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 60 or -60 depend on current angle and environment

!6

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

No.3  Ring

six membered ring

?6

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

No.4  Rotate current angle

<angle: rotate current angle

<30,14,<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: change bond type at Bn
vf: vector forward, vb: vector backward,
tm: triple, wv: waved, bd: broad single, ov: over line

<30,19,1=vf,2=vb,3=tm,4=dt,5=wv,
@(?bd=45’2,9’ov45’2)/Me
**No.7** Change bond length (1)

Bn'length : change bond length at Bn

<30,12,12'1.2,12

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

'length : change all bond length after

<30,12,'1.2,14

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

?n'length : change ring length

<30,76,3\,|,76'1.2,4=76

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

Insert hetero atom

<30,12,0,12

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

2:O : change A2 C to O

@[3,5]N : change A3,A5 C to N

<30,16,2:0,@[3,5]N

An(n:numeric): atom number

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

2:N : change A2 C to N

?6,4\,?6,2:N
No.13  Change atom (brock address)
2:N : change A2(brock address) C to N
\(?6,4\backslash,1,?6,2:N\)
| : divide brock

No.14  Change atom (absolute address)
#2:N : change A#2 C to N
\(?6,4\backslash,1,?6,#2:N\)

No.15  Change atom (relative address)
-2:N : change A(-2) C to N
\(?6,4\backslash,?6,?-2:N\)

No.16  Fuse ring (attached 1 bond)
\(?6,3=?5\) : fuse ?5 at B3
\(?6,3=?5\)

No.17  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.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
<30,16,4*,?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(<30,18,2\,!,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(<-30,16,2\-dr,!,4\-1.5,!,6\-15,-60)

No.23  Insert substituent (1)

Mcf(<30,!
,!/Me,!/Et,!/Pr,!/iPr,!/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

Mcf(<30,!/0,!/H,!/H,!/3,!,**3,!)
**No.25** Insert substituent(3)

\[~,^,`,> : \text{change type, angle, length, environment of substituent}\]

\[\text{MCf}(<30, !1', /Me^\sim zf '2^\sim 30, !1', /Me^\sim zf '2^\sim 30, !2'1, */Pr>lr,!2'1, */Pr>rl, !'1)\]

**No.26** Add substituent(1)

\[\text{sw\_numberA}:=1; \text{numberA\_end}:=\_\text{skeletonA\_end};\]

\[\text{MCf}(<30, !11, 2:/Me, 3:/Et, 6:/Pr, 7:/iPr, 10:/tBu, 11:/Ph^-30)\]

\[\_\text{skeletonA\_end} : \text{end number of molecular skeleton atom}\]

**No.27** Add substituent(2)

\[~,^,`,> : \text{change type, angle, length, environment of substituent}\]

\[\text{MCf}(<30, ?6, @(3`2^-30, 3^-wf, 4^-zf, 6^-wf^-30, 6^-zf^-30)/H)\]

**No.28** Add substituent(3)

\[~,^,`,> : \text{change type, angle, length, environment of substituent}\]

\[\text{MCf}(<30, !7'1, @(2, 3)/Me^\sim 2^-30, 5:/Pr>lr, 7:/Pr>rl)\]

**No.29** Chain stretch direction environment (1)

\[>hz : \text{horizontal environment (default)}\]
\[>vt : \text{vertical environment}\]

\?[4, \text{hz}, @(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)

\[>lr : \text{left-right environment}\]
\[>rl : \text{right-left environment}\]

\[<30, 16, @(3^-30, 3^-30)/'(!3, "\{>lr\}")>lr, @(5^-30, 5^-30)/'(!3, "\{>rl\}")>rl\]
No.31 Chain stretch direction environment (3)

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

<30,16,6(2>45)/'(13,"{>45}"),
@6(6>(-90,90,-90))/(12,"{>-90,90,-90}")

