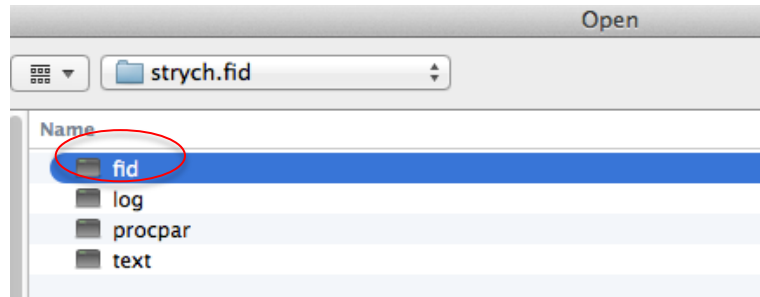


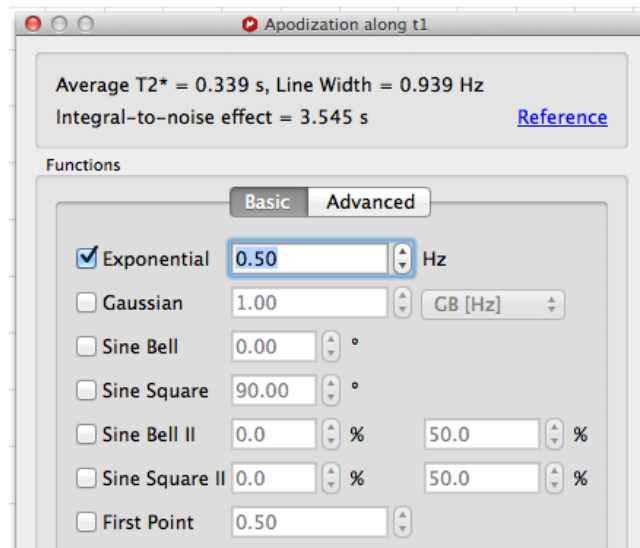
Mnova 1D NMR User Guide

To load and transform an FID data

(1) Click **File, Open**, then click the fid file to load the data. By default, the fid data will be automatically fourier transformed into spectrum.

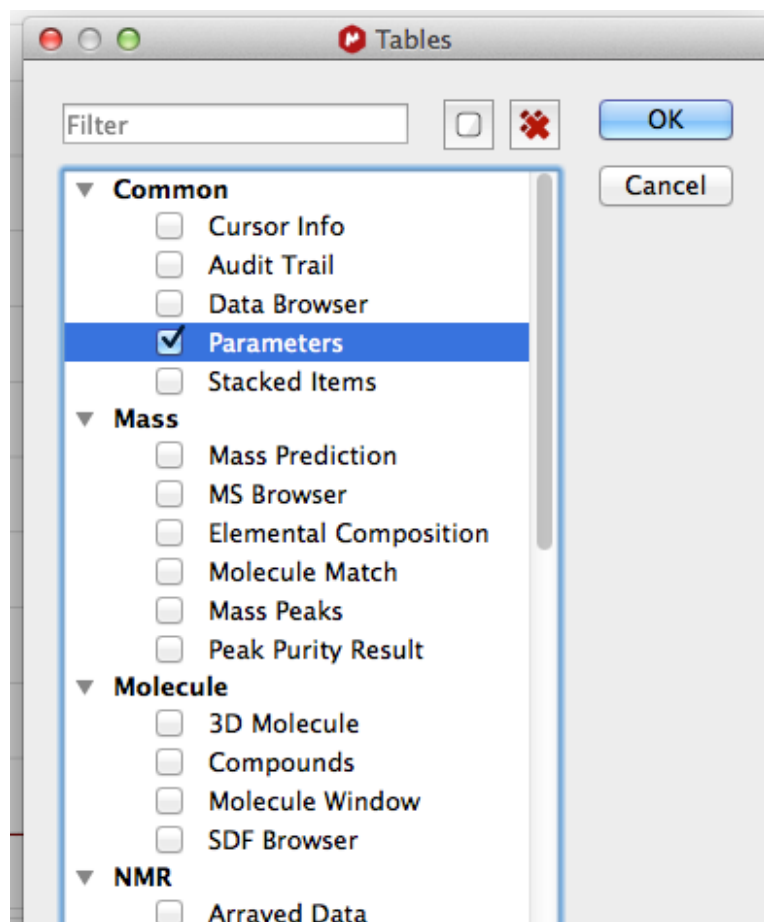


(2) If you would like to apply a different apodization than the default, simply click **Processing, Apodization**. In the pop-up window, choose the desired apodization function (e.g. exponential) and line broadening value (e.g. 0.5 Hz) and click **OK** to apply the new apodization settings.



