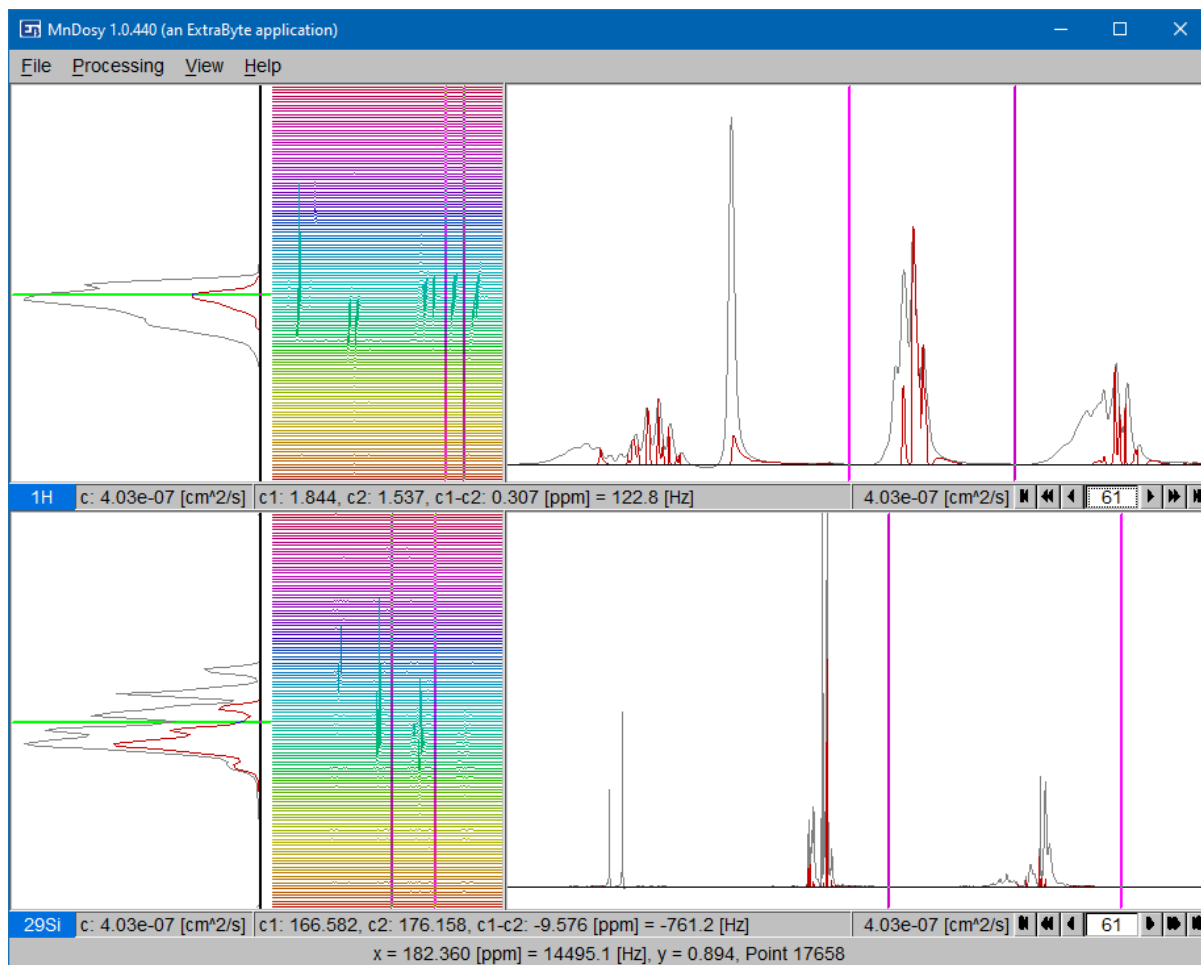


MnDOSY

User Manual

1.0.440



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What is MnDOSY

MnDOSY is a specialized software package for *processing NMR DOSY data*. It allows processing of a single-nucleus DOSY dataset, as well as correlated processing of two DOSY datasets obtained with the same sample but two different nuclei such as, for example, ^1H and ^{29}Si .

The highlights of MnDOSY include, apart from the capability to correlate DOSY data for two different nuclei, a very high degree of *automation*, rich *reporting* features, and a broad range of *data-export* modalities.

