NMDT_0064

Delta V5.3.1 Transfer Integral Tool

NMR data processing software Delta NMR Software v5.0

190816 3

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.

	💰 Transfer Integral Tool:benzyl_acet — 🛛 🛛 🗡
	File Options
🖉 Data Slate : benzyl_acetate_1h_090220-1.jdf — 🗆 🗙	
File Options Reports Project Slicing Expansion Process View Analyze Tools Actions	🔁 🐌 🛷 🐇
😑 🐌 💠 🗙 🚰 💺 💼 🗖 😓 🦉 🕲 🕽 🔶 🌳	
	Integral Range N
	2.40403[ppm] 1.74566[ppm]
	5.41696[ppm] 4.76002[ppm]
	7.80187[ppm] 6.90151[ppm]
8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0	Upper Limit Lower Limit
1 X : parts per Million : 1H	2.40403[ppm] to 1.74567[ppm]
	Normal 1 Norm All Un-norm All Sort

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- To transfer the integral ranges to another spectrum, click the solution 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.

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

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X : parts per Million : 1H

8 Click the spectrum to apply the integral ranges and

the normalization to, as shown in 4 and 5 .

🔗 Transfer Integral Tool:benzyl_acet — 🗌	\times	
File Options 8		
🔁 🐌 🌌 🌌	×	Data Slate: benzyLacetate_1h_090220-1.jdf - X File Options Reports Project Slicing Expansion Process View Analyze Tools Actions
Integral Range	N	
2.40403[ppm] 1.74566[ppm] 6	N	
5.41696[ppm] 4.76002[ppm]		
7.80187[ppm] 6.90151[ppm]		
Opper Limit Lower Limit		1 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0
2.40403[ppm] to 1.74567[ppm]		- X, parts per Pannon, 11
Normal 3 Norm All Un-norm All	Sort	



Number of protons:

9 Select Options - Show Column - [#H] to display the #H column

in the Transfer Integral Tool window.

Ø	Transfer Integral Tool:benzyl_acet	- 🗆	×	Transfer Integral Tool:benzyl_acetate_1h_090220	_		\times
Fil	eOptions			File Options			
	O Load Peak Integrals		Y				
Ľ	Copy to Clipboard						
	Apply All		N	Integral Range	#H	N	
	🥏 Overwrite						
$\ $	Show Column	_[#H]		2.4041[ppm] 1.74573[ppm]	1		
	Sort List ^+T	○[R]	H	5.41703[ppm] 4.76009[ppm]	1		μ
	7.80194[ppm] 6.90158[○[#U], [#L]	7.80194[ppm] 6.90158[ppm]	1		

(1) Input the number of protons into the **#H** box and select the spectrum to apply the

changes as shown in ④ and ⑤.

Transfer Integral Tool:benzyl_acetate_1h_090220	_	×	🖉 Data Slate : benzyl_acetate_1h_090220_chk-7.jdf — 🗆 🗙
File Ontions			File Options Reports Project Slicing Expansion Process View Analyze Tools Actions
			┢╸┝╴╲╴╔╩╚╔╗╔╗╗
		X	
Integral Range		N	60.7 91.4
2.4041[ppm] 1.74573[ppm]	3		ੑੵੵੑੑੑ <u>ੑ</u> ੑੑੑੑਸ਼ੑੑੑੑਸ਼ੑੑੑੑੑਸ਼ੑ
5.41703[ppm] 4.76009[ppm]	2		
7.80194[ppm] 6.90158[ppm]	۶Į		8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 X : parts per Million : 1H X

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.

🖉 Transfer Integral Tool:20190606_qNMR_experime — 🛛 🛛 🛛	Data Slate : 20190606_qNMR_experiment-1-2.jdf
	File Options Reports Project Slicing Expansion Process View Analyze Tools Actions
File Options	😑 🐌 🕂 🗙 🚰 💁 🖬 🖯 🗧 😓 🗳 🚳 🕤 🖕 🍁
	9 T
Integral Range #H N	
1.08134[ppm] -0.58888[ppm] 18	A 00 00 00 00 00 00 00 00 00 00 00 00 00
9.43255[ppm] 7.47322[ppm] 3	
	0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 -1.0 -2
	1 X : parts per Million : Proton

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Set the slope and offset of integration baseline to 0:

(1) Select Options – Show Column – [R] to display the R column in the Transfer Integral

Tool window.

💋 т	ransfer Integral Tool:benzyl_acet	- 🗆	×	👂 Transfer Integral Tool:benzyl_acetate_1h 🚽 🗌	\times
File	Options	_		File Options	
	O Load Peak Integrals		Y		
	Copy to Clipboard				
	⊖ Apply All		N	Integral Range	
	🧭 Overwrite				<u> </u>
	Show Column	○[#H]		1.63773[ppm] 1.57388[ppm]	
	Sort List ^+T	○[R]		1.71846[ppm] 1.65805[ppm]	٦U
	1.93891[ppm] 1.75969[○[#U], [#I	L]	1.93891[ppm] 1.75969[ppm]	

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

💋 Transfer Integral Tool:benzyl_acetate_1h	—		×					
File Options								
📔 🐌 🌌 🌌			×					
Integral Range	Integral Range							
1.63773[ppm] 1.57388[ppm]	12	R						

(1) Select the spectrum to apply the changes as shown in (4) and (5).

Data Slate : gibberellic_acid_proton-2.jdf	- • ×
File Options Reports Project Slicing Expansion Process View Analyze Tools	Actions
1.75 1.73 1.71 1.69 1.67 1.65 1.63 1.61 1.59	
1 X : parts per Million : 1H	
Press files a sile and anotae 214	
Eile Ontions Reports Project Slicing Expansion Process View Applying Tools	Action
Image: A the state of the s	
0 0 0 0 0 0 0 0 0 0 0 0 0 0	

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

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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:

Select Options - Show Column - [#U],[#L] to display the #U and #L columns

in the Transfer Integral Tool window.

🔗 Transfer Integral Tool:20190606 – 🗆 🗙	Stransfer Integral Tool:20190606_qNMR_experiment	-1-2.j	df	-	
File Options	File Options				
 Load Peak Integrals Copy to Clipboard 	📔 🐌 🌌 🌋				×
O Apply All N	Integral Range	N	#U	#L	
Show Column	2.4041[ppm] 1.74573[ppm]		11	11	
Sort List ^+T Q[R]	5.41703[ppm] 4.76009[ppm]		11	11	
7.80194[ppm] 6.90158[,,	7.80194[ppm] 6.90158[ppm]		11	11	

(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))

	#U			#L		_	#L		
	11			11			11		
	11			11	◀		41	◀	
	11			11	◀		11		
	11			11			11	Ī	
C	Defaul	lt v	al	ue = 1	1				

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



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