Delta Tips

NMR data processing software

Delta
NMR Software
v5.0

NMDT_0057
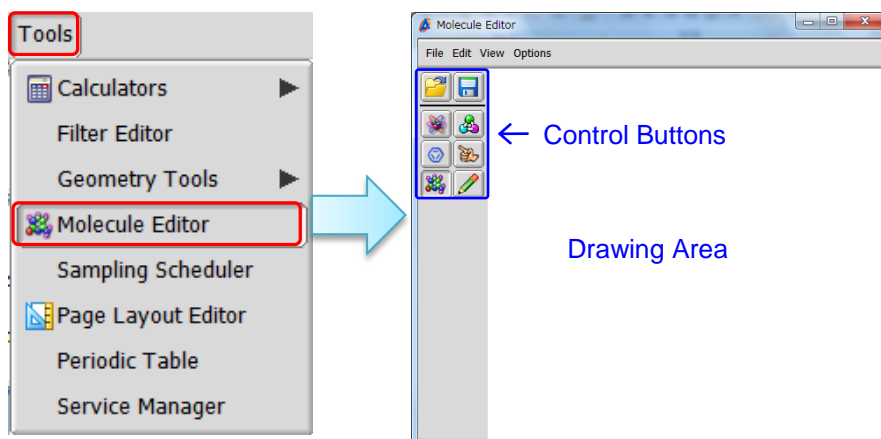
Molecule Editor

Delta software has a function to draw structural formula by using **Molecule Editor** and to display structural formulae together with NMR spectra as shown in the figure below.
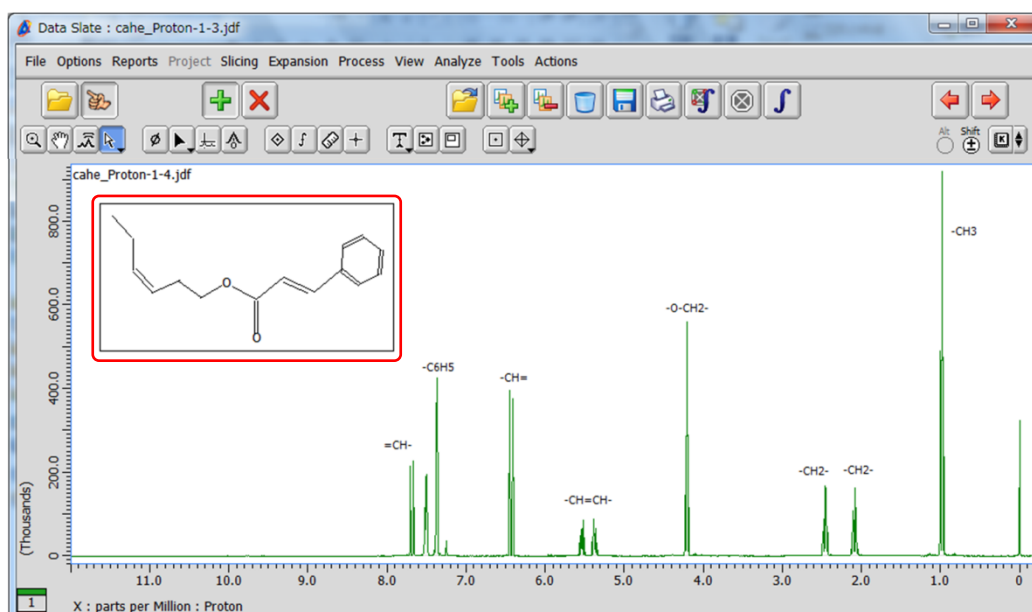
An example of structural formula displayed in ^{1}H spectrum

In the example below, we will demonstrate basic functions of **Molecule Editor** on 1-propanol.

① Select **Tools** - **Molecule Editor** in the **Delta** window to open the **Molecule Editor** window.
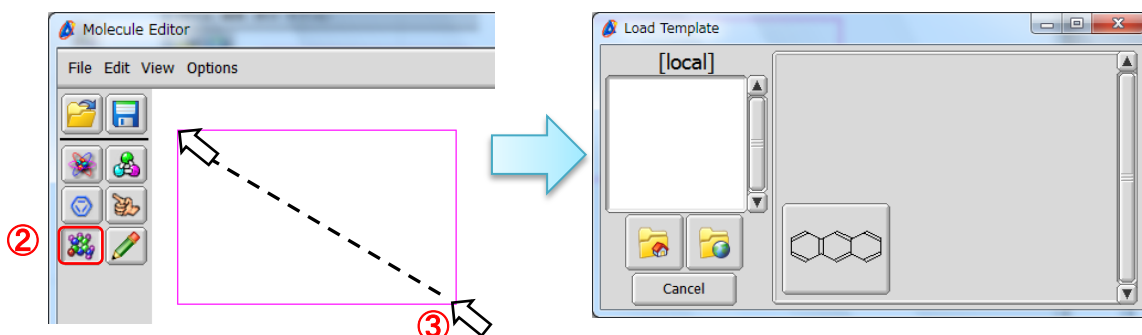

Molecule Editor window

★ You can also open **Molecule Editor** from the **Data Slate** and **Data Processor** windows.