An MnDOSY user does not need to be an NMR expert. All spectra pre-processing is done automatically, and so is the fast DOSY transform. While MnDOSY provides access to the pre-processing choices for NMR experts, most MnDOSY users will use it as a black-box and rely on the utility's intrinsic capability to choose and apply the most suitable processing methods.

MnDOSY allows the user to export the data in various formats and produce various kinds of reports, from a synthetic summary to extremely detailed, depending upon user-defined configurations.

At present, MnDOSY reads only data acquired on Bruker NMR spectrometers, but we plan to extend this to instruments of any make, produced by any OEM.

Glossary:

NMR	Nuclear Magnetic Resonance
DOSY	Diffusion Ordered Spectroscopy
MnDOSY	Multi-Nuclear DOSY
OEM	Original Equipment Manufacturer

Further reading:

Overview

Main menu

MnDOSY main window includes a menu bar at the top (see Figure 1), whose items are: "File", "Processing", "View" and "Help".

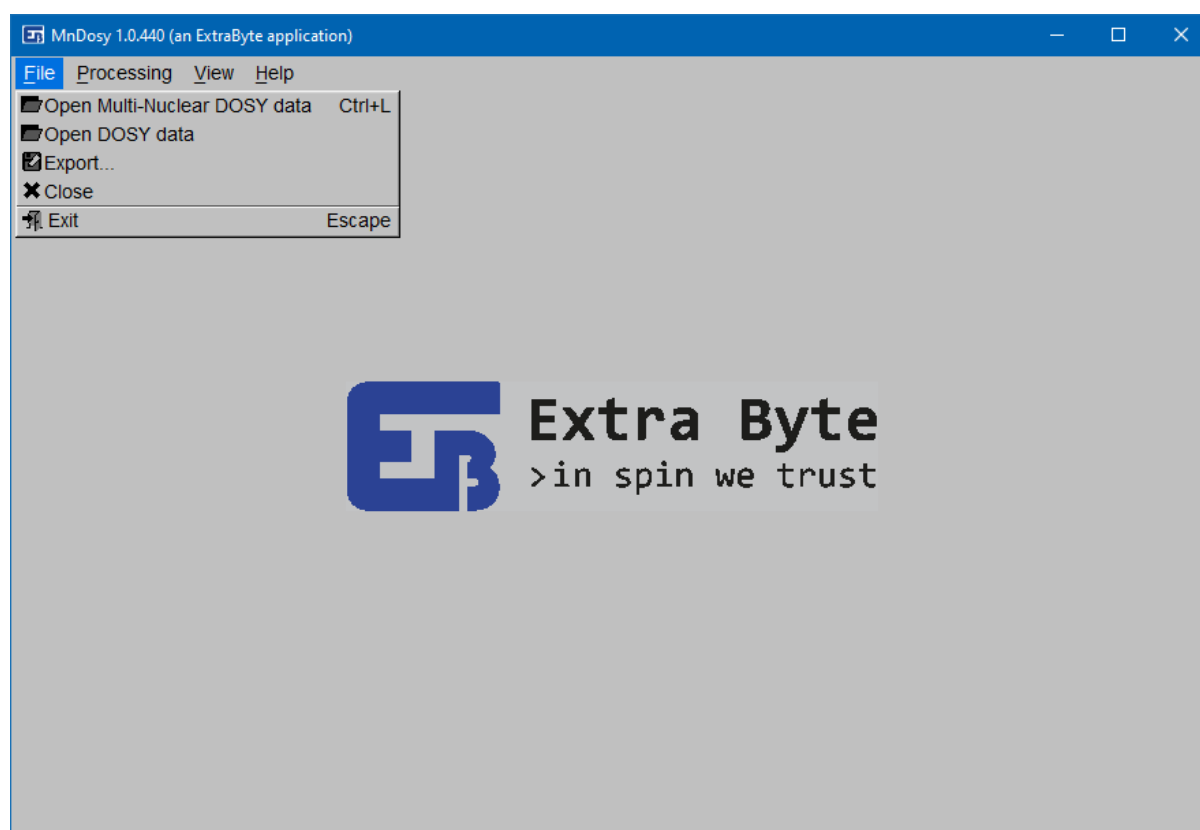


Figure 1. Main window appearance at program launch

File

- "Open Multi-Nuclear DOSY Data"
User is asked to load two Bruker 2D data files (*ser*). There is no test if the selected data come from a DOSY experiment or not. The order of selection is not important.
- "Open DOSY Data"
This allows to open just one Bruker 2D data file.
- "Export..."
When data have been loaded, this opens a very simple interface where user can decide what to export (1D or 2D data or 2D projection) and the destination file format (Scalable Vector Graphic image (.svg) or Comma-Separated Values text (.csv)). Also, it's possible to export into Bruker TopSpin format.
- "Close"
Close the opened file(s).

