Delta Tips

NMDT_0064

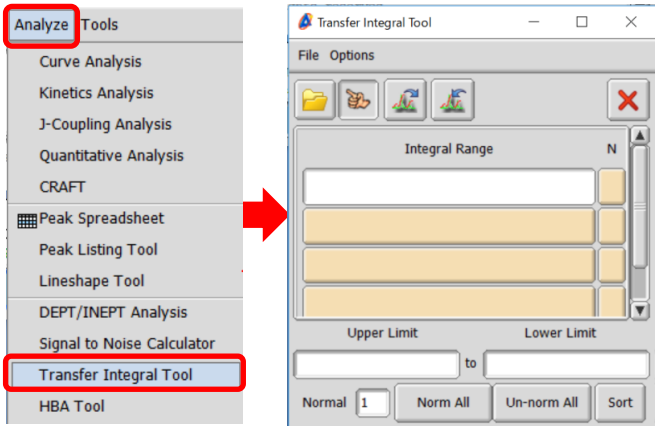
Delta V5.3.1 Transfer Integral Tool

This issue of Delta Tips explains functions of **Transfer Integral Tool** in Delta V5.3.1.
New **Transfer Integral Tool** allows us to set the number of data points around the start and the end of the selected integration interval, which is used to automatically estimate the baseline.

★ For **Transfer Integral Tool** in Delta V5.3.0 and lower versions, please refer to Delta Tips **Integration: Transfer Integral Tool** (⇒NMDT_0037).

The **Transfer Integral Tool** can save and copy integral ranges from one spectrum to another one. This function is very useful if you need to integrate several to many spectra in the same way.

① Select **Analyze – Transfer Integral Tool** to open the **Transfer Integral Tool** window.

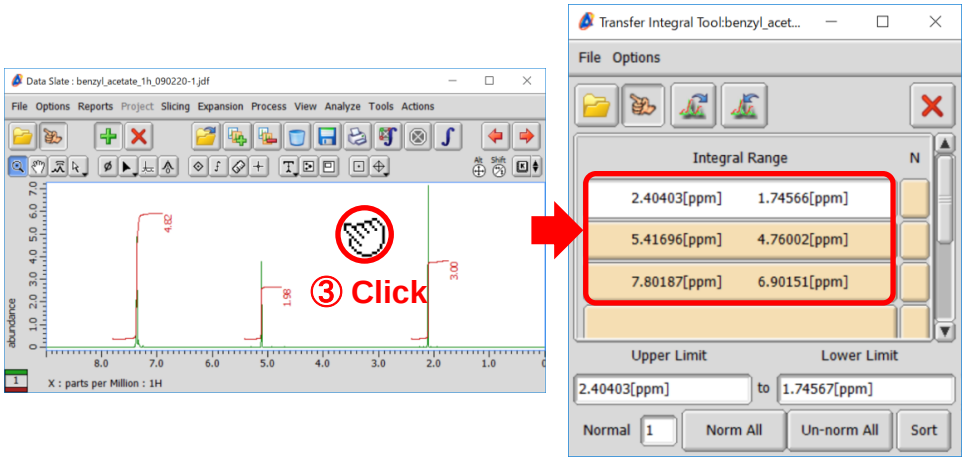


② Click the  button in the **Transfer Integral Tool** window.

Note that the cursor has changed into the **Finger symbol**  .

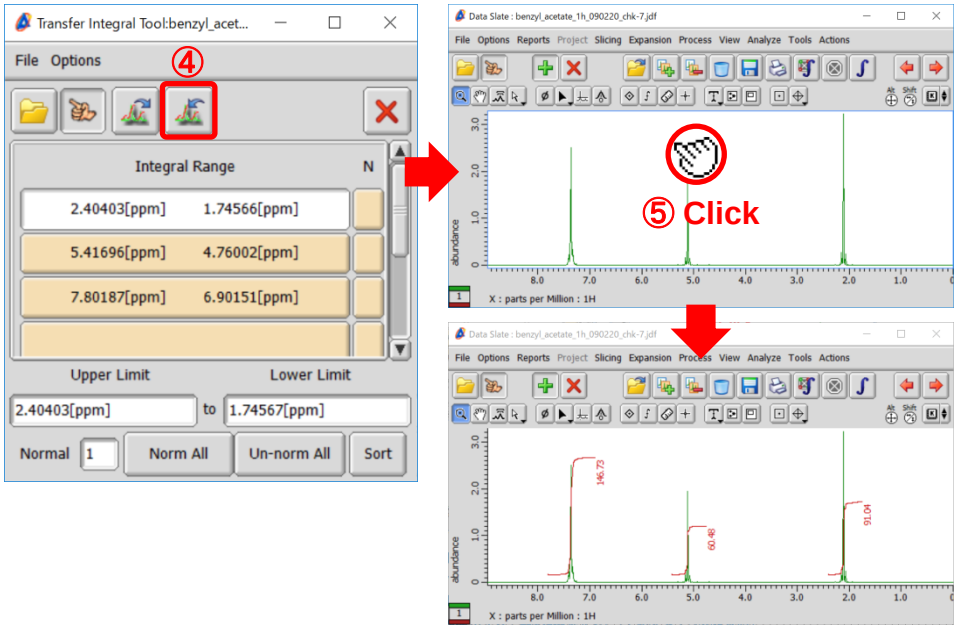
③ Click the spectrum to load the integral ranges from with the cursor.