To view experimental parameters


To check/view the experimental parameters such as relaxation delay, acquisition time, receiver gain, etc., click **View, Tables**. In the pop-up window, click **Parameters** and **OK**, then you will see a list of all experimental parameters. You may also click **Report** in the Parameters window to report the parameters in a text box on the spectrum.

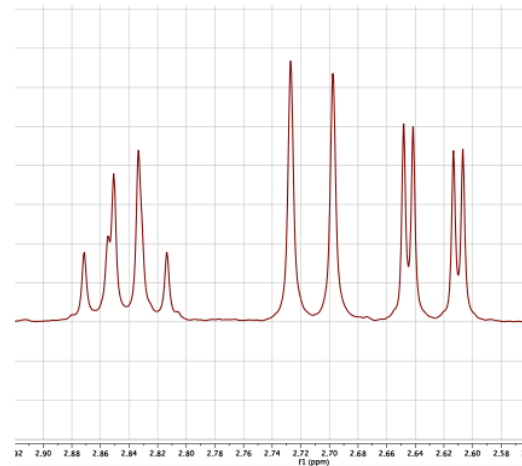
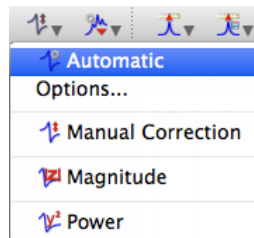
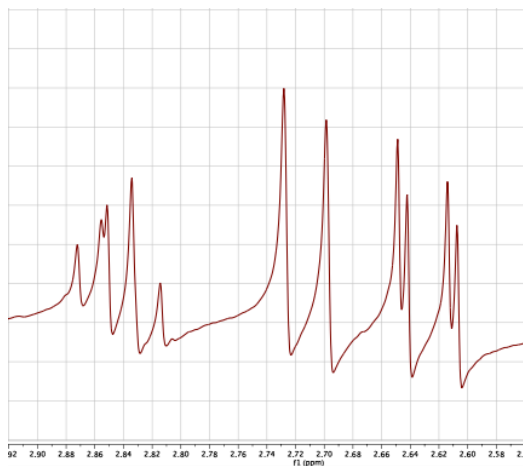


The 'Parameters' window displays a table of experimental parameters. The 'Report' button in the top toolbar is circled. The table lists 14 parameters and their values.


	Parameter	Value
1	Data File Name	/Volu...
2	Title	strych
3	Comment	STAN...
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	uplus
8	Author	
9	Solvent	CDCl3
10	Temperature	25.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	nsw500
14	Number of Scans	4

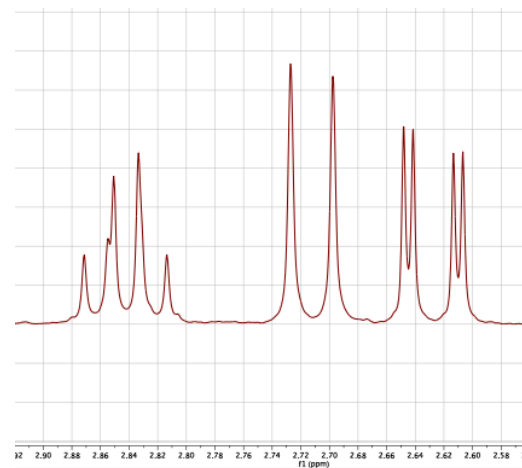
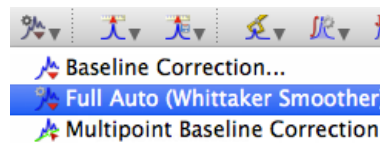
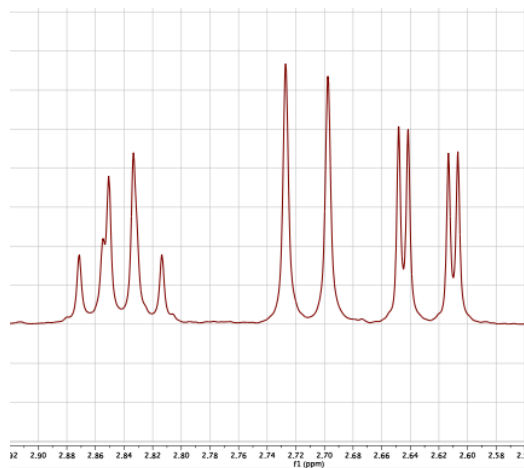
To correct the phasing

Click the icon  to correct phasing if needed. You may choose either **Automatic** or **Manual Correction** to phase the spectrum.



