Delta Tips

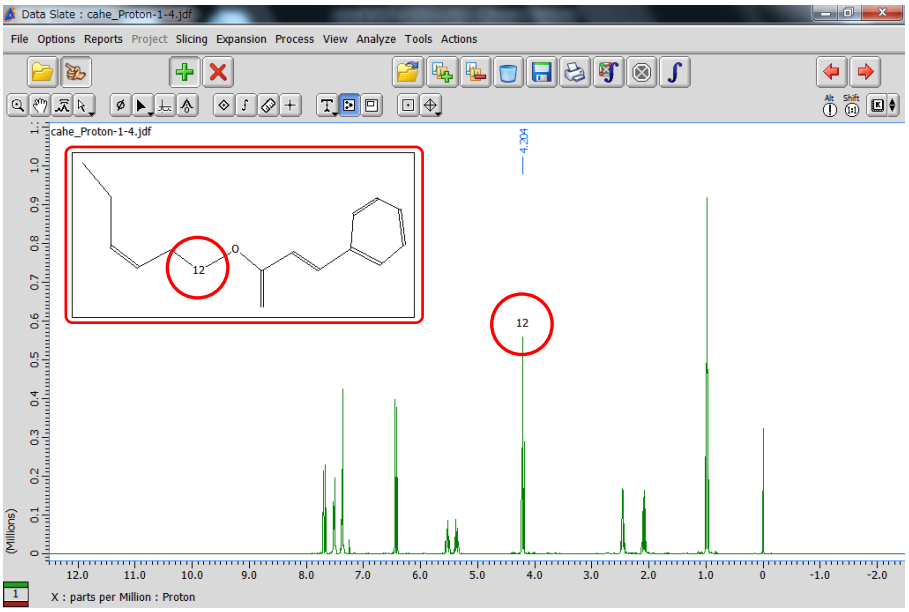
NMDT_0058

Peak Assignment Function

NMR data processing software

Delta NMR Software v5.0

Delta software has a peak assignment function by using structural formula. In the example below, a triplet signal at 4.20 ppm is assigned to methylene protons **H12** of CAHE (Cinnamic Acid cis-3-Hexen-1-yl Ester). Refer to NMDT-0057 on the use of **Molecule Editor**.



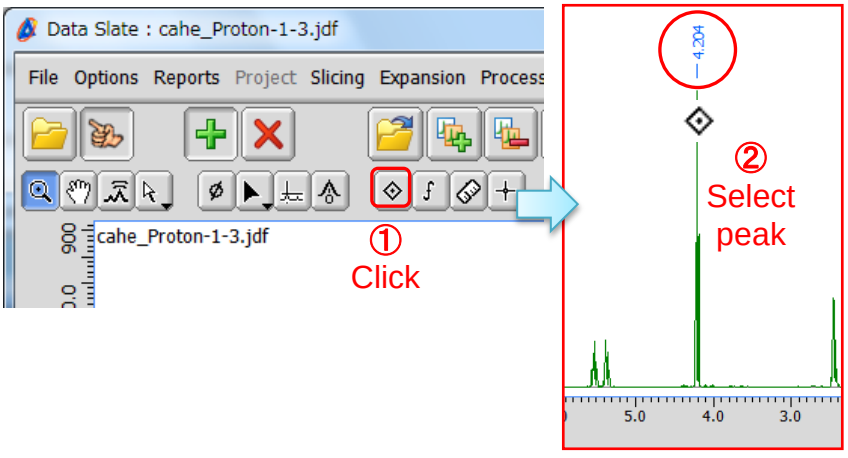
Triplet at 4.20 ppm is assigned to methylene protons **H12** of CAHE.

① Open data in the **Data Slate** window and push the **Create peak** button  .

Note that the cursor has changed into the **peak** symbol ◈ .