- "Exit"
Exit the application.

Processing

- "Setup..."
Open an interface where user can select the processing steps and options (see paragraph [Processing](#) for details).
- "Run FID processing"
Run basics processing of all loaded experiments from raw data up to spectra phase and baseline correction, according to what has been set in the Setup interface.
- "Run DOSY transform"
Run DOSY transform of current data, according to the Setup. This tests if current data have already been processed with the previous command (that is necessary to run DOSY).
- "Run all"
Run both FID processing and DOSY transform according to the Setup.
- "Undo"
Undo last operation (shortcut 'Ctrl+Z').
- "Restart"
Undo all operations up to original data (shortcut 'Ctrl+Home').

View

- "Preferences..."
Change graphic preferences (some are under development).
- "Data info..."
View a brief description of the loaded data

Help

- "Manual"
A link to the user Manual, which must be in the application folder.
- "License"
Show information about license. Also, user can register and activate a license. Registration occurs through email exchange with Extra Byte, which will provide all the payment details. After the payment, user will receive a proper key to activate the license.
- "About"
Open a window with some information about MnDOSY and Extrabyte.

Graphic interface

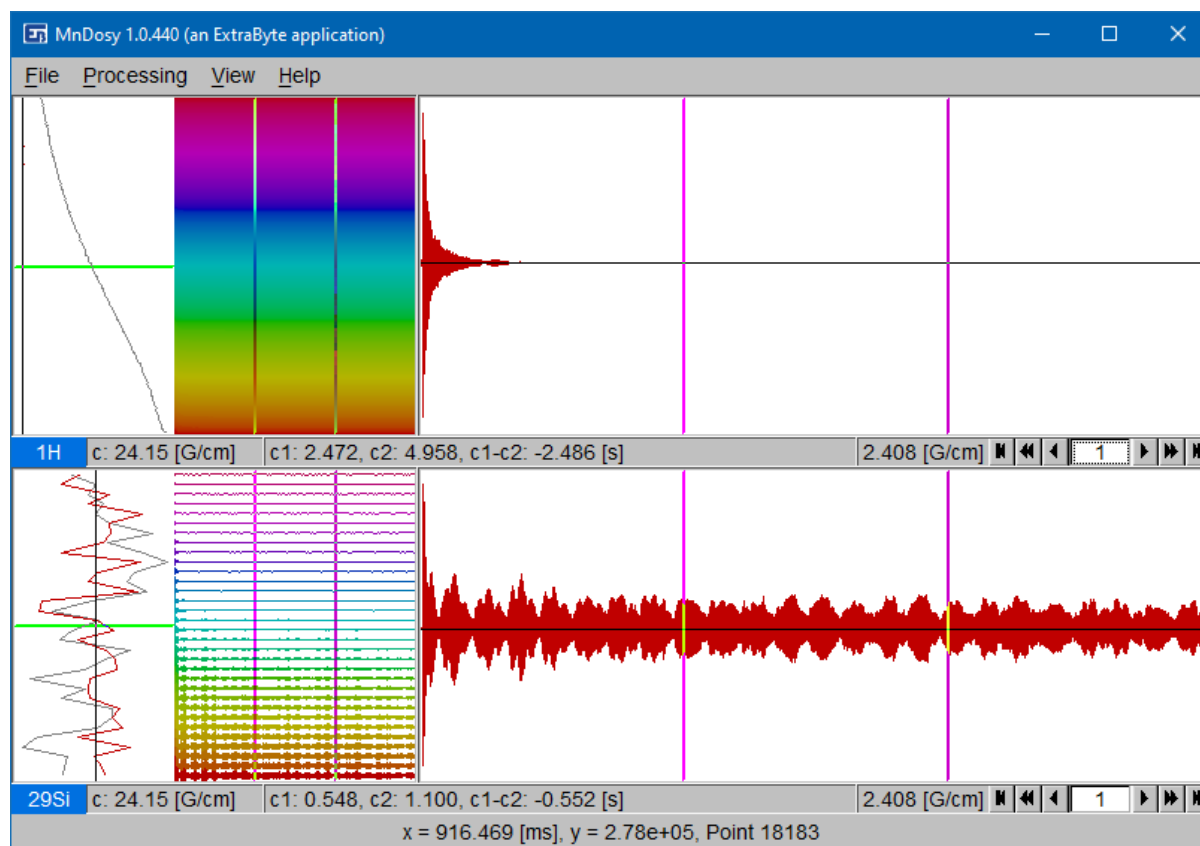


Figure 2. Main window appearance when data are loaded

General appearance

When data are loaded successfully, data are displayed in the space in the main window between the menu bar and the status bar. If user loaded two files, this space is divided equally into two horizontal layers (see Figure 2). Each layer is made of two canvases for 2D and 1D plots, and a bar for some information at the bottom. Canvases for 2D plots are at the left side, while those for 1D are at the right. All the canvases are resizable and their size are synchronized between the layers. Status bar always shows the mouse position coordinates. Frequency units are expressed both in *ppm* and *Hz*. All plots zoom state can be reset with a mouse double click.

2D map

2D canvas displays all the data in stacked horizontal lines equally separated, one for each trace (FID or spectrum). This dimension is fixed while one can zoom in along the horizontal dimension by dragging the mouse (zoom out by pressing 'Ctrl'), or vertically with the mouse wheel. In this canvas are present two vertical cursors synchronised with the correspondent 1D canvas x-axis. Their position is shown in the centre of the bar, along with their difference.

2D Projection

At the left side of the 2D canvas are plotted the projections of either all the spectrum points (grey) and those comprised between the cursors (red). In the "Preferences" interface (in "View" submenu)

one can set the projection mode (maximum value or arithmetic average). This projection can be zoomed with mouse wheel only. A horizontal cursor, synchronized to the other layer, can be moved vertically over this projection, and its real value position is shown in the bar, at left. After DOSY transform the cursor is synchronized also with the trace shown in the 1D canvas.