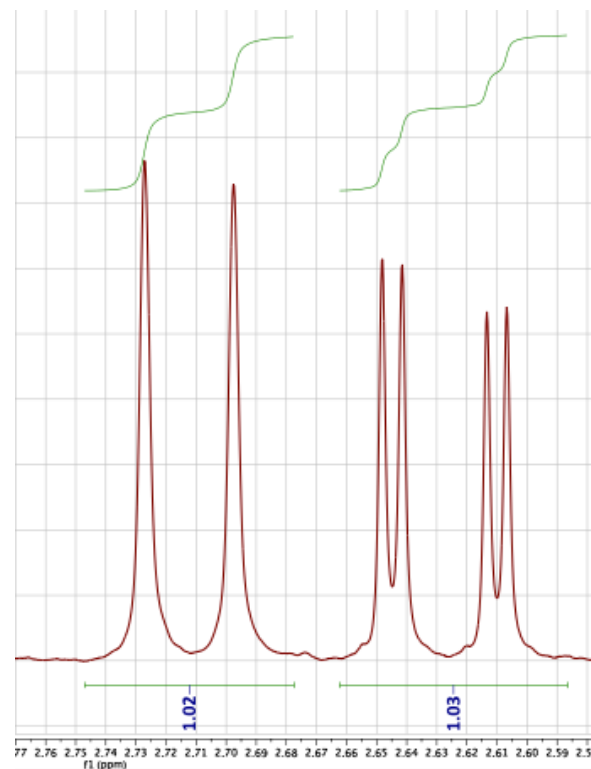
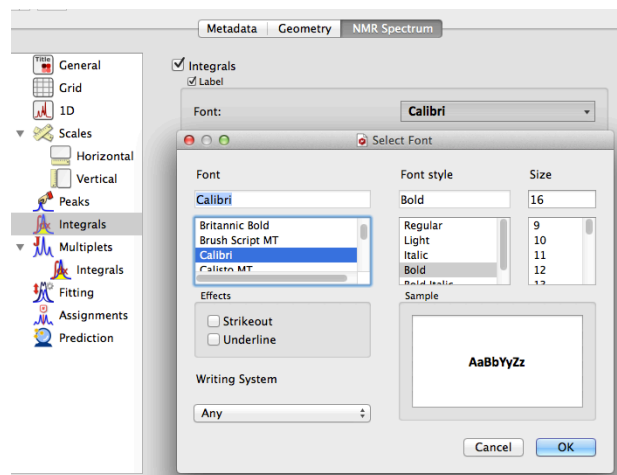
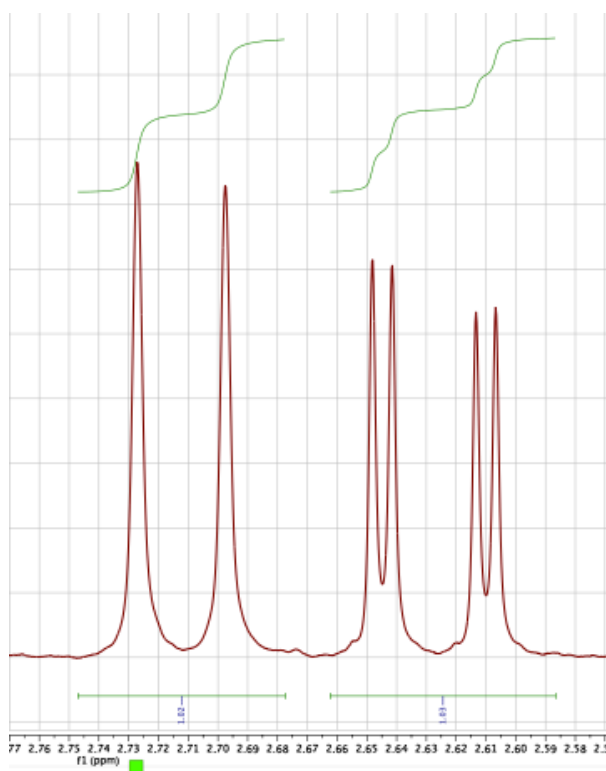
To apply baseline correction

Click the icon  to correct the baseline if needed. In most cases, the method **Whittaker Smoother** works very well. If not, try another method such as **Multipoint Baseline Correction** or **Polynomial Fit**.

