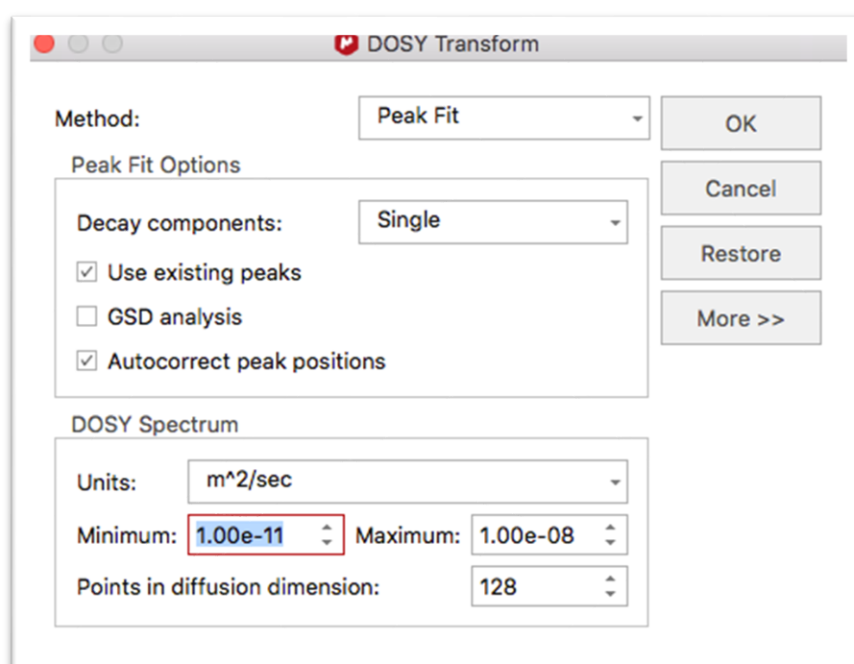


DOSY Processing with Mnova 14.0

- Open the DOSY spectrum
- Open the following Tables: *Stacked items* ; *Peaks* ; *Data Analysis*
- Select all spectra in *Stacked items* table > Processing > autobaseline correction

Pseudo-2D DOSY spectrum: peak by peak analysis

- **Analysis > Peak by Peak:** Perform a peak picking manually by selecting, on the stacked spectra (first one of the series), the signals to be considered for the DOSY transform.
In the Peaks table: delete every existing peak (if there are peaks) before selecting the right ones.
Note: If we do not select manually the peaks before the DOSY processing, then Mnova applies an automatic peak peaking over the full spectrum.
- **NMR > Stacked > DOSY Transform**



>> Values of D in m²/s

Integration mode with curves

Data Analysis:

- **Edit Model Options** > select « **Best fit** » Function
(or from the Data Analysis table : screwdriver)

Y-Filling Options

Y-Filling Policy

Replace Active Column

Auto Adjust Regions

Number of Handlers:

Automatic Y'-Filling Policy

Fit Function:

Peak Intensities

Parabolic Interpolation

f1 +/-:

Apply Local Phase Correction

- **New > Integrals Graph**
- Integration of the corresponding signals (select “integration” in the Data Analysis table)
- Click on the [Y'(X)] column to open the Y'-Column model function window and choose **Three Parameter Exponential Fit**.
- Click on Report
- From the equation, G gives the diffusion coefficient value and the error.

Functions

	Name	Function	Initialization	Report	Description
1	Linear Fit	$A+B*x$	A= 0, B= 0		Zero Order Reaction Rate
2	Mono-exponential Fit	$B*\exp(-x*F)$			Exponential Decay, First Order Reaction Rate
3	Three Parameter Exponential Fit	$B+F*\exp(-x*G)$			Exponential Decay, First Order Reaction Rate With Offset
4	Inverse Linear Fit	$1/(A+B*x)$	A= 1, B= 0		Second Order Reaction Rate
5					

Fitted Parameters

B= -8172.34, F= 392118, G= 1.48738e-05
rError = 1.60981e-06, probnotmono = 0.99379

>> Values of D in cm²/s

Note: the plot is also possible with peaks (rather than integrations)