

Delta Tips

NMDT_0017


How to Report Diffusion Coefficient

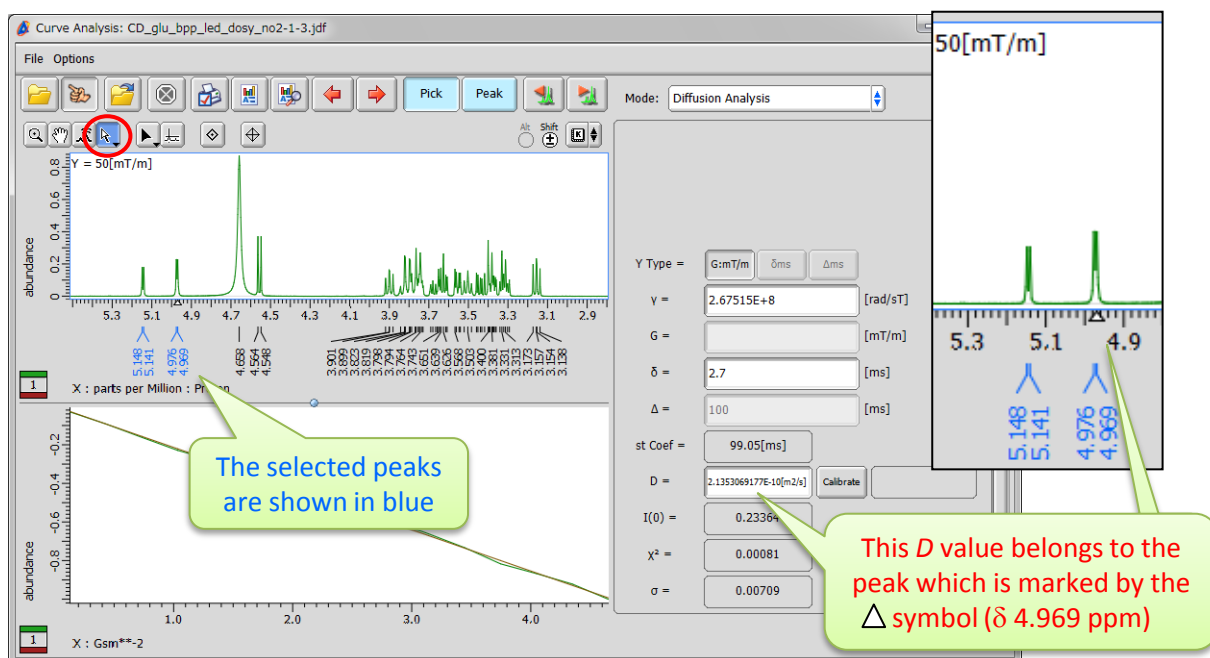
NMR data processing software



Delta
NMR Software
v5.0



This issue of Delta Tips demonstrates how to report diffusion coefficient (D) of multiple peaks at once.


- Click the  button to activate the selection mode in the Curve Analysis window. Select the peaks of interest to calculate and report their D values. We have selected two doublets.

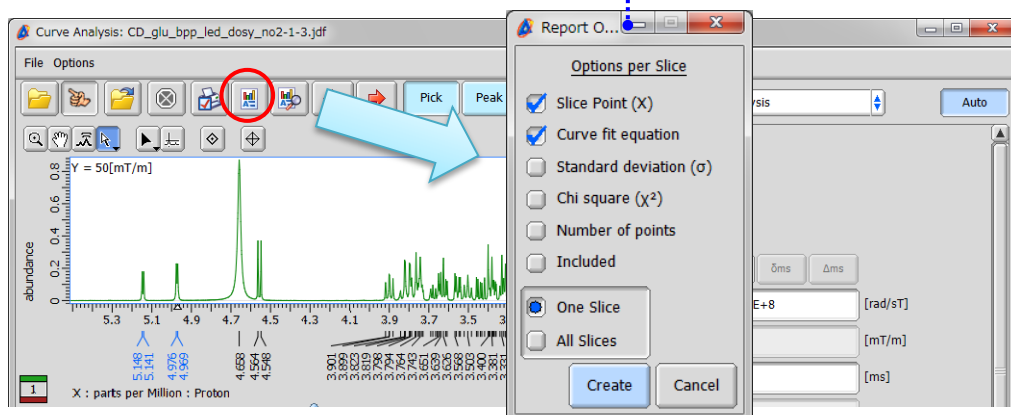


- ★ If a group of peaks is selected, it is possible to switch from one peak to another one within the group by clicking the   buttons.