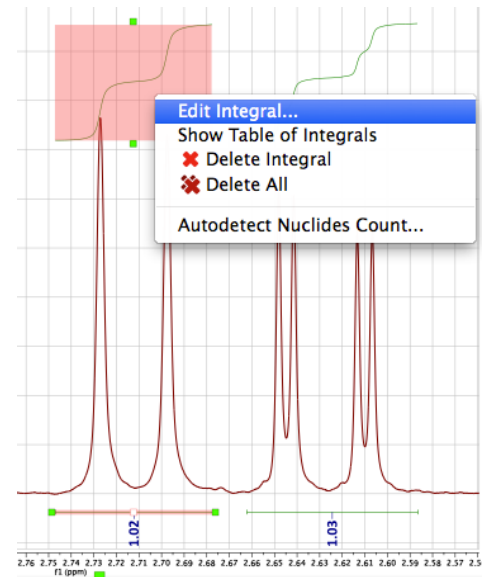


To integrate peaks

Note that before integrating peaks, you need to first perform baseline correction to the spectrum. To integrate peaks in a spectrum, click **Analysis, Integration**. You may choose either **Autodetect Regions** or **Manual**. If you choose **Manual**, left click and drag the mouse to select peaks to integrate, the integral of each selected peak will be automatically displayed. By default, the integral values have a very small font size. To change the font size, double click left mouse, in the pop-up window, click **Integrals**, then you can set a larger font size such that the integral values are more legible.

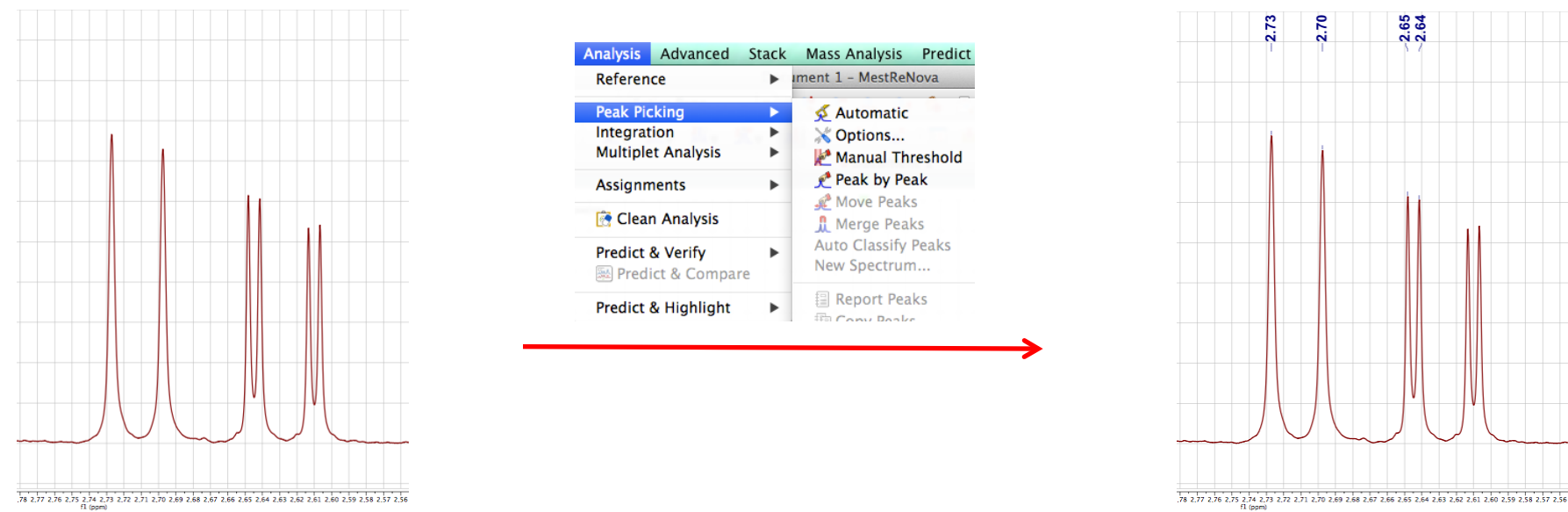


To set the integral of a peak to a specific value, hover over the integration line, then right click the orange shaded area and click **Edit Integrals**, then you can set the integral of that peak to a specific value.