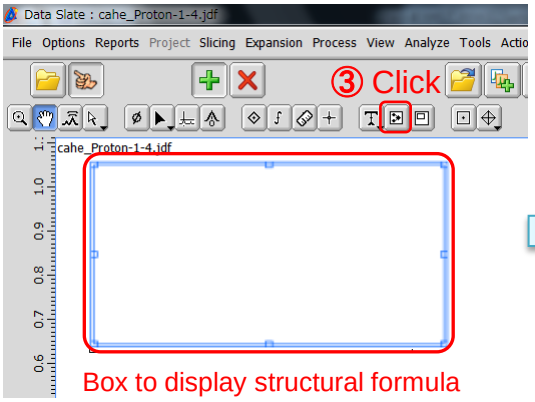
② Select the peak which you wish to assign. It is the triplet at 4.20 ppm in the example.

Note that a peak mark and chemical shift have been displayed above the selected peak.

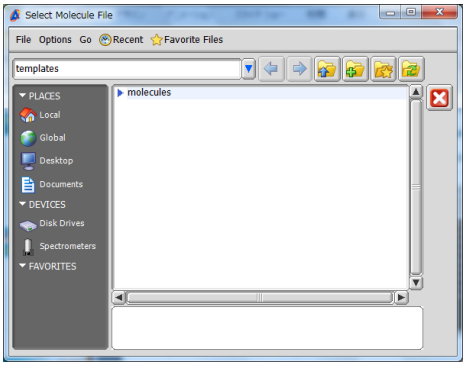


★ You can also use the **peak assignment function** in the **1D Processor** window.

③ Push the **Create Molecule Window** button and create a box in the **Data Slate** window. Note that the cursor has changed into the **Molecule** symbol . After the box has been created by Drag & Drop, the **Select Molecule File** window opens automatically.

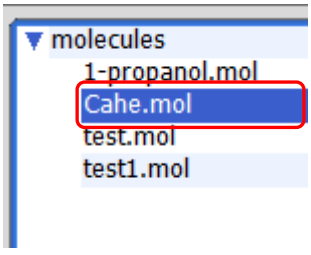


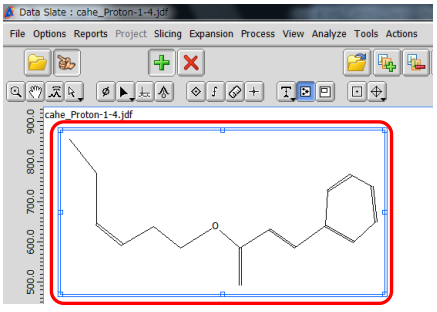
Box to display structural formula



Select Molecule File window

④ Select a file in the **Select Molecule File** window and push the **Open** button .
Note that the selected structural formula has been displayed in the box.

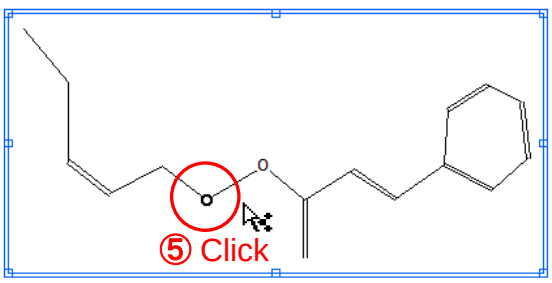




Structural formula of CAHE.

★ You can select files in the molfile format in **Select Molecule File** window.

