

Delta Tips

NMDT_0059



Deconvolution Function

NMR data processing software

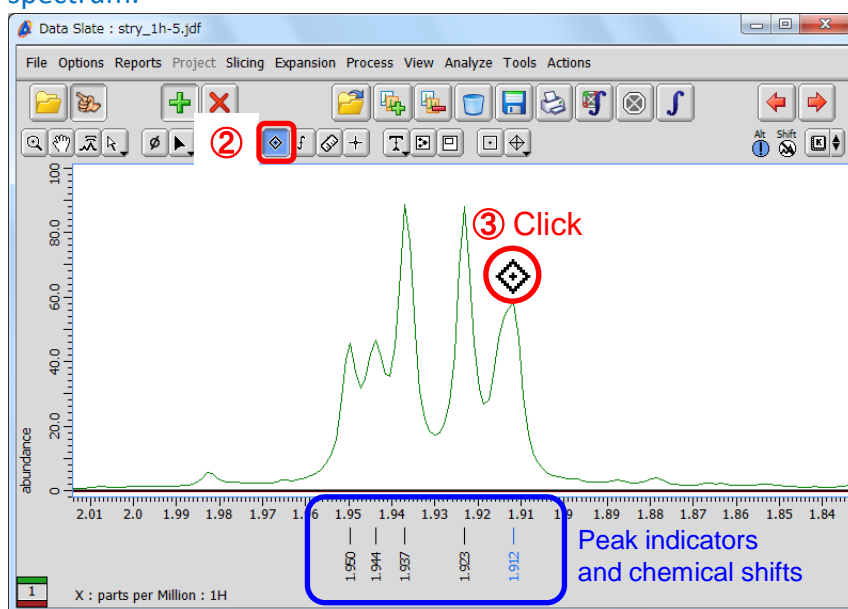
Delta
NMR Software
v5.0



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

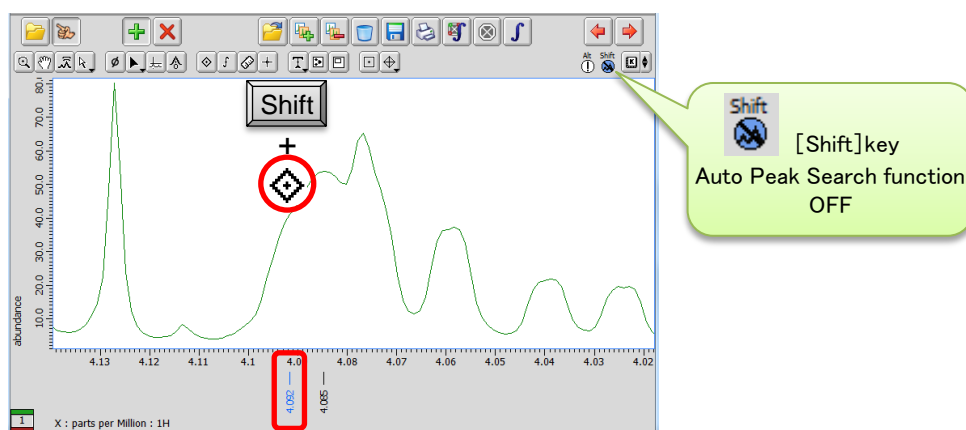
- ① Display a spectrum in the **1D Processor** or **Data Slate** window.
- ② Click the **Peak** button  to activate the peak picking mode.
- ③ Pick peaks in the spectrum with the cursor indicated by the **Peak symbol** .

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.

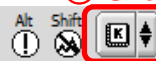


Selected a shoulder peak (create peak anywhere)

