

Delta Tips

NMDT_0065

How to Pick Peaks in 2D Spectra


NMR data processing software

Delta
NMR Software
v5.0





This issue of Delta Tips shows how to pick peaks in 2D spectra in the **2D Viewer** window.

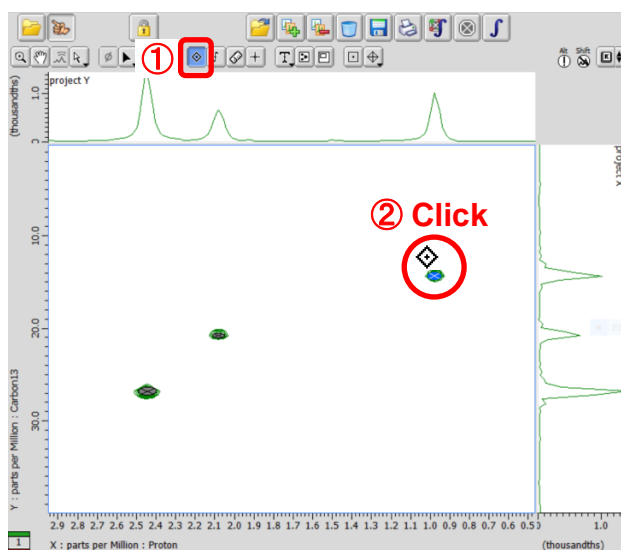
Automatic Peak Picking:

Click the  button to automatically pick the peaks which are above the peak threshold level.

Manual Peak Picking:

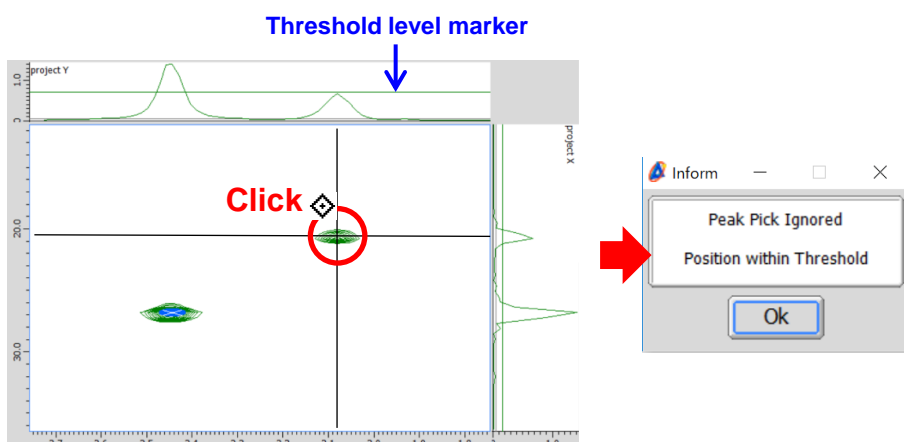
- ① Click the  button. Note that the cursor has changed into the **Peak symbol** .
- ② Click the 2D data with the cursor.

It is possible to pick the peaks which are above the peak threshold level.



Peak picking in 2D spectrum

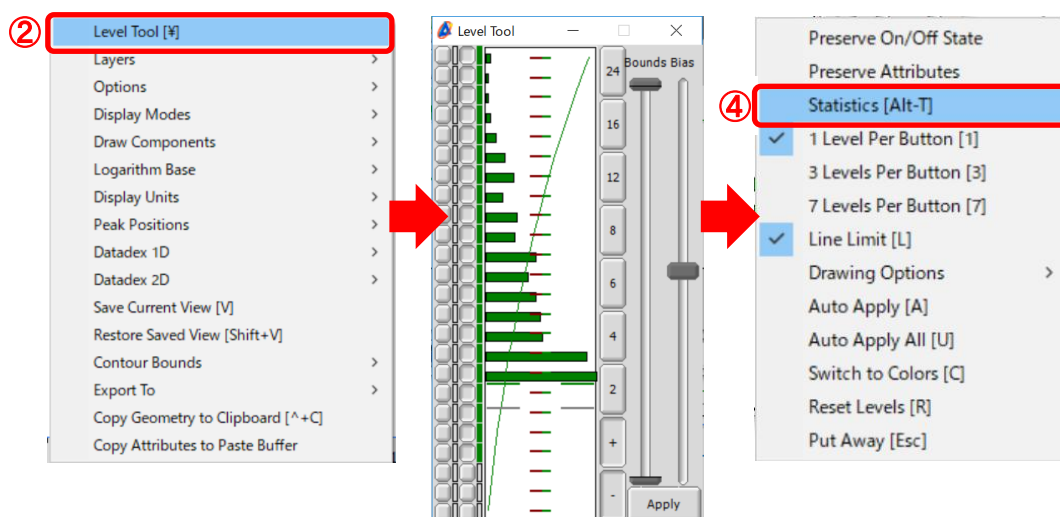
- ★ It is impossible to select the peaks which are below the peak threshold level. If you try to select this peak, an **Inform** dialog box appears and the peak is ignored.