The integral ranges are displayed in the **Transfer Integral Tool** window.



④ To transfer the integral ranges to another spectrum, click the  button in the **Transfer Integral Tool** window. Note that the cursor has changed into the **Finger symbol**  .

⑤ Click the spectrum to set the integral ranges into with the cursor.
The integral data is shown on it.

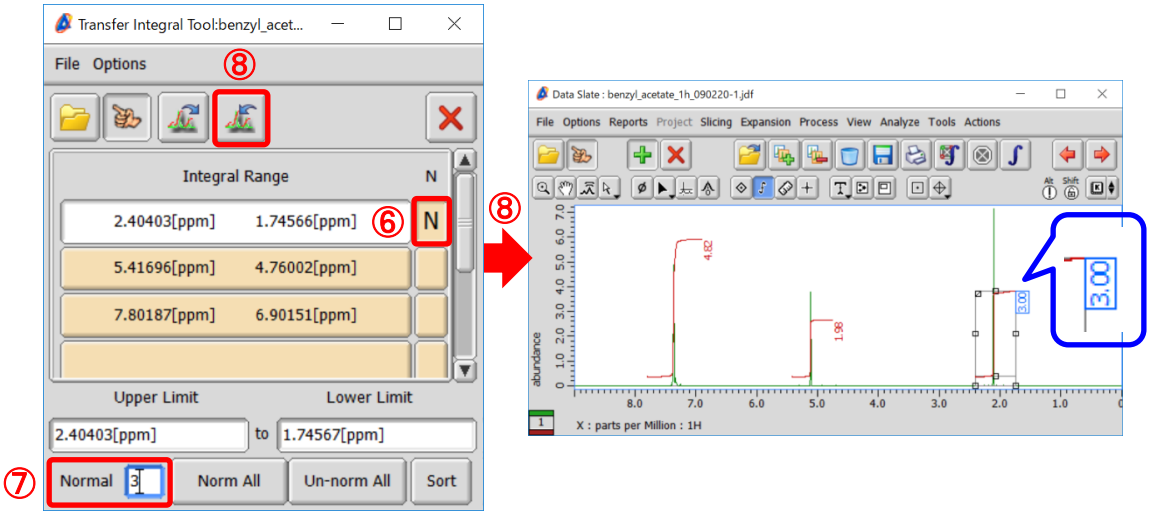


Normalization:

⑥ Click the **N** button of the integral range which you would like to normalize in the **Transfer Integral Tool** window. Note that **N** is displayed on the button.

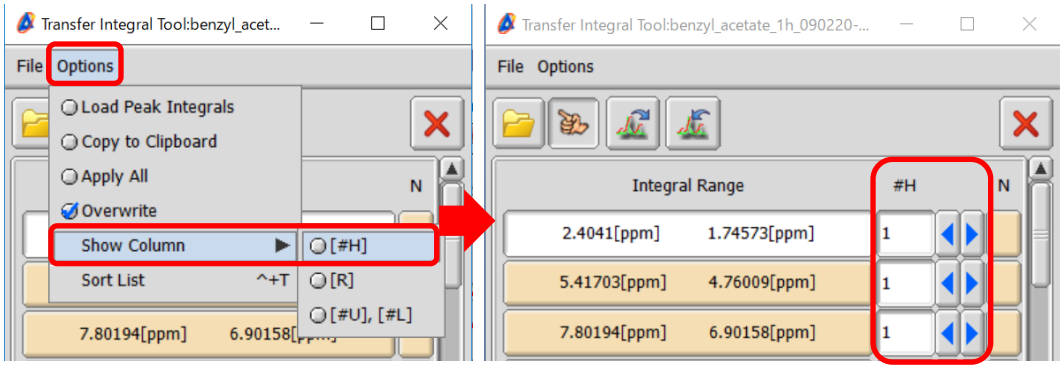
⑦ Input the normalization value into the **Normal** box. We set 3 in the example below.

⑧ Click the  button and then select the spectrum to apply the integral ranges and the normalization to, as shown in ④ and ⑤ .