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② Push the **Template** button .

③ Create a box by Drag & Drop.

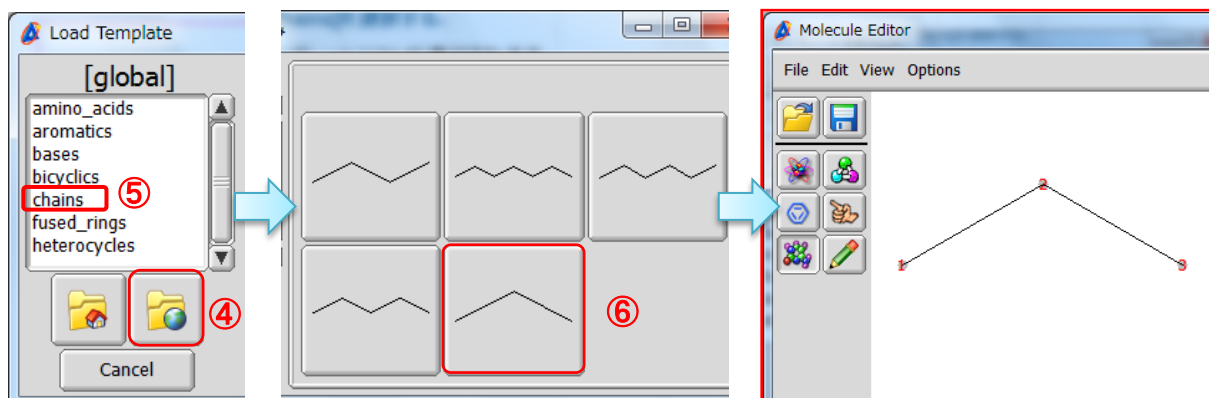Note that the **Load Template** window has automatically opened.

The drawing box has been created.

Load Template window

④ Push the **Global Directory** button in the **Load Template** window.

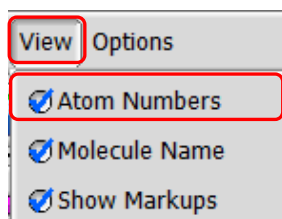⑤ Select the *chains* template group from the list.

⑥ Push the **propyl** template button.

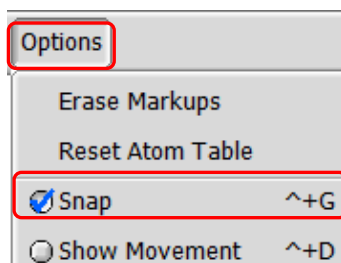**Global template list – chains – propyl**

The **propyl** template has been loaded.

★ You can display atom numbering by selecting **View** ― **Atom Numbers** in the **Molecule Editor** window.
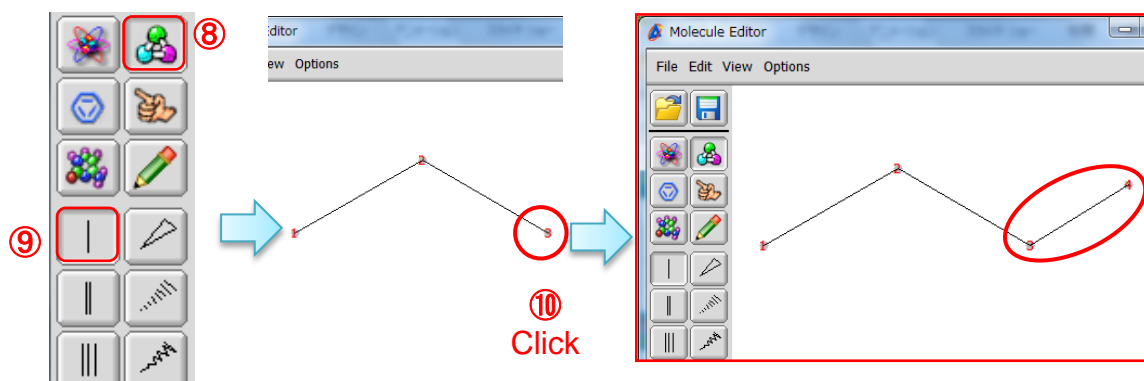

View – Atom Numbers

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⑦ Select **Options** ─ **Snap** in the **Molecule Editor** window.