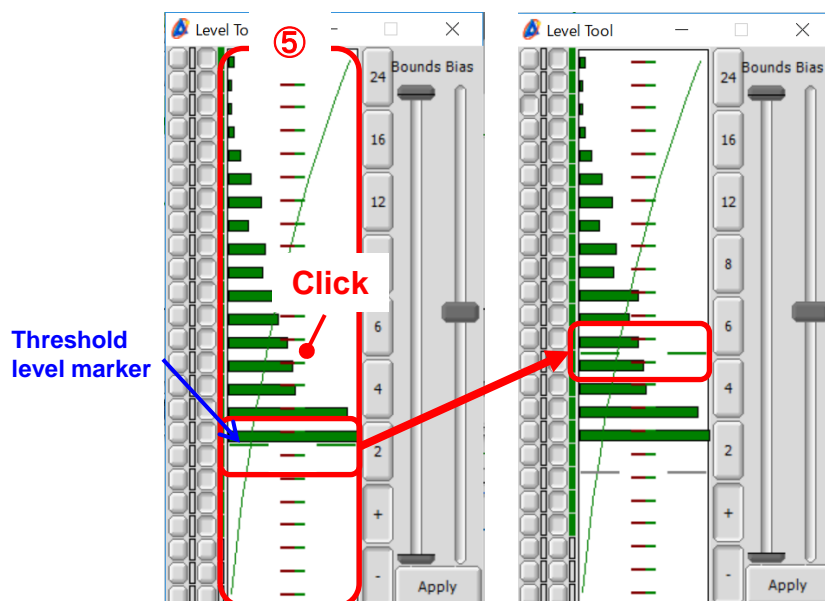
It is possible to set the peak threshold level manually as follows.

A. Using the **Level Tool**:

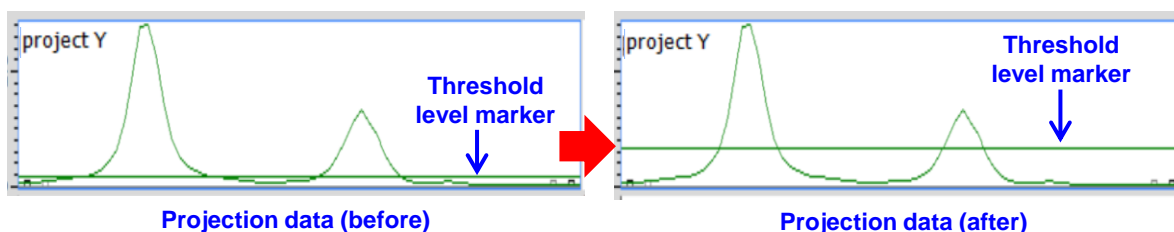
- ① Push and hold the right mouse button on the 2D data to display the context menu.
- ② Select **Level Tool** to display the **Level Tool** window.
- ③ Push and hold the right mouse button in the **Level Tool** window to display the context menu of the **Level Tool** window.
- ④ Select **Statistics** in the context menu of the **Level Tool** window.





- ⑤ Select a point in the ⑤ area in the **Level Tool** window to set the peak threshold level.




