NYU Department of Chemistry
MNova User Guide – T1/T2 Analysis

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Open Data:

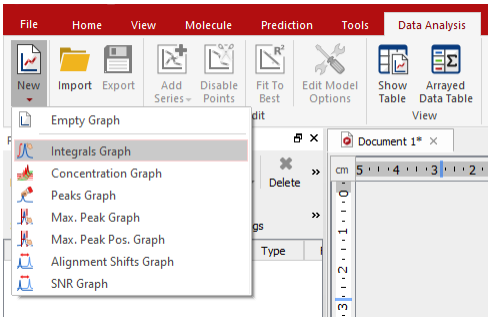
- Open your data set through the File -> Open menu.
- Browse to your data location and select the *ser*.
- MNova will read the processing parameter files from Topspin and process the data. A stacked plot of the spectra will be made.
- Once opened, the STACK and NMR menus will appear at the top.
- Inspect the spectrum and determine if further processing is required.

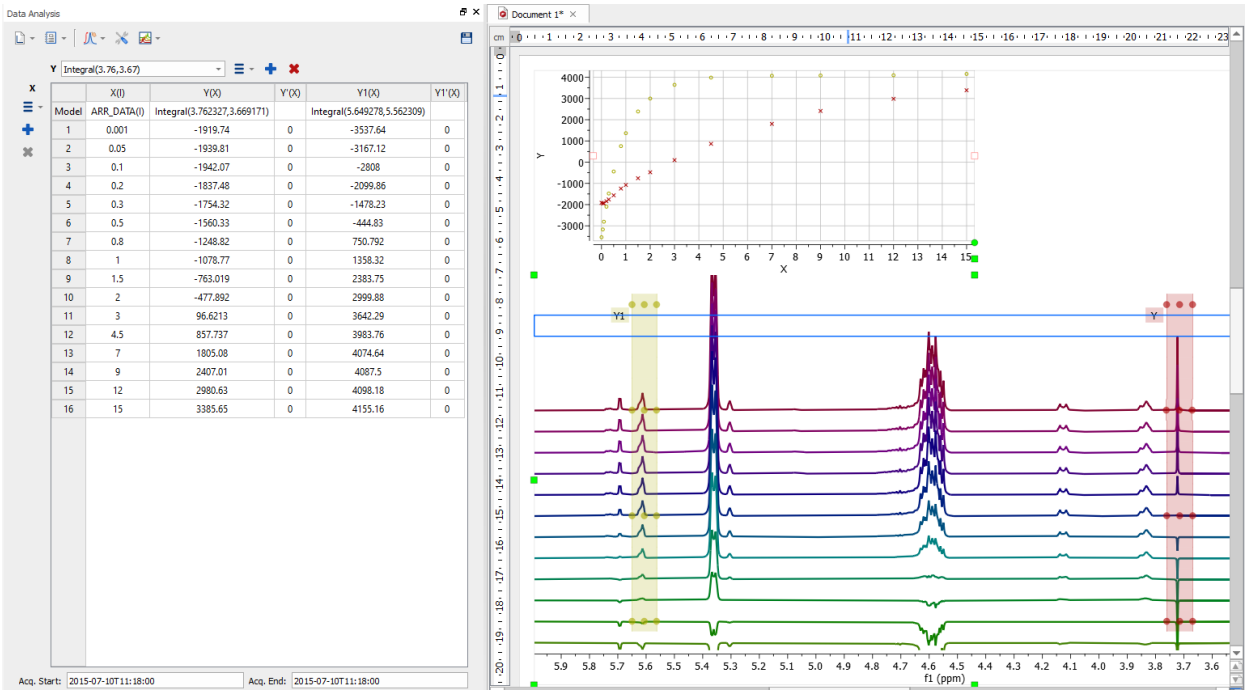
Processing:

- Processing is only required in the f1 dimension.
- Click on one of the spectra of the stacked plot and perform all 1D processing procedures as usual (See 1D Processing manual). Any changes made to the selected spectrum will automatically be applied to all other spectra.
- Always perform baseline correction to ensure that integrations are calculated correctly.