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

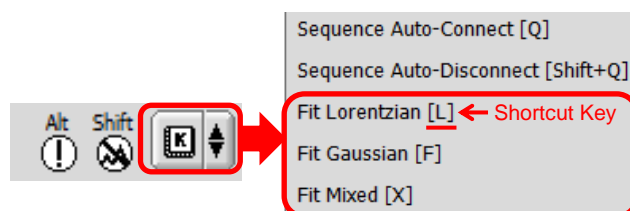


④ Click



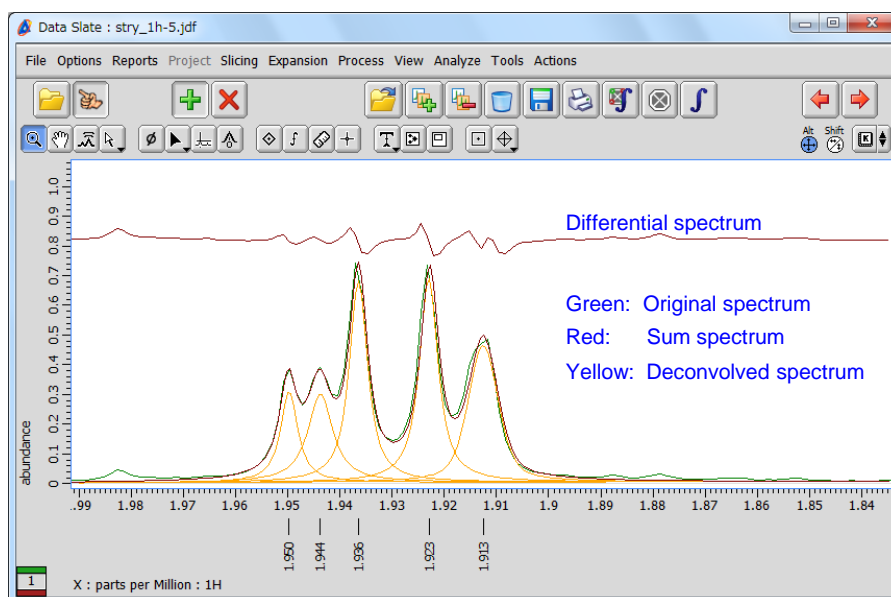
⑤ Select a curve fitting function for deconvolution from the menu.

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



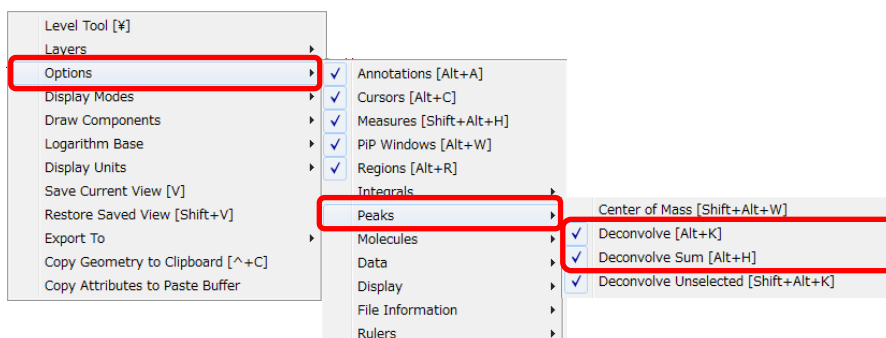
★ **Fit Mixed** is the Voigt fitting function which is a combination of Lorentzian and Gaussian functions.

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



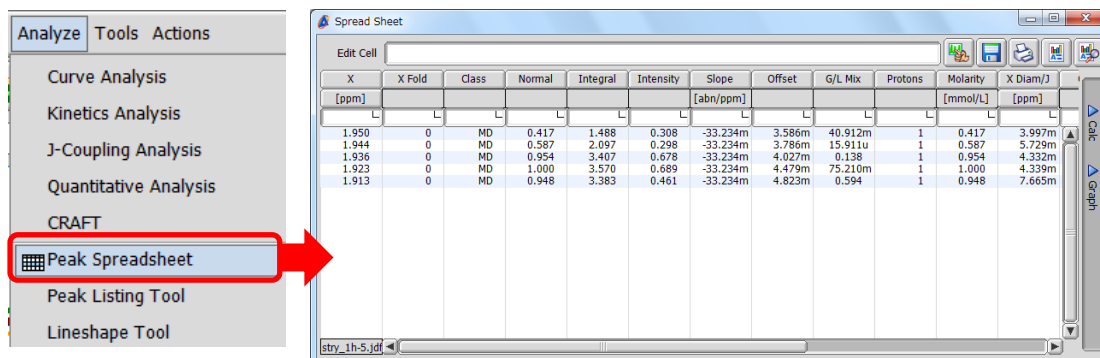
Deconvolution of overlapping peaks

★ 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.



