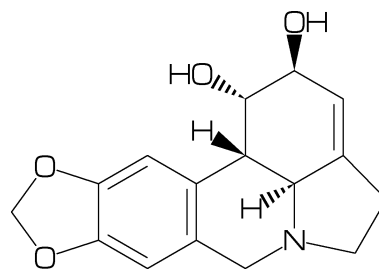
**No.78 Example(4) Colchicine**

```
<30,Ph,@(1,2,6)/OMe,l,-4=?7,
l,-5=?7,$(-1,-4,-6)d1,-2://0,-3:/OMe,
#9\,NH,! ,//0,! ,
```



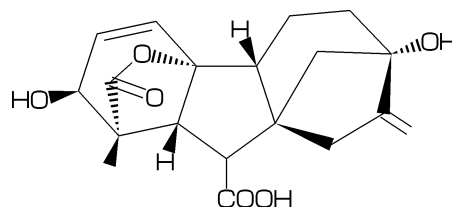
No.79 Example(5) Lycorine

<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



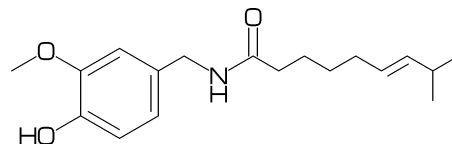
No.80 Example(6) Gibberellin

<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



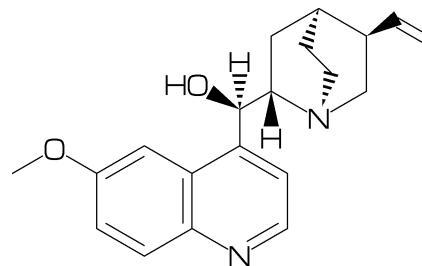
No.81 Example(7) Capsaicin

<30,Ph,
1:/OH,6:/OMe,4\,!,NH,!,//O,
|,!8,-3=dr,-1:/Me



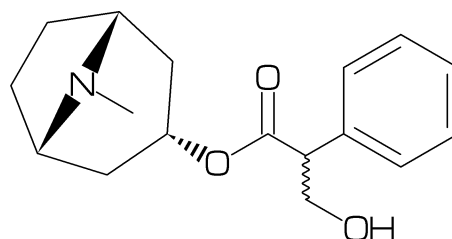
No.82 Example(8) Quinine

<30,Ph,3=Ph,7:N,6:/OMe,
10\,*/OH,/H~zf^-60,!,
|,?6,2:N,1:*/H^60,
4*\,!~dr,
2*,165~zf,60,&5~zb



No.83 Example(9) Atoropin

<-30,0,!,//O,!,!,Ph,
#1\~zb^-120,
|,?7^1.1,6*\^190^1.25,N,/Me,&3~wb,
#3\~wv,!,OH



No.84 Example(10) Paclitaxel

?6,5=d,3*,{,'^1,36,45,45,45,45,},,
-4=?6,-4=?4,-1=wb,-3=wf,-1:O,||,
@(4^35,4^-35,6)/Me,@(3^-60,15)*/OH,
8:/*H^-60,9:*/Me^60,10://O,
1\,O,!,//O,!,*/OH,!,/Ph,
60~wf,NH,-60,//O,60,Ph,
7*,0,-45,//O,60,Ph,11*\,0,-60,//O,60,
12*^-15,0,60,//O,-60