No.32 Change atom and Substituent

NH,SOO : inset hetero atom and substituent
simultaneously

<30,13,NH!,SOO,13

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,10,13,COOH)
MCd(.8,1)(0.3,0.1)<30,COOH,14,COOH)

No.35 User definition

iBuOH : user defined substructure

iBuOH:='(!,/Me,!,OH)
Mcf<30,76, @(4,6)/iBuOH)

No.36 Inline definition

Insert user defined substructure

<30,13,'(!,/Me,!,OH),13
No.37 Example(1) Ampicillin

<45,?4,2:z5,1:S,
\(\omega(3^-45,4^-45)/\omega H,1://\omega H^15,
5://COOH^18,\omega(6^35,6^-35)/\omega Me,
4\^75,NH,1://0,1,NH,1:Ph

No.38 Example(2) Cholesterol

<30,76,1:z4,2=76,3=76,-4=75,7=dl,
1://OH,\omega(4,12)//Me^60,9://H^60,
10://H^180,\omega(11,-1)://H^-60,
-1://Me,14://Me,1,

No.39 Example(3) alfa-Tocopherol

<30,Ph,13=76,
7:0,\omega(1,2,5)/\omega Me,8://Me^60,6://OH,
8\,1,12,\omega(4,8)//Me,12://Me

No.40 Example(4) Caffeine

<30,76,-4=75,2:s7,3=76,4=75,6://Me,
\omega(2,6,7,9)N,\omega(2,6,9)/\omega Me,
\omega(1,5)//0

No.41 Example(5) Lycorine

<30,Ph,-4=76,-2=76,6=75,(9,12)=75[3],
13=dl,8:N,\omega(15,17)0,

No.42 Example(6) Gibberellin

<12,76\,1.3,3=75,9=77,12://160\,1.6,8,
4://155^-zf\,1.2,0.55,://0^-180\,1.&2^-zb,
5=dl,11=wf,13=ub,7://COOH,11://Me,1://OH,
12://OH,2://Me,\omega(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)//0)
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#; 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

![Doublebond Gap Diagram](image1)

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

ratio_atom_bond:= 0.25;  
MCD(1,.6)(0,.5)<30,76,0(2,5)>0)
ratio_atom_bond:= 0.36; %<<== default  
MCD(1,.6)(.5,.5)<30,76,0(2,5)>0)
ratio_atom_bond:= 0.45;  
MCD(1,.6)(1,.5)<30,76,0(2,5)>0)

![Atom/Bond Length Diagram](image2)

**No.51** Offset of atom width

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

![Atom Width Diagram](image3)

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

ratio_wedge_bond:=0.10;  
MCD(1,.6)(0,.5)<30,76,5:*Me)  
ratio_wedge_bond:=0.12; %<<== default  
MCD(1,.6)(.5,.5)<30,76,5:*Me)  
ratio_wedge_bond:=0.20;  
MCD(1,.6)(1,.5)<30,76,5:*Me)

![Wedge/Bond Length Diagram](image4)

**No.53** Offset of wedge width

beginfont("EN:Offset_wedge")  
offset_wedge#=0.0pt#;  
MCD(1,.3)(0,.5)<30,76,5:*Me) endfont
beginfont() offset_wedge#:=0.4pt#; %<<== default  
MCD(1,.3)(.5,.5)<30,76,5:*Me) endfont
beginfont() offset_wedge#:=1.0pt#;  
MCD(1,.3)(1,.5)<30,76,5:*Me) endfont

![Wedge Width Diagram](image5)

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

ratio_atomgap_atom:=0.0;  
MCD(1,.6)(0,.5)<30,76,0(2,5)>0)  
ratio_atomgap_atom:=0.050; %<<== default  
MCD(1,.6)(.5,.5)<30,76,0(2,5)>0)  
ratio_atomgap_atom:=0.12;  
MCD(1,.6)(1,.5)<30,76,0(2,5)>0)

