Delta Tips

NMDT_0017

NMR data processing software

140121-1

How to Report Diffusion Coefficient

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

① 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.

Curve Analysis: CD_glu_bpp_led_dosy_no2-1-3.jdf	50[mT/m]							
File Options	30[111/11]							
	Mode: Diffusion Analysis)						
80 graph 90								
	Y Type = G:mT/m Oms Δms y = 2.67515E+8	d/sT]						
5.3 5.1 4.9 4.7 4.5 4.3 4.1 3.9 3.7 3.5 3.3 3.1 2.9		<u>mhmhmhml</u> wuhm						
RAAAABBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	G = [m]	^{7/m]} 5.3 5.1 4.9						
	δ = 2.7 [ms	s] 📈 📈						
	Δ = [100 [ms	^{s]} 844 88						
	st Coef = 99.05[ms]							
I ne selected peaks	D = 2.1353069177E-10[m2/s] Calibrate							
are shown in blue	I(0) = 0.23364							
dance -0.8	χ ² = 0.00081 Tł	This <i>D</i> value belongs to the						
abun	σ = 0.00709 peak which is marked by the							
1.0 2.0 3.0 4.0 \triangle symbol (δ 4.969 ppm)								

- ★ 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
- ② 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

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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.
The File Information

& Curve Analysis: CD, alu ban led dosy, no2-1-3.1df	window
File Options	
📔 🐌 🚰 🛞 🍰 🖩 🚯 🗢 🔿 Pick Peak 🭕	1 Mode: Diffusion Analysis
	File Information: [CD_glu_bpp_led_dosy_no2-1-3.jdf]
8 = Y = 50[mT/m]	File View Formatting
ree 04 0.6	
	Parameters Reports Peaks Processing Rulers Experiment Molecules
	Reports in this file
Image: State of the s	DIFFUSION ANALYSIS (4.96891[PPM]) : CURVE_ANALYSIS (16-JAN-2017 17:25:43)



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6 Select 'CURVE_ANALYSIS' to display the report.

ĺ	💰 File Inform	nation: [CD_gl	u_bpp_led_d	osy_no2-1-3.jdf]		
	File View					
The Reports tab	Paramete	ers Reports	Peaks Proc	cessing Rulers Experiment Molecules		
	Reports in th	nis file				
List of reports	DIFFUSION	ANALYSIS (4.9	6891[PPM]):	CURVE_ANALYSIS (16-JAN-2017 17:25:43)		
				•	-	
	CD_glu_bpp	led_dosy_no	2-1-3.jdf			
	Vector at	4.96891[ppm]				
	Diffusion	Analysis				
	st Coef = 99.05[ms]					
	D = 2.1353	069177E-10[m:	2/s]			
	1(0) = 0.2	3364				
	x	Y	Intensity			
				•	• • • • • • • • • •	Report
	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]	0.161[T/m]	0.136			
	4.969[ppm]	0.178[T/m]	0.165			
	4.969[ppm]	0.194[T/m]	0.155			
					2	

 \bigcirc 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).