To display peak frequencies

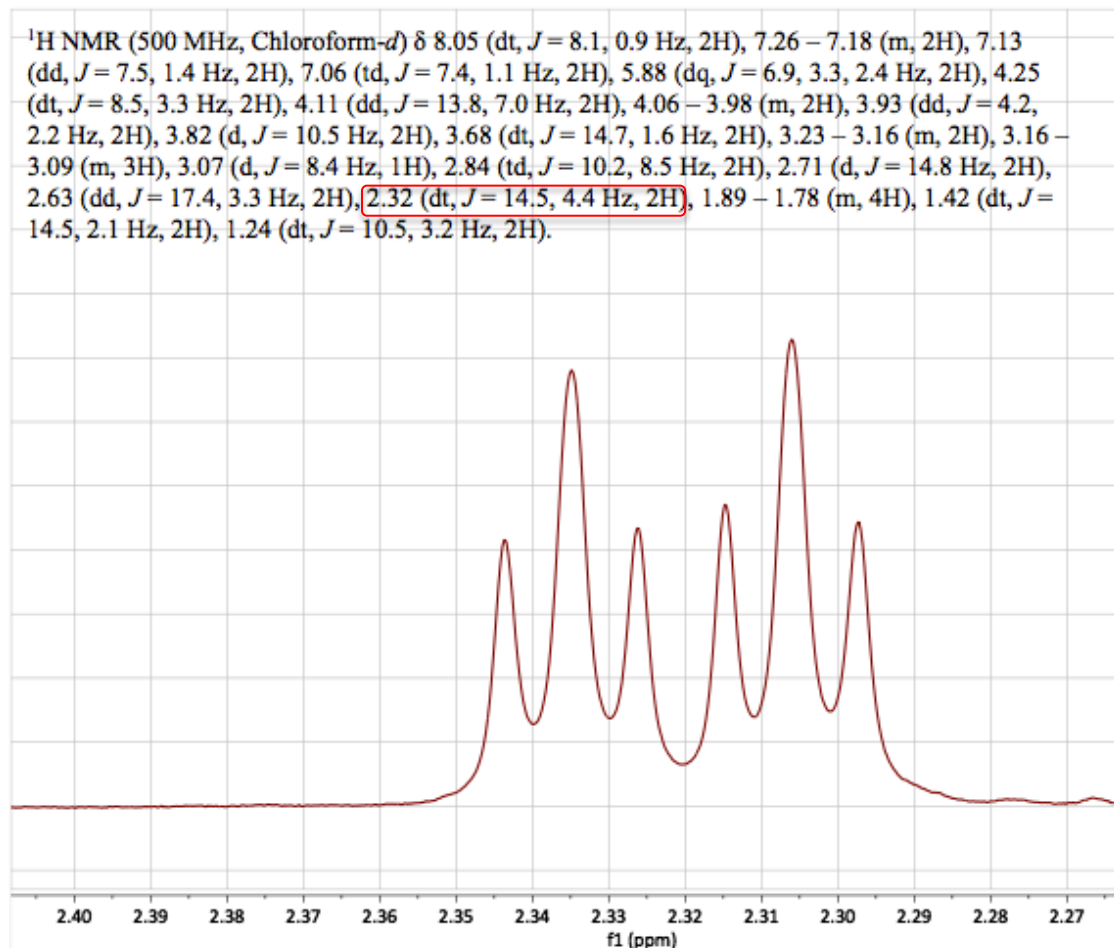
Click **Analysis, Peak Picking**. You may choose **Automatic**, **Manual Threshold**, or **Peak by Peak** to display peak frequencies. By default, the peak frequency values have a small font size. To make the frequencies more legible, double click left mouse and then click **Peaks** in the pop-up window where you can change the font size.