Options
  Erase Markups
  Reset Atom Table
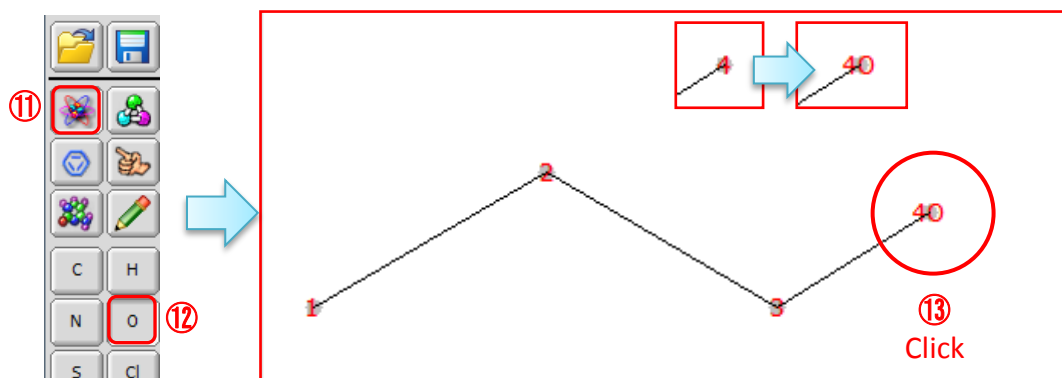 ☑ Snap   ^+G
  ○ Show Movement ^+D

Options – Snap

⑧ Push the **Draw Bond** button and ⑨ the **Single Bond** button .

⑩ Click on the terminal group **3** of propane to draw a new single bond.

⑩
Click

A new single bond has been added.

⑪ Push the **Draw Atom** button and ⑫ the **Oxygen** button .

⑬ Select the terminal group **4** of butane to replace the carbon atom (rather CH_3) by oxygen.

⑬
Click

The carbon atom has changed into oxygen.

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⑭ Refer to steps ⑧ - ⑬ in order to draw a new bond from the oxygen atom **4** and to replace the new carbon atom by hydrogen. The hydroxyl group of 1-propanol has been created.
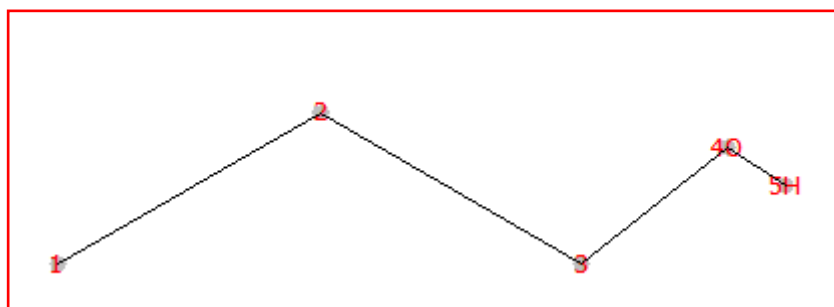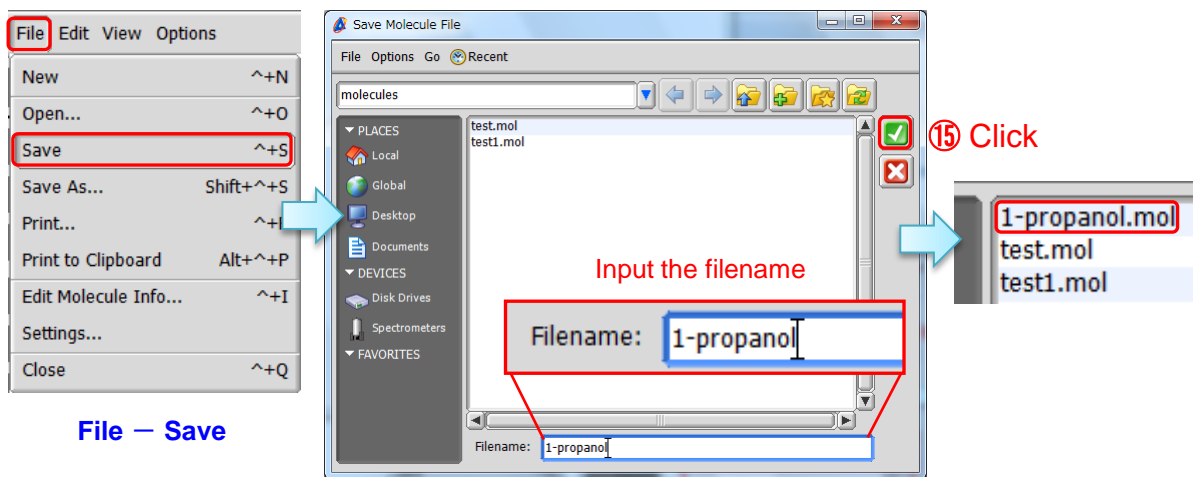

Structural formula of 1-propanol, C_3H_7OH.

⑮ Select **File** — **Save** to open the **Save Molecule File** window.

Input a file name into the **Filename** input box and push the **Save** button.

Note that the file has been saved in the molfile format (.mol).

File — **Save**

Save Molecule File window

⑮ Click

Input the filename

Filename: 1-propanol

1-propanol.mol
test.mol
test1.mol

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