X	X Fold	Class	Normal	Integral	Intensity	Slope	Offset	G/L Mix	Protons	Molarity	X Diam/J
[ppm]						[abn/ppm]				[mmol/L]	[ppm]
1.950	0	MD	0.417	1.488	0.308	-33.234m	3.586m	40.912m	1	0.417	3.997m
1.944	0	MD	0.587	2.097	0.298	-33.234m	3.786m	15.911u	1	0.587	5.729m
1.936	0	MD	0.954	3.407	0.678	-33.234m	4.027m	0.138	1	0.954	4.332m
1.923	0	MD	1.000	3.570	0.689	-33.234m	4.479m	75.210m	1	1.000	4.339m
1.913	0	MD	0.948	3.383	0.461	-33.234m	4.823m	0.594	1	0.948	7.665m

★ The **Spread Sheet** table

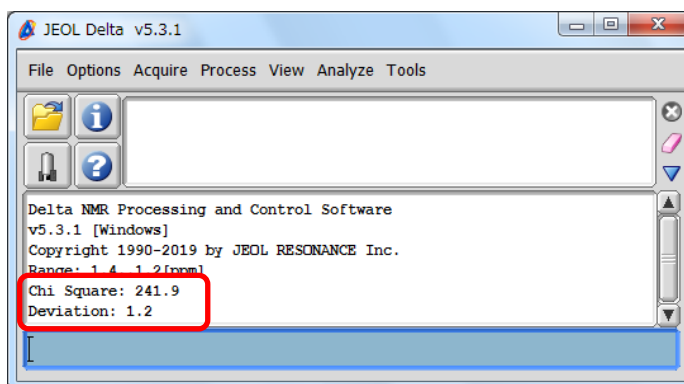
Class MD
 └─ Deconvolution
 └─ Peak Picking (A: Automatic, M: Manual)

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.



JEOL Delta v5.3.1

File Options Acquire Process View Analyze Tools

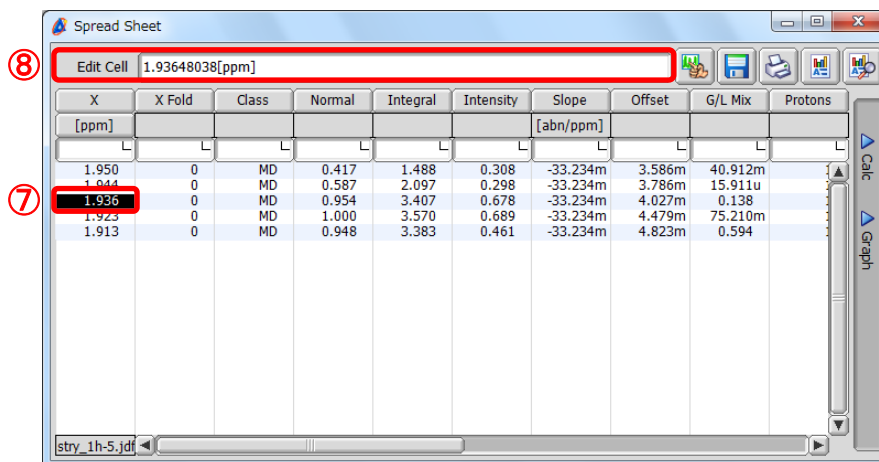
Delta NMR Processing and Control Software
 v5.3.1 [Windows]
 Copyright 1990-2019 by JEOL RESONANCE Inc.
 Range: 1.4 - 1.2 [ppm]
Chi Square: 241.9
Deviation: 1.2

★ 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.

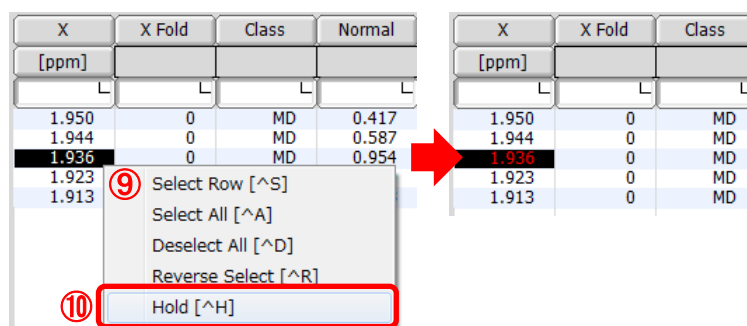
⑦ Select a cell in the **Spread Sheet** window.

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.