![Atom Gap/Length Diagram](image6)
No.55 Ratio chain/ring length

\[
\text{ratio\_chain\_ring} = 0.4; \\
\text{MCd}(1, 0.6)(0, .5)(<30,76,5:/Et)
\]
\[
\text{ratio\_chain\_ring} = 0.66; \quad \%<= \text{default} \\
\text{MCd}(1, 0.6)(.5, .5)(<30,76,5:/Et)
\]
\[
\text{ratio\_chain\_ring} = 1.0; \\
\text{MCd}(1, 0.6)(1, .5)(<30,76,5:/Et)
\]

No.56 Ratio zebra gap/bond length

\[
\text{ratio\_zebragap\_bond} = 0.06; \\
\text{MCd}(1, 0.6)(0, .5)(<30,\text{Ph},5:/*\text{Me`1})
\]
\[
\text{ratio\_zebragap\_bond} = 0.12; \quad \%<= \text{default} \\
\text{MCd}(1, 0.6)(.5, .5)(<30,\text{Ph},5:/*\text{Me`1})
\]
\[
\text{ratio\_zebragap\_bond} = 0.20; \\
\text{MCd}(1, 0.6)(1, .5)(<30,\text{Ph},5:/*\text{Me`1})
\]

No.57 Margin left and right

\[
\text{margin\_left\_right} = 0\text{mm}; \\
\text{MCd}(1, 1)(0.5,0.9)(<30,\text{CH}_3,10,17,\text{CH}_3)
\]
\[
\text{margin\_left\_right} = 0.4\text{mm}; \quad \%<= \text{default} \\
\text{MCd}(1, 1)(0.5,0.5)(<30,\text{CH}_3,10,17,\text{CH}_3)
\]
\[
\text{margin\_left\_right} = 5\text{mm}; \\
\text{MCd}(1, 1)(0.5,0.1)(<30,\text{CH}_3,10,17,\text{CH}_3)
\]

No.58 Margin top and bottom

\[
\text{margin\_top\_bottom} = 0\text{mm}; \\
\text{MCd}(1, 1)(0.1,0.5)(<30,\text{Ph},2:/\text{OH},5:/\text{NH}_2)
\]
\[
\text{margin\_top\_bottom} = 0.4\text{mm}; \quad \%<= \text{default} \\
\text{MCd}(1, 1)(0.5,0.5)(<30,\text{Ph},2:/\text{OH},5:/\text{NH}_2)
\]
\[
\text{margin\_top\_bottom} = 5\text{mm}; \\
\text{MCd}(1, 1)(0.9,0.5)(<30,\text{Ph},2:/\text{OH},5:/\text{NH}_2)
\]

No.59 Switch Start Vector

\[
\text{Mc}(1,.8)(0,0.5)(<30,\text{Ph},4:/\text{Cl},3:/F)
\]
\[
\text{sw\_start\_vector} = 1; \\
\text{MCd}(1,1)(0.5,.9)(<30,19)
\]
\[
\text{sw\_start\_vector} = 2; \\
\text{MCd}(1,1)(.5,5)(<30,19)
\]
\[
\text{sw\_start\_vector} = 3; \\
\text{MCd}(1,1)(.5,1)(<30,19)
\]
\[
** \text{default: numberA\_start=1 numberA\_end=4095}
\]
No.61 Switch Numbering bond

\[\text{numberB}_{\text{start}}:=3; \text{numberB}_{\text{end}}:=8;\]

\[\text{sw}_{\text{numberB}}:=1; \text{MCd}(1,1)(0.5,0.9)<30,19\]
\[\text{sw}_{\text{numberB}}:=2; \text{MCd}(1,1)(0.5,0.5)<30,19\]
\[\text{sw}_{\text{numberB}}:=3; \text{MCd}(1,1)(0.5,1)<30,19\]