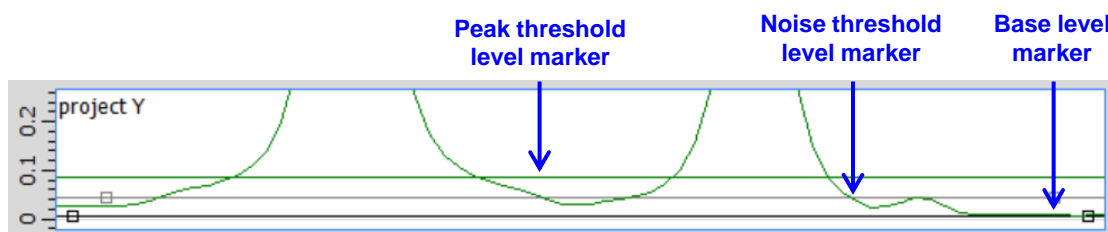
⑥ Click the  button in the **Level Tool** window to apply the change.






★ It is possible to apply changes automatically as follows:
Select **Auto Apply** in the context menu of the **Level Tool** window (see above).
Note that the  button has changed into the  button.

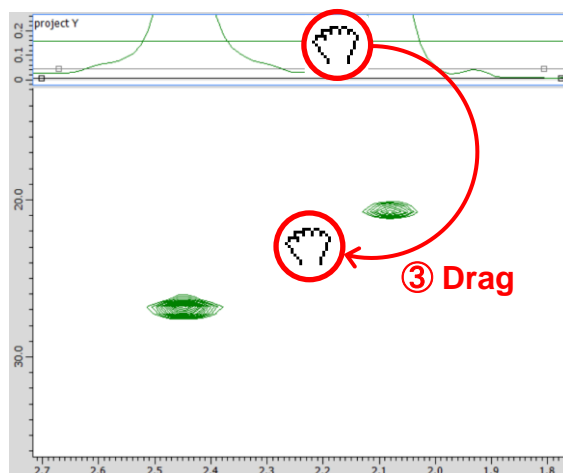
B. Using the **Projection data**:


① Click inside the **Projection data** area and click the  button in the **2D Viewer** window to display the threshold level markers on the projection data.

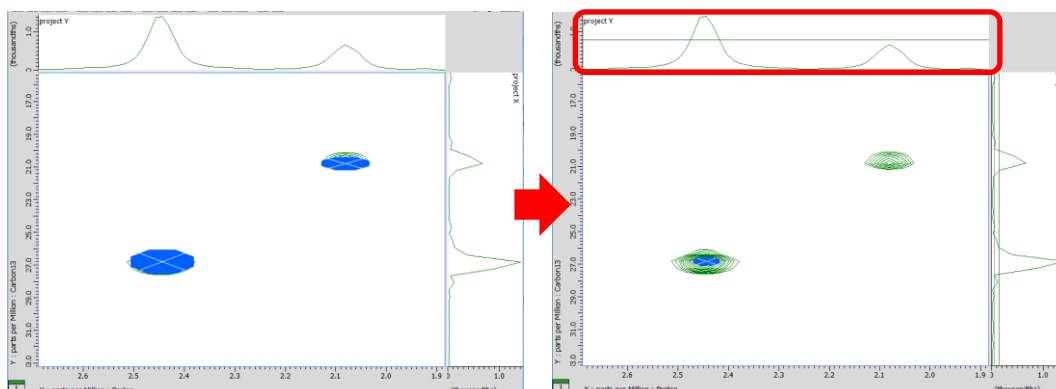


② Select the peak threshold level marker and note that the cursor has changed into . Drag and drop it where needed.

③ Right-click the projection data and drag onto the 2D data to apply the changes to the 2D data. It is possible to use this function only when the  button is selected and has changed into the .

