Delta Tips

NMDT_0059

Deconvolution Function

NMR data processing software

Delta NMR Software v5.0

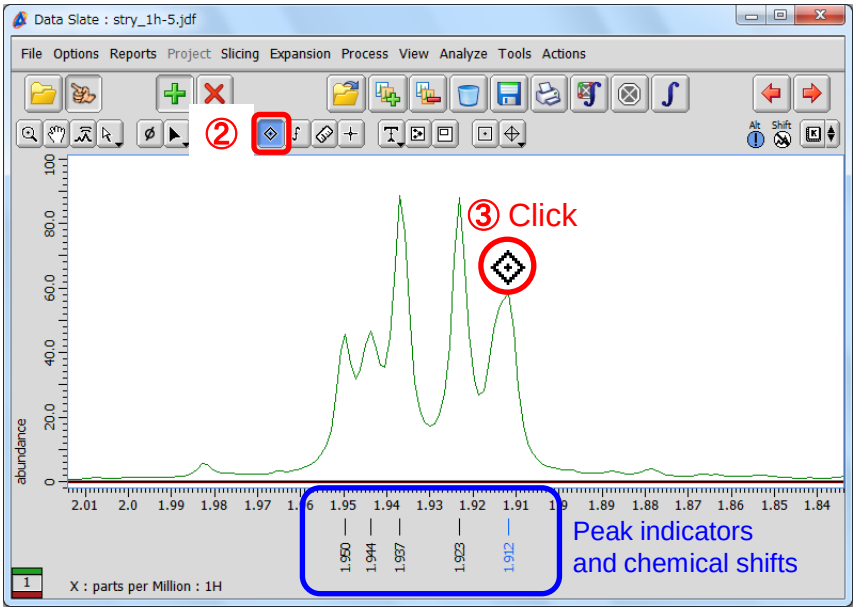
In Delta software, it is possible to deconvolve overlapping peaks with Lorentzian, Gaussian and a combination of Lorentzian and Gaussian functions.

① Display a spectrum in the **1D Processor** or **Data Slate** window.

② Click the **Peak** button  to activate the peak picking mode.

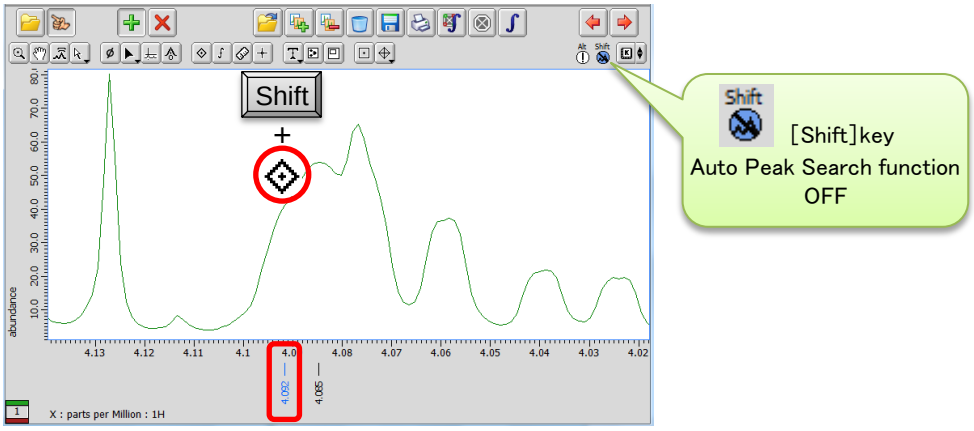
③ Pick peaks in the spectrum with the cursor indicated by the **Peak** symbol  .

Peak indicators (marks) and chemical shifts of the selected peaks have been displayed below the spectrum.



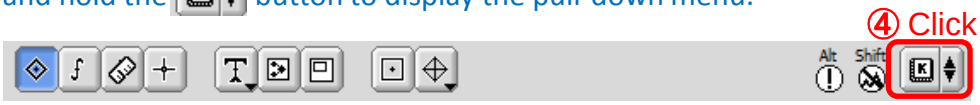
Peak Picking

★ If you need to pick up some shoulder or broad overlapping peaks manually, push and hold the Shift key and create the peak.



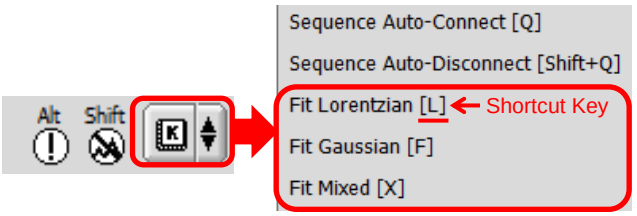
Selected a shoulder peak (create peak anywhere)

④ Push and hold the button to display the pull-down menu.