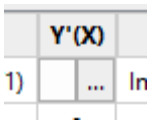
T1 Relaxation Analysis:

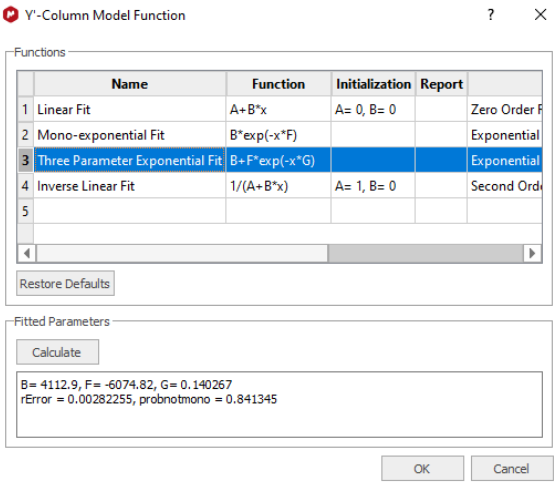
- Enter the Data Analysis tab and create a new Integrals Graph.
- This will bring you into integration mode. Select the peaks/regions to integrate.
- An integration table (Data Analysis window) with time points (X(I)) and integration values (Y(X)) as well as an XY-plot (in the spectrum page) will be generated as shown below.