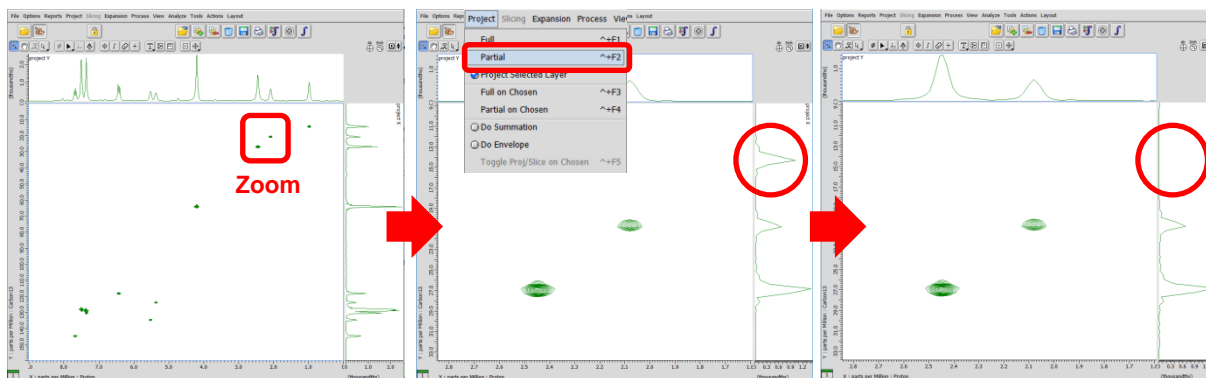


④ Click the  button or the  button (please see page 1) to pick peaks which are above the threshold level.



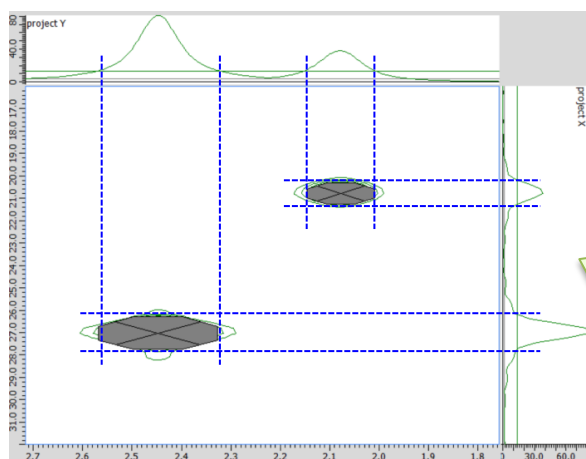
Picked peaks in the 2D spectrum after resetting the threshold level

★ The projection data display full projection as default. It is possible to display the projection data of the currently displayed area as follows:
Zoom your 2D data and select **Project — Partial** in the **2D Viewer** window.



Full projection data (projection of entire 2D spectrum)

Partial projection data (projection of displayed area)

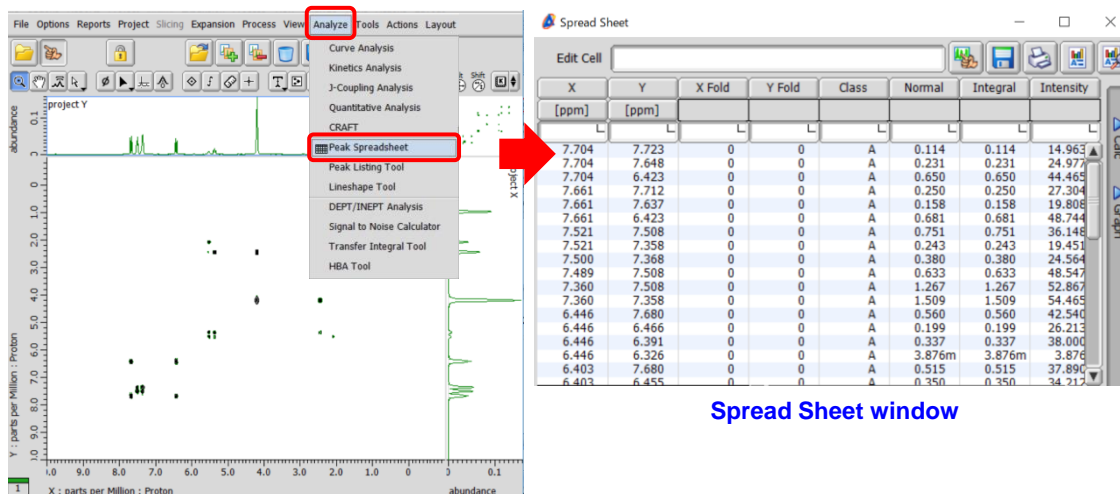


About the Size of Peak Marker

It is determined by the points of the threshold level and the projection data spectrum.



- ★ Details for all picked peaks can be summarized in the **Spread Sheet** window as follows:
Select **Analyze — Peak Spreadsheet** to open the **Spread Sheet** window.



Spread Sheet window

- ★ For the details of the **Spread Sheet** window, refer to Delta Tips **Spread Sheet (Part 1)** and **Deconvolution Function** (\Rightarrow NMDT_0008 and 0059).