To analyze and report multiplets

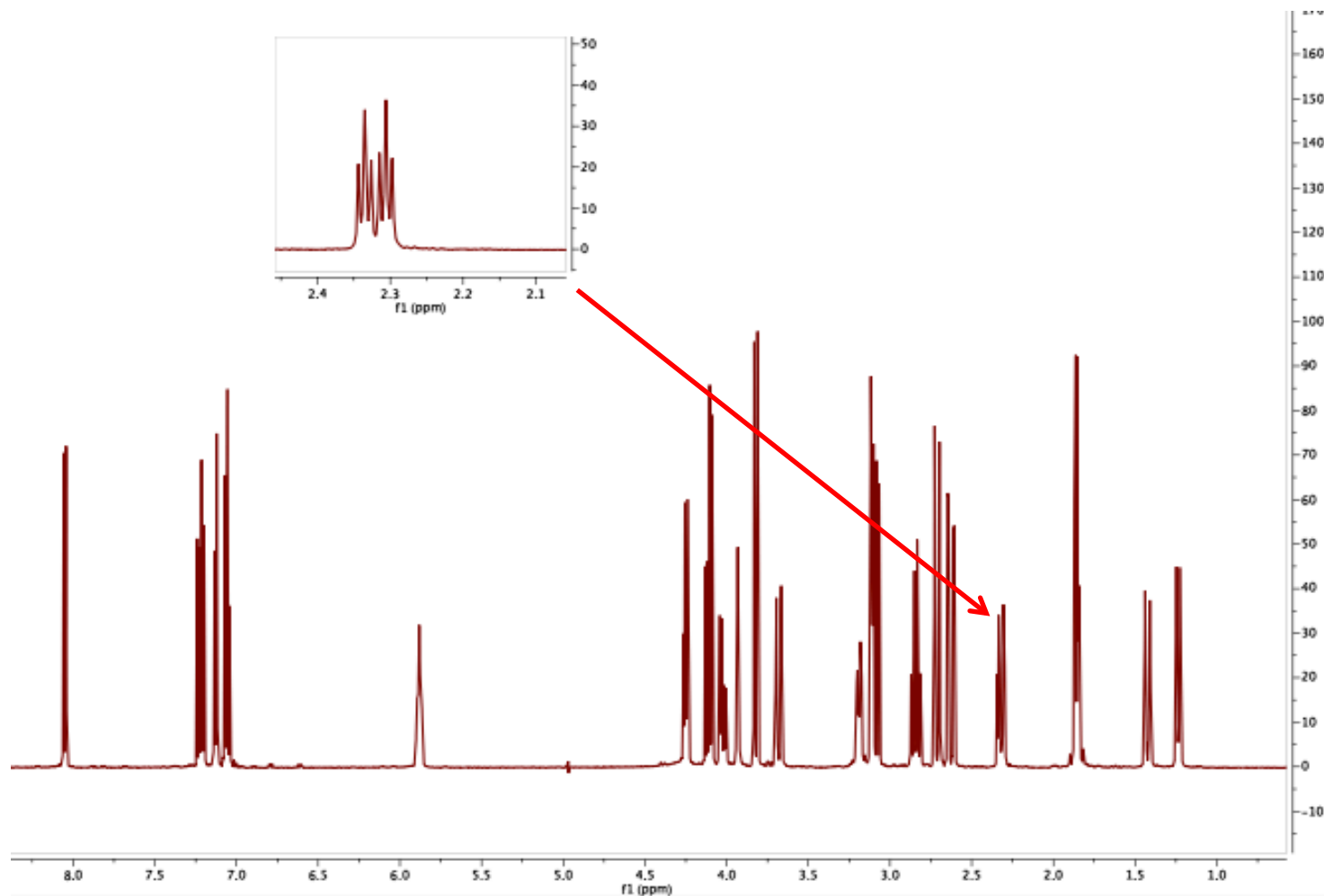
Mnova can analyze and report multiplets in terms of chemical shift, splitting pattern, J-coupling(s), and # of protons.

Click **Analysis, Multiplet Analysis, Automatic**, then Mnova will automatically select and analyze all peaks in the spectrum. Next, click **Analysis, Multiplet Analysis, Report Multiplets**, then all peaks will be reported in a text box. You may also manually select a specific peak for multiplet analysis. To do so, click **Analysis, Multiplet Analysis, Manual**, then drag the mouse to select the peak of interest. Note that you can also report multiplets in a specific journal format. To do that, first click **Analysis, Multiplet Analysis, Automatic (or Manual)** to select peaks in the spectrum, then click **Scripts, Report, Multiplets**, in the pop-up window, you can choose a specific journal format to report the multiplets, e.g. JACS, Tetrahedron, etc.