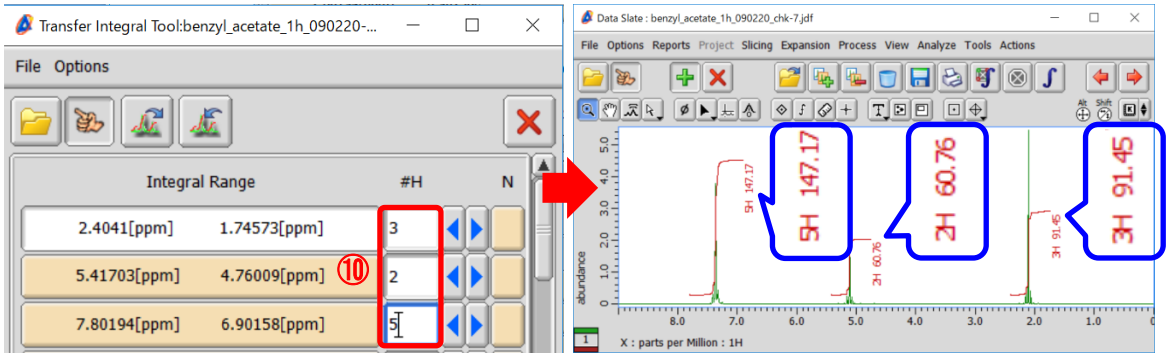


Number of protons:

⑨ Select **Options**—**Show Column**—**[#H]** to display the **#H** column in the **Transfer Integral Tool** window.



⑩ Input the number of protons into the **#H** box and select the spectrum to apply the changes as shown in ④ and ⑤.

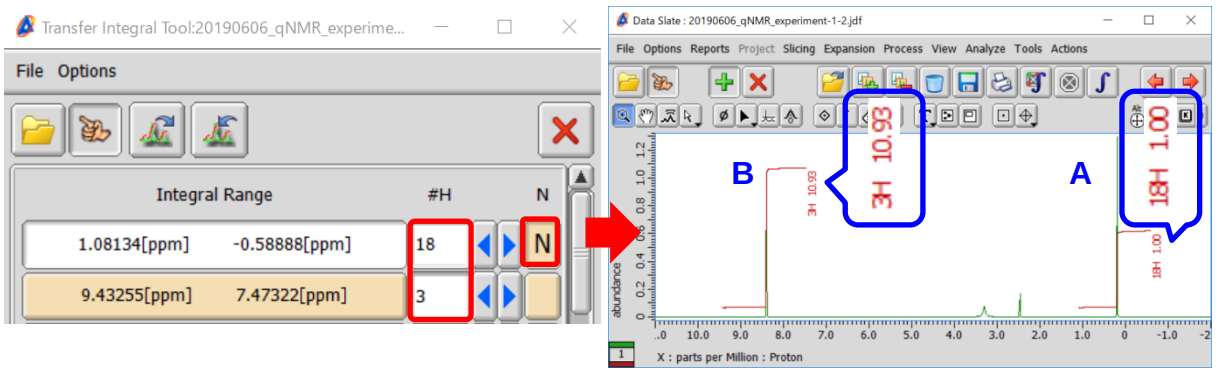


★ How to calculate the relative ratio of components in a mixture

If your sample contains several molecules, it is possible to determine the relative ratio as follows:

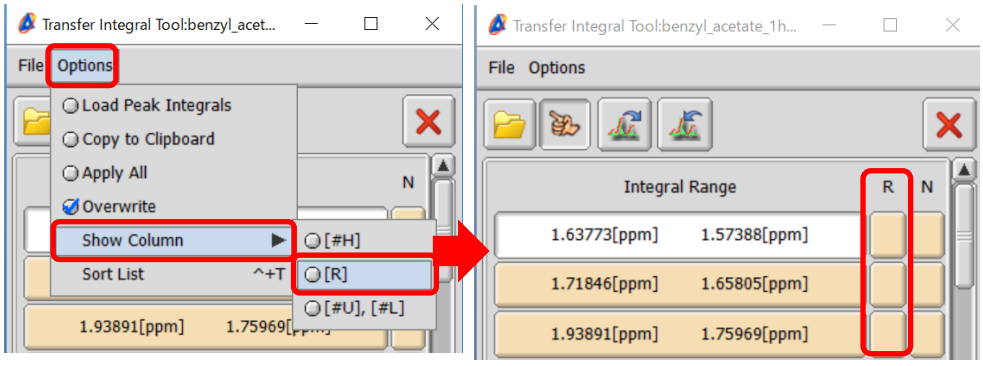
Set the number of protons and the **N** button in the **Transfer Integral Tool** window.

In the example below, the sample is composed of components A and B. The relative ratio of A and B is shown as 1.00 : 10.93.