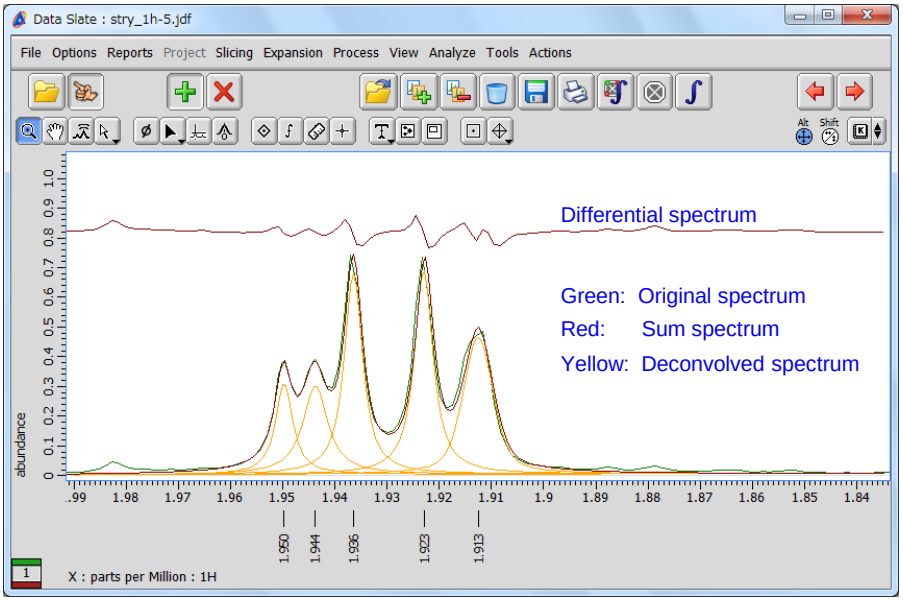
⑤ Select a curve fitting function for deconvolution from the menu.

Deconvolution has been executed and the fitting result has been shown on the data.



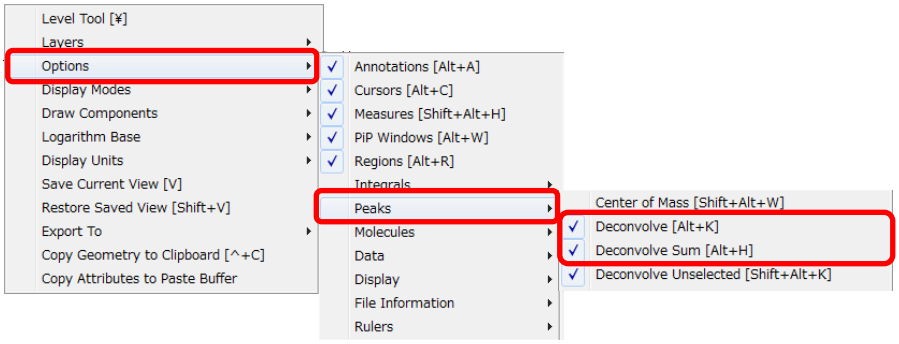
★ **Fit Mixed** is the Voigt fitting function which is a combination of Lorentzian and Gaussian functions.

★ The shortcut key is shown for each fitting function on the right.



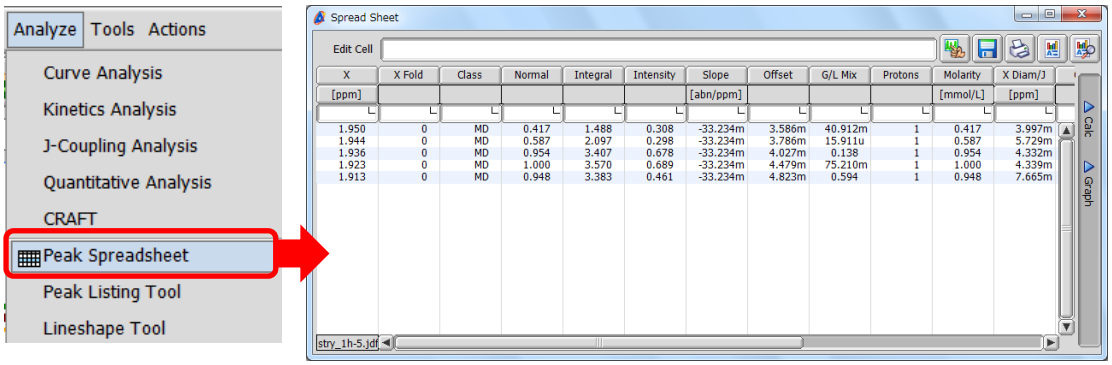
Deconvolution of overlapping peaks

★ It is possible to display or hide the deconvolution result from the context menu as follows: Push and hold the right mouse button to display the menu. Then select **Options** – **Peaks** – **Deconvolve** and **Deconvolve Sum** as shown below.