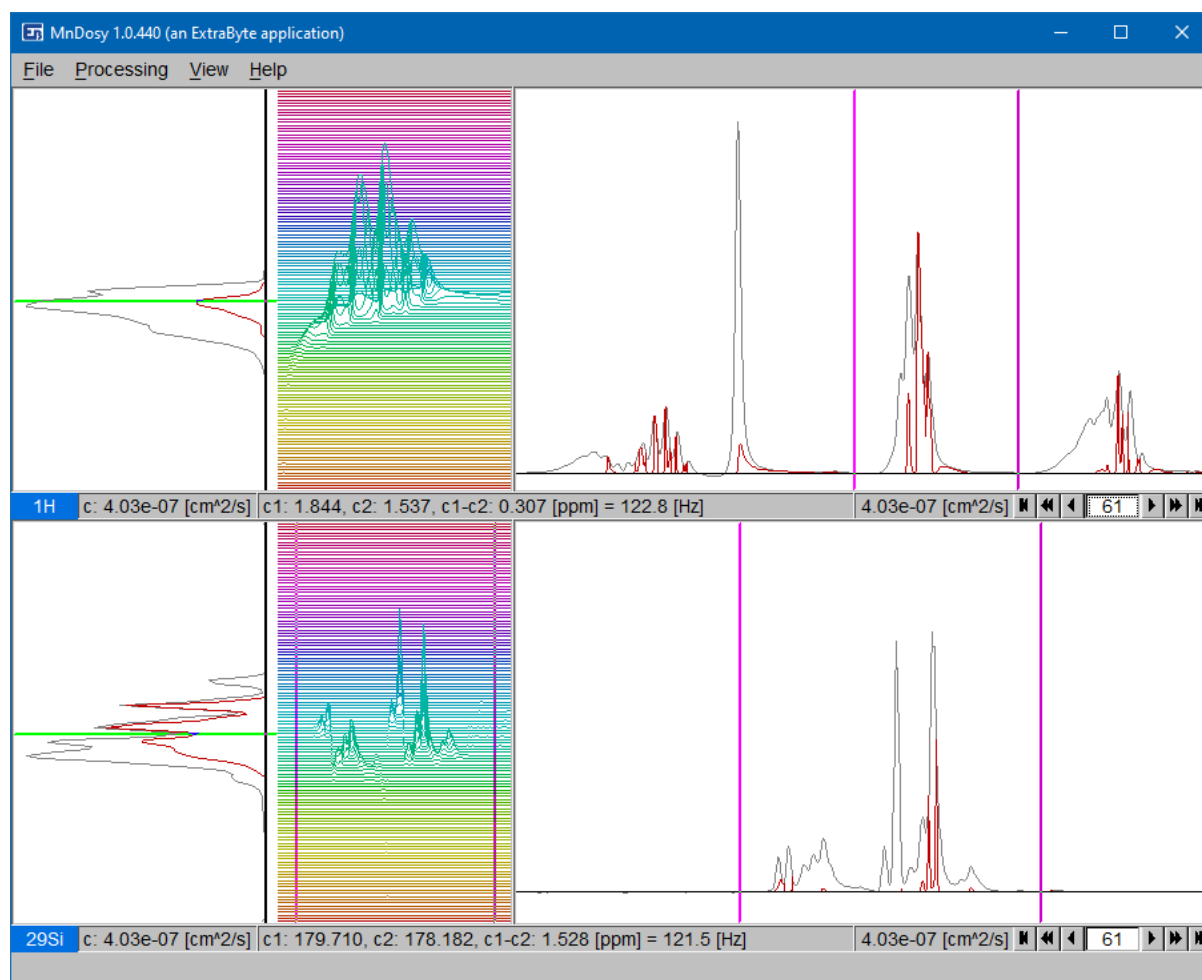


Figure 3. Example of main window appearance after DOSY transform

1D canvas

1D canvas displays each trace singularly, coloured in red. The arrows at the right side of the bar allow to switch trace (previous/next, 10 previous/next, first/last). DOSY traces are accompanied by a reference spectrum, coloured in black, that is the first frequency spectrum. DOSY traces are normalized on this spectrum. This plot can be zoomed in both horizontal and vertical directions by selecting a rectangle area with the mouse, zoomed out horizontally by dragging the mouse and pressing 'Ctrl', or zoomed in/out vertically with the mouse wheel. Also, 1D plot can be translated in any direction dragging the mouse together with pressing down 'x' on the keyboard.

Information bar

The bar at the bottom of the layer shows, from left to right: the nuclide name, the position of the projection cursor, the vertical cursors and their difference, the parameter correspondent to the trace selected in the 1D plot (that is the field gradient before the DOSY transform and the diffusion coefficient after).

Processing

"Setup" menu item opens a window, as shown in Figure 4, where user can prepare the processing settings.