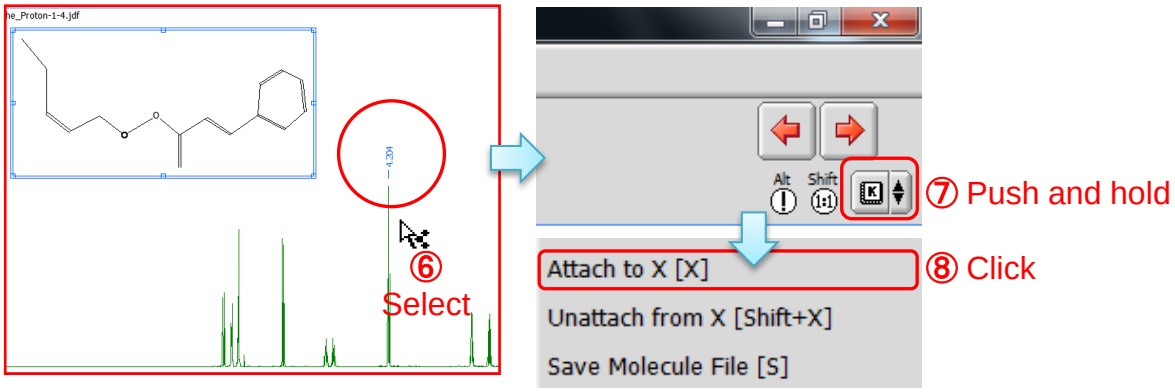
⑤ Push and hold the Ctrl **[Ctrl]** key to select an atom (group). Note that the cursor has changed into the **Select** symbol . Select the atom which you wish to assign to the peak in the **Data Slate** window. The selected atom is represented by an **open circle**.



⑥ Push and hold the Shift **[Shift]** and Ctrl **[Ctrl]** keys. Note that the cursor has changed into the **Select** symbol . Select the peak which you wish to assign to the atom (group) in the structural formula.

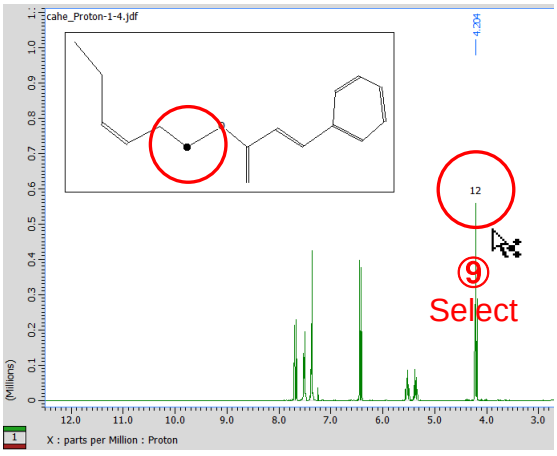
⑦ Push and hold the button to display the pull-down menu.

⑧ Select **Attach to X**. The selected atom (group) has been assigned to the peak.

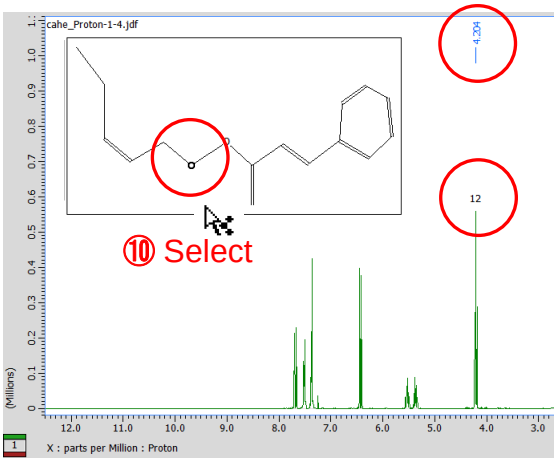


⑨ Push and hold the Ctrl **[Ctrl]** key, and select the peak in the spectrum. Note that a **closed circle** highlights the atom in the structural formula (see the **left figure** below).

⑩ Push and hold the Ctrl **[Ctrl]** key and select the atom in the structural formula. Note that an **open circle** highlights this atom (group). At the same time, the atom number and peak mark of the assigned peak are displayed (see the **right figure** below).



Select the peak: the closed circle highlights the assigned atom (group)



Select the atom: the atom number and chemical shift of the peak are displayed

★ It is possible to display or hide atom numbering in the **Molecule** box from the context menu as follows: Push and hold the right mouse button to display the menu, and select **Options - Molecules - Atom Numbers** or **Options - Molecules - Atom Select Numbers**.