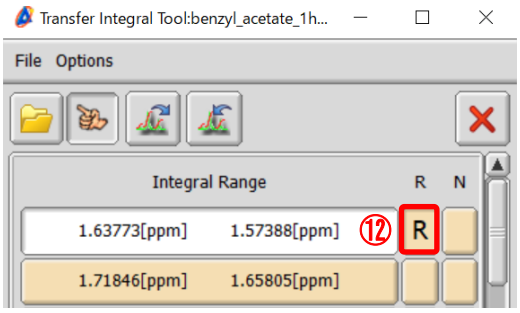


Set the slope and offset of integration baseline to 0:

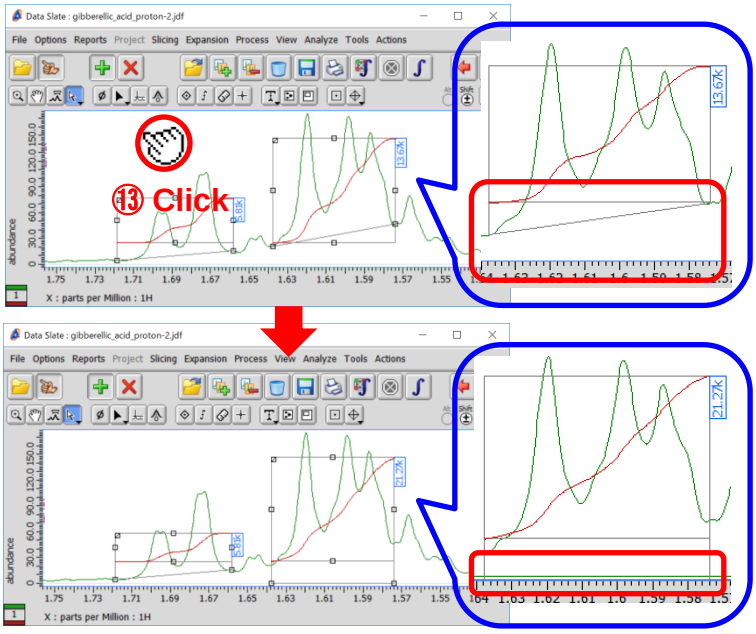
⑪ Select **Options**—**Show Column**—**[R]** to display the **R** column in the **Transfer Integral Tool** window.



⑫ Click the **R** box of the integral range which you wish to reset.



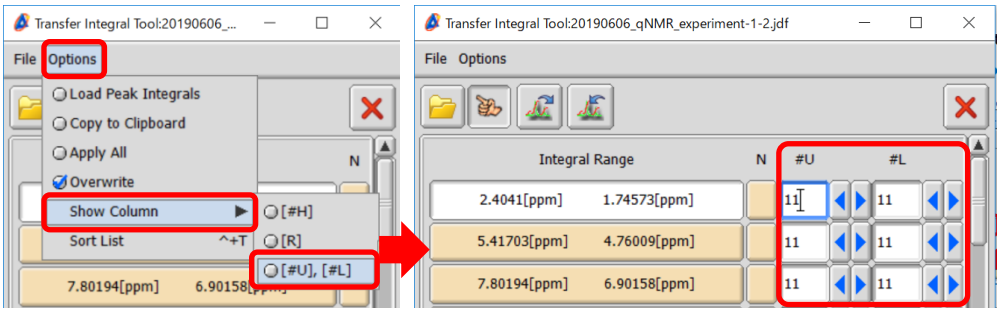
⑬ Select the spectrum to apply the changes as shown in ④ and ⑤.



★ For the details on the baseline of integration,
refer to Delta Tips **Interval and Baseline of Integration** (⇒NMDT_0060).

Baseline is automatically estimated from the average intensity of data points around the start and the end of the selected integration interval.
It is possible to set the number of data points as follows:

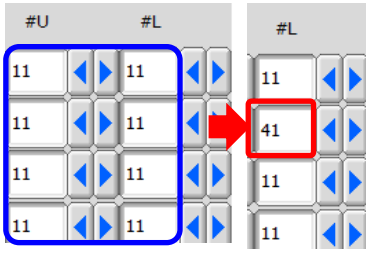
⑭ Select **Options**—**Show Column**—**[#U],[#L]** to display the **#U** and **#L** columns in the **Transfer Integral Tool** window.



⑮ Input the number of data points into the **#U** and **#L** input boxes.

#U: the upper limit of the integral interval
(low field (high frequency), the left side of the ruler (chemical shift))

#L : the lower limit of the integral interval
(high field (low frequency), the right side of the ruler (chemical shift))



Default value = 11

⑯ Select the spectrum to apply the changes as shown in ④ and ⑤.