** default: \text{numberB}_{\text{start}}=1 \text{ numberB}_{\text{end}}=4095

No.62 Switch font frame

\[\text{sw}_{\text{font_frame}}:=1;\]

\[\text{MCf}<30,\text{Ph},4:/\text{Cl},3:/\text{F}\]

No.63 Switch molecular frame

\[\text{MCd}(1,0.8)(0,0.5)<30,\text{Ph},4:/\text{Cl},3:/\text{F}\]
\[\text{sw}_{\text{mol_frame}}:=1;\]
\[\text{MCd}(1,0.8)(1,0.5)<30,\text{Ph},4:/\text{Cl},3:/\text{F}\]

No.64 Switch atom frame

\[\text{sw}_{\text{atom_frame}}:=1;\]

\[\text{MCf}<30,\text{Ph},4:/\text{COOH},3:/\text{OH}\]

No.65 Switch solid mode

\[\text{MCd}(1,0.8)(0,0.5)<30,\text{Ph},4:/\text{Cl},3:/\text{F}\]
\[\text{sw}_{\text{solid}}:=1; \text{ratio_bond_width}:=0.08;\]
\[\text{MCd}(1,0.8)(1,0.5)<30,\text{Ph},4:/\text{Cl},3:/\text{F}\]

No.66 Switch Expand

\[\text{MCd}(1,0.6)(0,0.5)<30,\text{Ph},4:/\text{COOH},3:/\text{NH}_{2}\]
\[\text{sw}_{\text{expand}}:=1;\]
\[\text{MCd}(1,0.6)(1,0.5)<30,\text{Ph},4:/\text{COOH},3:/\text{NH}_{2}\]
**No.67** 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.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

\[ \text{beginfont}("NO:1") \]

- **sw_mol_frame**: 1

\[ MCd(1,0.5)(0.0,0.5)(<30,Ph,\Phi(2)N) \]

\[ \text{endfont} \]

\[ \text{beginfont}("NO:2") \]

\[ MCd(1,0.5)(0.5,0.5)(<30,Ph,\Phi(2,4)N) \]

\[ \text{endfont} \]

\[ \text{beginfont}("NO:3") \]

\[ MCd(1,0.5)(1.0,0.5)(<30,Ph,\Phi(2,4,6)N) \]

\[ \text{endfont} \]

**No.70** Global setting

- **sw_mol_frame**: 1

\[ \text{beginfont}("NO:1") \]

\[ MCd(1,0.5)(0.0,0.5)(<30,Ph,\Phi(2)N) \]

\[ \text{endfont} \]

\[ \text{beginfont}("NO:2") \]

\[ MCd(1,0.5)(0.5,0.5)(<30,Ph,\Phi(2,4)N) \]

\[ \text{endfont} \]

\[ \text{beginfont}("NO:3") \]

\[ MCd(1,0.5)(1.0,0.5)(<30,Ph,\Phi(2,4,6)N) \]

\[ \text{endfont} \]

**No.71** Output molecular information

\[ \text{beginfont}() \]

- **sw_info_weight**: 1
- **sw_info_formula**: 1

\[ MCf(...) \]

\[ \text{endfont} \]

\[ \%\%\text{Output to mcf_man_soc-info.aux}\%\%
\]

\[ \text{INFO}{\{F:mcf_man_soc}\{C:82\}{MWc:194.19174}\{FCM:C8H10N4O2}\%} \]

- **MWc**: calculated molecular weight
- **FMc**: calculated molecular formula

**No.72** Output additional information

\[ \text{beginfont}("EN:Caffeine","CAS:58-08-2") \]

\[ MCf(...) \]

\[ \%\%\text{Output to mcf_man_soc-info.aux}\%\%
\]

\[ \text{INFO}{\{F:mcf_man_soc\{C:83\}{EN:Caffeine}\{CAS:58-08-2\}\%} \]

- **F**: filename
- **C**: character number
- **EN**: molecular name
- **CAS**: CAS number
- ***: default output