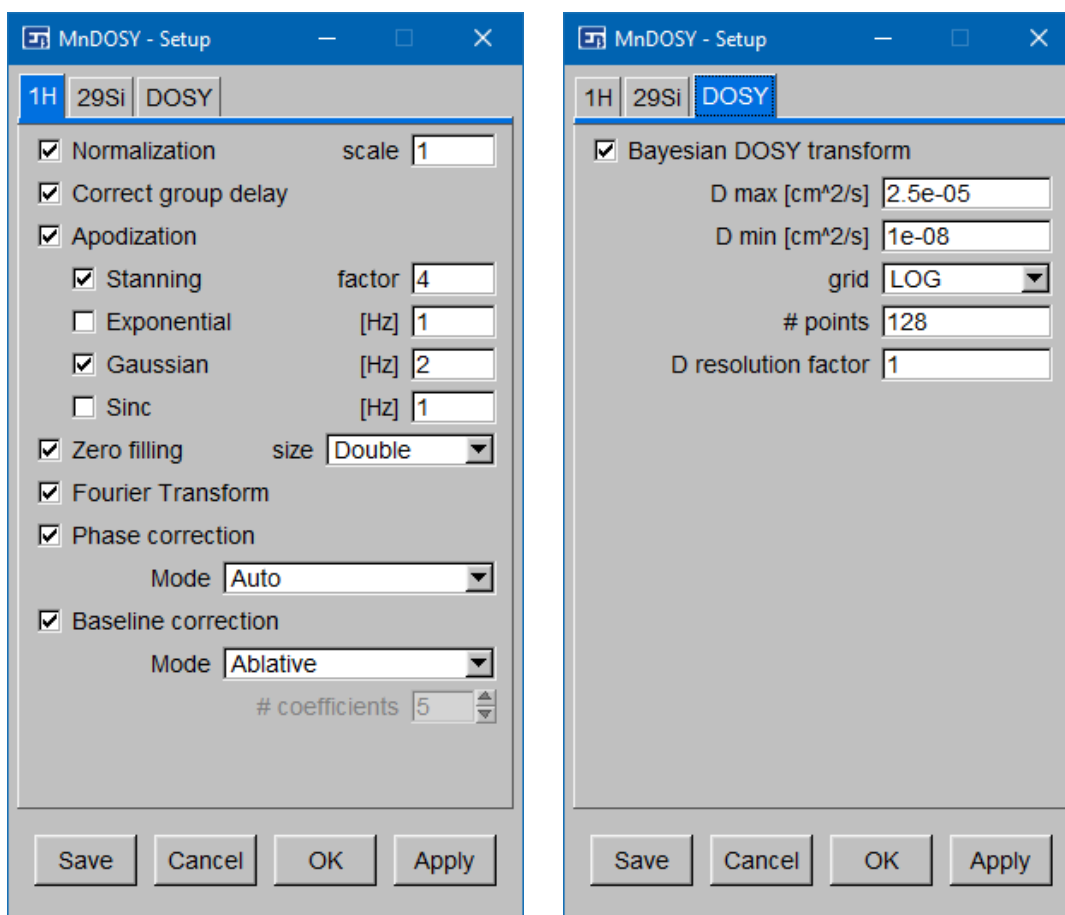


Figure 4. Processing setup interface

A three panels tab is shown: two of them allow to set the options for raw data processing up to spectra phase and baseline correction for the corresponding nuclide (1H or 29Si), while on the third tab the options for the DOSY transform. "Apply" button set the current input parameters for the next command calls. "OK" does the same and closes the interface, while "Save" saves all the parameters for the next MnDOSY session. "Cancel" button closes the interface and restore the last parameters saved with the other buttons.

In the main window menu bar, buttons "Run FID processing" and "Run DOSY transform" execute all the commands selected in the first two and third panels, respectively. Running the first command is necessary to run the second one. Undo any command with 'Ctrl+Z'. During execution, the setup interface can remain opened.

Description of the commands is following.

- "Normalization"
Better keep selected in order to avoid numerical overflow during successive evaluations.
- "Correct group delay"
Remove the group delay artifact that causes the known spectrum smiles.
- "Apodization"
Different apodization modes are available and can be combined. Modes and functions are described.

- Stanning

$$A(t) = \begin{cases} \cos^2(\alpha t) & \text{for } \alpha t < \pi/2 \\ 0 & \text{for } \alpha t \geq \pi/2 \end{cases}$$

Input parameter: number of times the mean decay time at which is $\alpha t = \pi/2$.

- Exponential

$$A(t) = e^{-\alpha t}$$

This apodization corresponds to a convolution product in the frequency domain between the spectrum and a Lorentz function, whose width is the input parameter.

- Gaussian

$$A(t) = e^{-\alpha t^2}$$

This apodization corresponds to a convolution product in the frequency domain between the spectrum and a Gauss function, whose width is the input parameter.