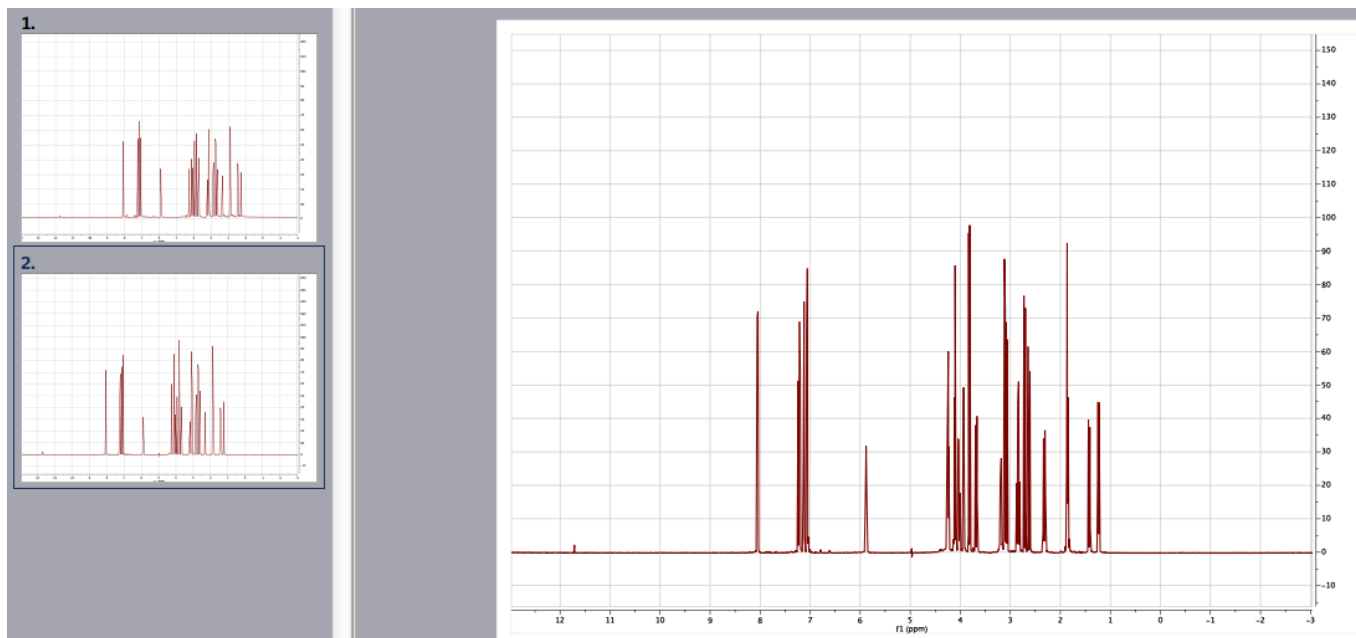
To create an inset in the spectrum

To create an inset for a specific region in the spectrum, click the icon  and then drag to select the region to expand and create the inset. If the peak intensity in the inset is too low, first scroll up the overall spectrum, then click the icon  and drag to select the region to re-create the inset, now the peak intensity in the inset should be higher.

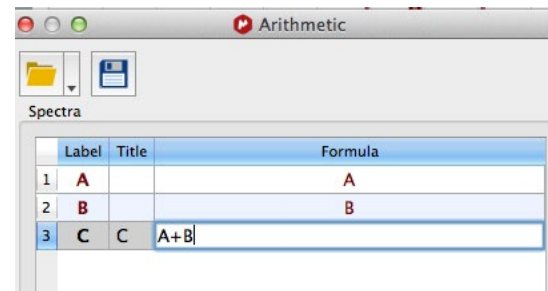


To stack, add, or subtract two spectra



First click **File, Open** to open the 1st spectrum and then do the same to open the 2nd spectrum. You should see two spectra on the left side of the display window, as shown below. If not, click **View, Pages** to display the two spectra. Next, highlight both spectra and then either click the icon  to stack the selected spectra or click the icon  to superimpose the selected spectra.