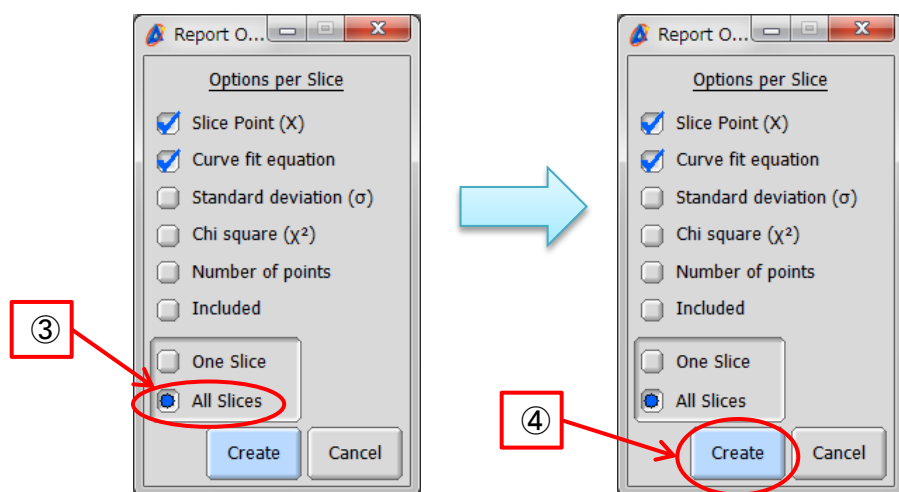
 Move to left


 Move to right

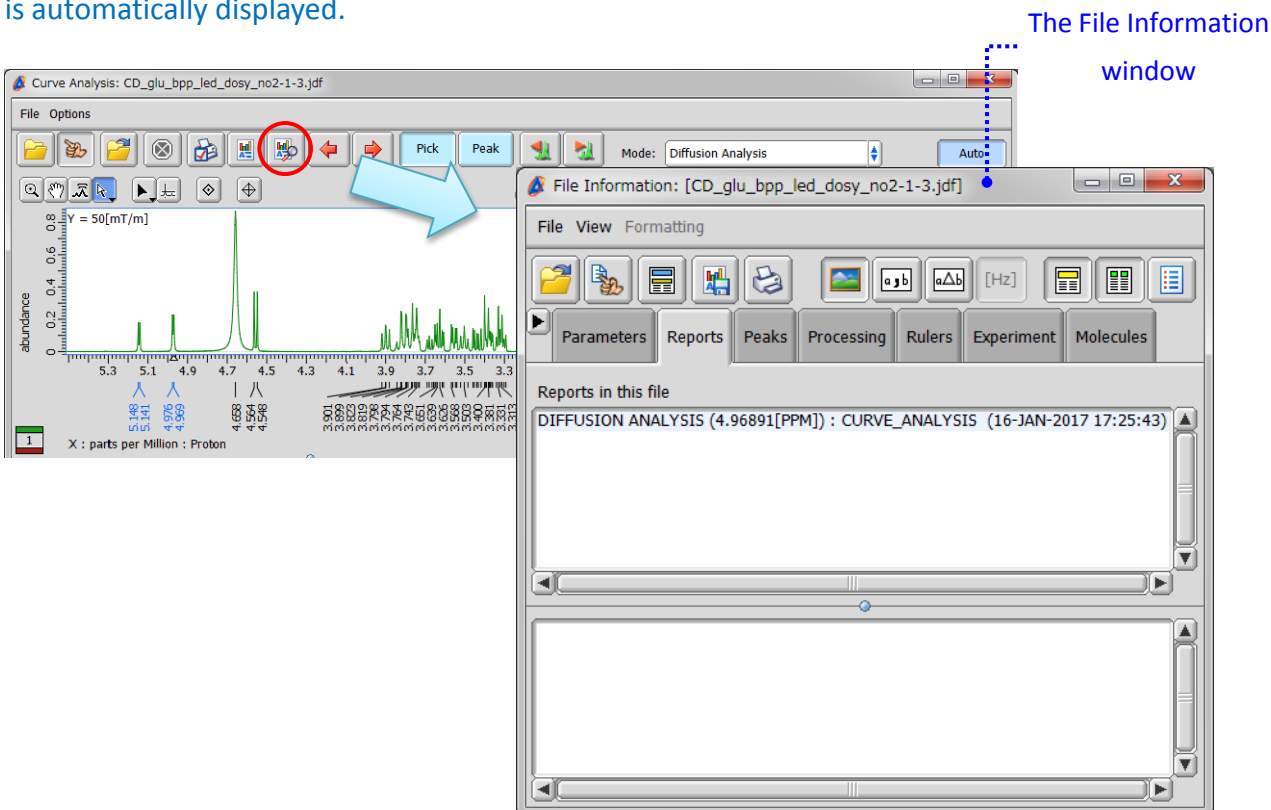
- Click the  button in the Curve Analysis window to create a report. The Report Options window opens.



- ③ Select the 'All Slices' option in the Report Options window. The other check boxes allow you to customize the contents of the report.
- ④ Click the **Create** button to create the report on all the peaks selected above.



- ⑤ Click the  button to view the report. The **File Information** tool opens and the **Reports** tab is automatically displayed.





⑥ Select 'CURVE_ANALYSIS' to display the report.


The Reports tab

List of reports

Report

X	Y	Intensity
4.969 [ppm]	50.0 [mT/m]	0.227
4.969 [ppm]	91.29 [mT/m]	0.213
4.969 [ppm]	0.119 [T/m]	0.199
4.969 [ppm]	0.141 [T/m]	0.186
4.969 [ppm]	0.161 [T/m]	0.177
4.969 [ppm]	0.178 [T/m]	0.165
4.969 [ppm]	0.194 [T/m]	0.155

⑦ Save the report in a file as shown below.

- ★ Click the  button to save the report on diffusion data as a text file (*.txt).
- ★ Select **File – Save Report As** to save the report as a text file (*.txt), comma separated value file (*.csv) or tab separated value file (*.txt).

Text File

Database (CSV)

Database (CSV) with no units

Database (Tab Delimited)

Database (Tab Delimited) with no units