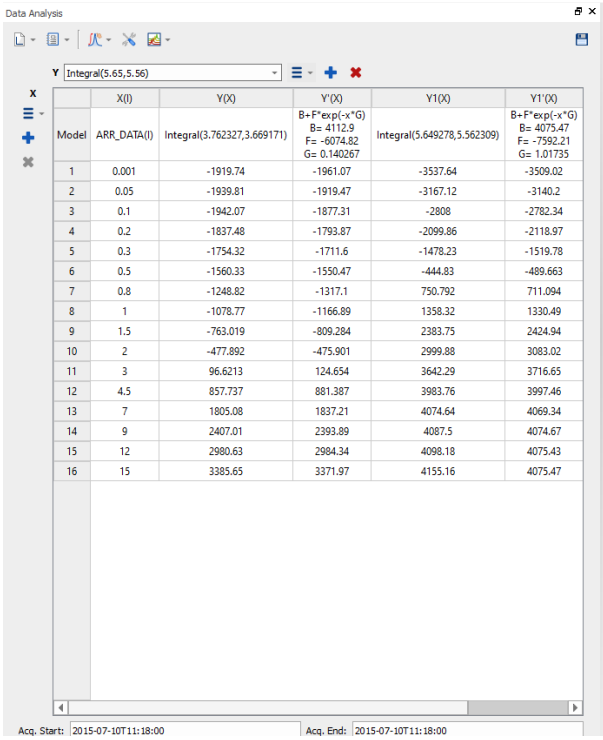


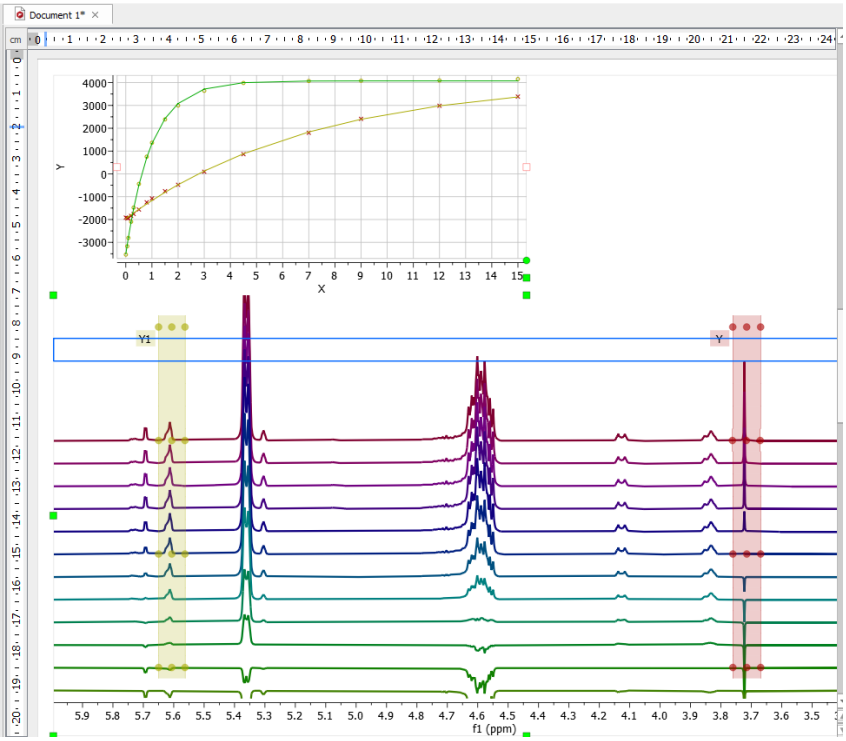


- In the Data Analysis window, click on the empty cell just below the Y'(X) column title to reveal a three dots menu.
- Press the three dots to open the Model Function menu.
- Select Three Parameter Exponential Fit and press calculate. The Fitting Parameters box will show the fitted values.
- The signal intensity at time (t) is defined by the equation $M(t)=M_0(1-2e^{-t/T1})$. The fitting function used here is $S=B+Fe^{-xG}$. Therefore, to calculate the relaxation rate, **T1 = 1/G**.
- Perform the above procedure to other peaks of interest.



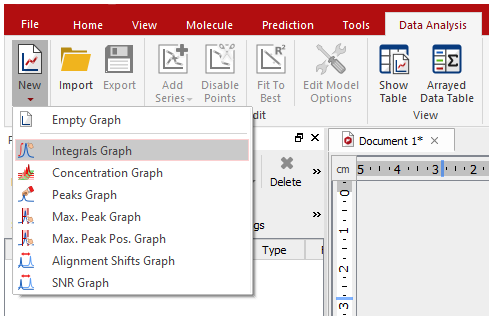


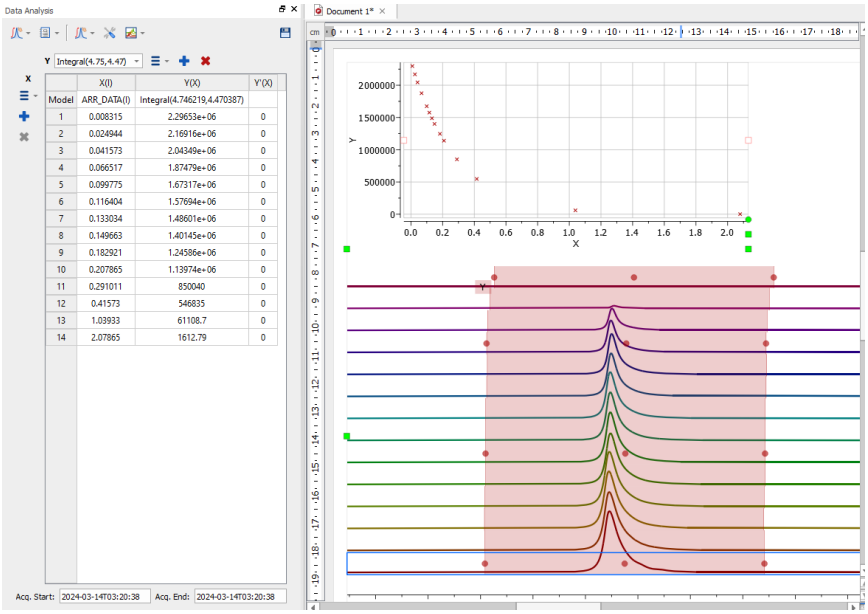




T2 Data Analysis:

- Similar to T1 analysis, create a new Integrals Graph and integrate the regions of interest.





- In the Data Analysis window, click on the empty cell just below the Y'(X) column title and press the three dots to open the Model Function menu.
- Select Mono-exponential Fit and press calculate. The Fitting Parameters box will show the fitted values.
- In the mono-exponential equation $B*e^{-xF}$ B is the magnetization at time 0 and F is 1/T2. Therefore, to calculate the T2 relaxation rate, **T2 = 1/F**.