- Sinc (Cardinal Sine)

$$A(t) = \sin(\alpha t) / \alpha t$$

This apodization corresponds to a convolution product in the frequency domain between the spectrum and a rectangle function, whose width is the input parameter.

- "Zero filling"
Resize data points. New size is set by default as double the original one, but can be chose a power of 2 (necessary to switch to frequency domain). If the new size is greater, data are zero filled, otherwise truncated.

- "Fourier Transform"
Switch from time to frequency domain through the Fourier transform.
- "Phase correction"
Available modes:
 - Automatic (default)
 - Magnitude
 - Power (square magnitude)
- "Baseline correction"
Available mode:
 - Ablative
 - PcBc
Automatic Phase and Baseline Correction (Vasini, Sykora, & Cobas).
Parameter: number of coefficients to fit the baseline.
- "Bayesian DOSY transform"
Run DOSY transform through Bayesian method (Cobas & Sykora, 2010).
Parameter: minimum and maximum values of the diffusion coefficient, in cm^2/s , the grid type (linear or logarithmic) and the number of points necessary to calculate the DOSY map. The resolution factor is set to 1 as default.

Suggestion

You may start with a raw DOSY transform to quickly locate the DOSY spectrum range: set a wide diffusion range and not too many points. Then repeat with more precise parameters. Though this may be fast, if the grid is not enough fine then the peaks might be missed.

Bibliography

Cobas, C., & Sykora, S. (2010). *Progress in Bayesian DOSY and ROSY Transforms*. 51st ENC Conference, Daytona Beach, Florida (USA). doi:10.3247/SL3Nmr10.001

Vasini, E. M., Sykora, S., & Cobas, C. (n.d.). *PcBc - Novel Automatic Phase & Baseline Correction Algorithm*. 6th Practical Applications of NMR in Industry (PANIC 2018). doi:10.3247/SL7Nmr18.001