⑥ Select **Analyze**—**Peak Spreadsheet** to open the **Spread Sheet** window.

The detailed results for all deconvolved peaks have been summarized in the **Spread Sheet** table.



★ The **Spread Sheet** table

Class — MD
- Deconvolution
- Peak Picking (A : Automatic, M: Manual)

X — Peak position

Integral — Integral value

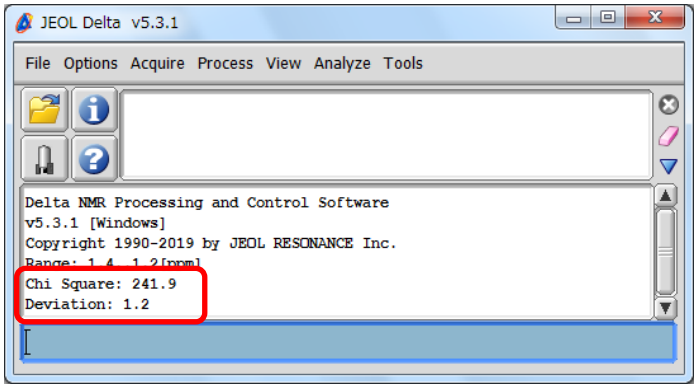
Intensity — Peak intensity

G/L Mix — Gauss/Lorentz ratio

X Diam/J — Peak half width

★ The result of deconvolution

The Chi square value and the standard deviation value are shown in the **Delta Console** window.

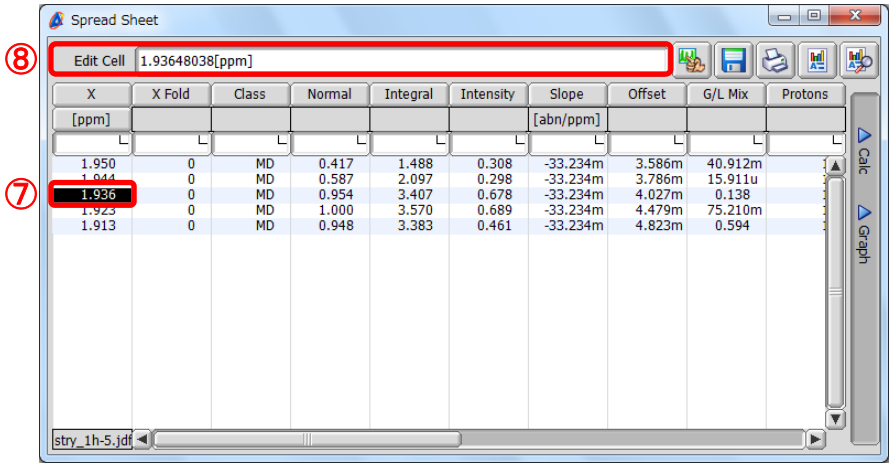


★ Recalculation

It is possible to set and fix the value of **X** (peak position), **Intensity** (peak intensity) and **X Diam/J** (peak half width) in a deconvolution result in the **Spread Sheet** window and execute deconvolution again.

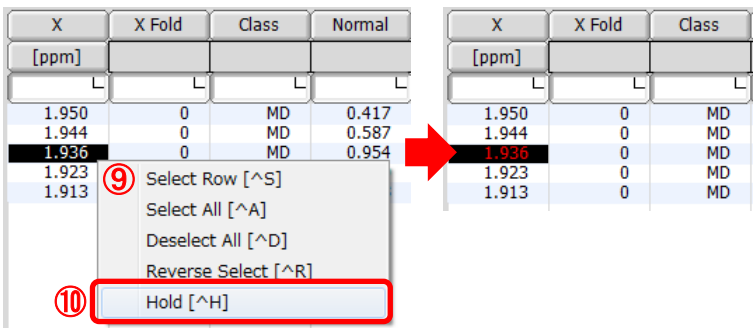
⑦ Select a cell in the **Spread Sheet** window.

⑧ Input a value into the **Edit Cell** box.



⑨ Push and hold the right-mouse-button over the cell to display the context menu.

⑩ Select **Hold** from the menu. The chemical shift value in the cell has turned red.



⑪ Select a curve fitting function from the menu.

The recalculated result has been shown on the data.