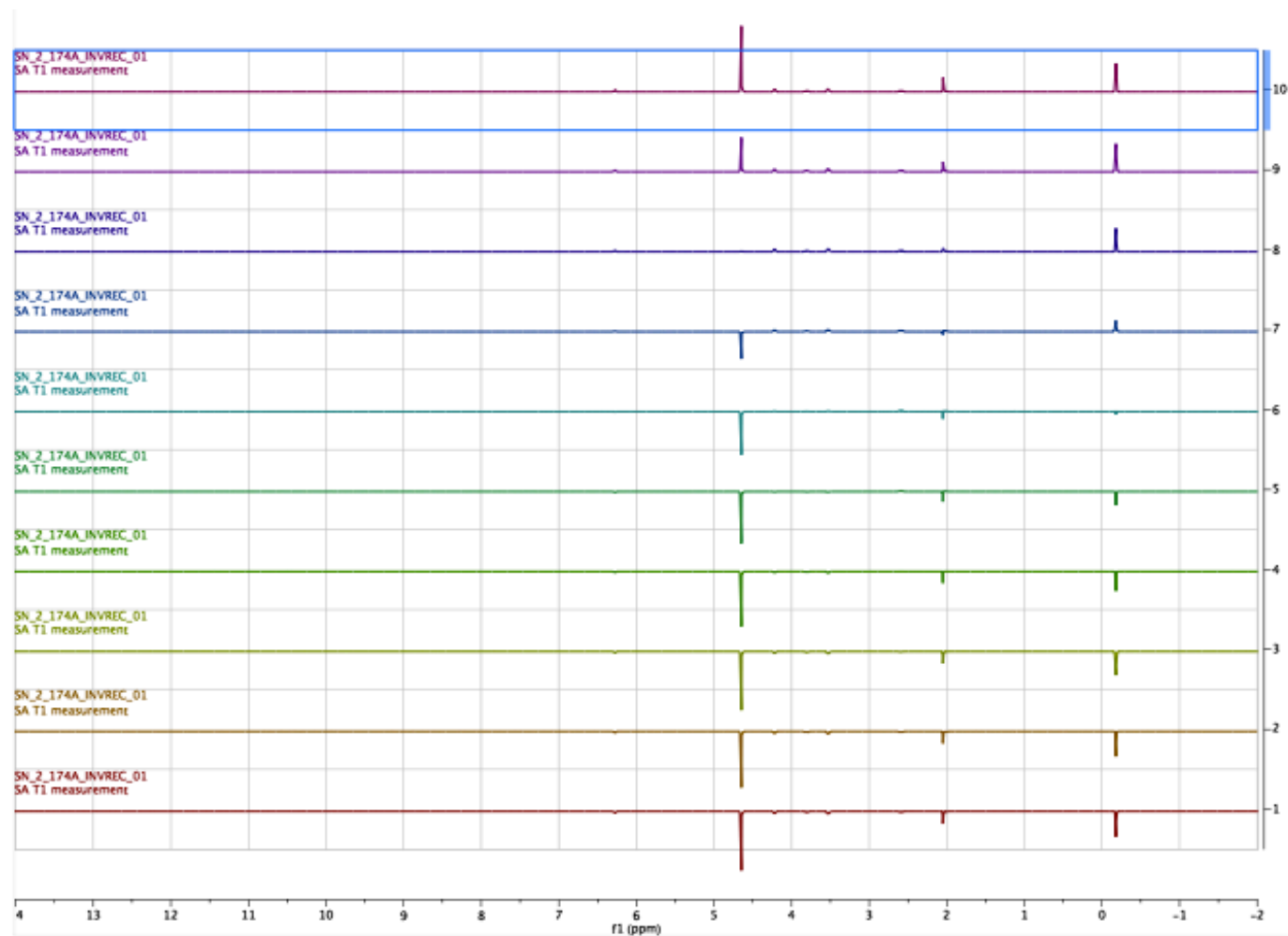
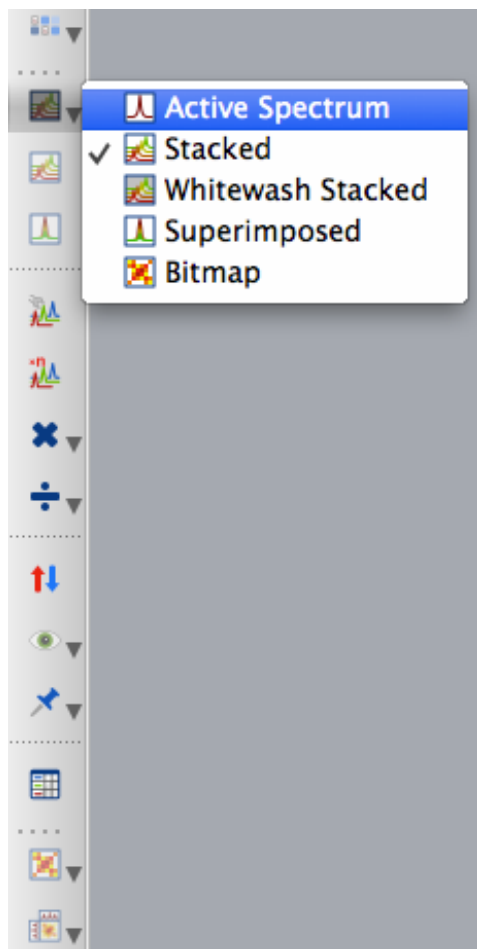


To add or subtract two spectra, first highlight both spectra and then click **Advanced, Arithmetic**. In the pop-up window, enter the formula of $A+B$ or $A-B$ to add or subtract the two spectra, respectively. The sum or difference spectrum will be displayed in a separate window (e.g. window 3).

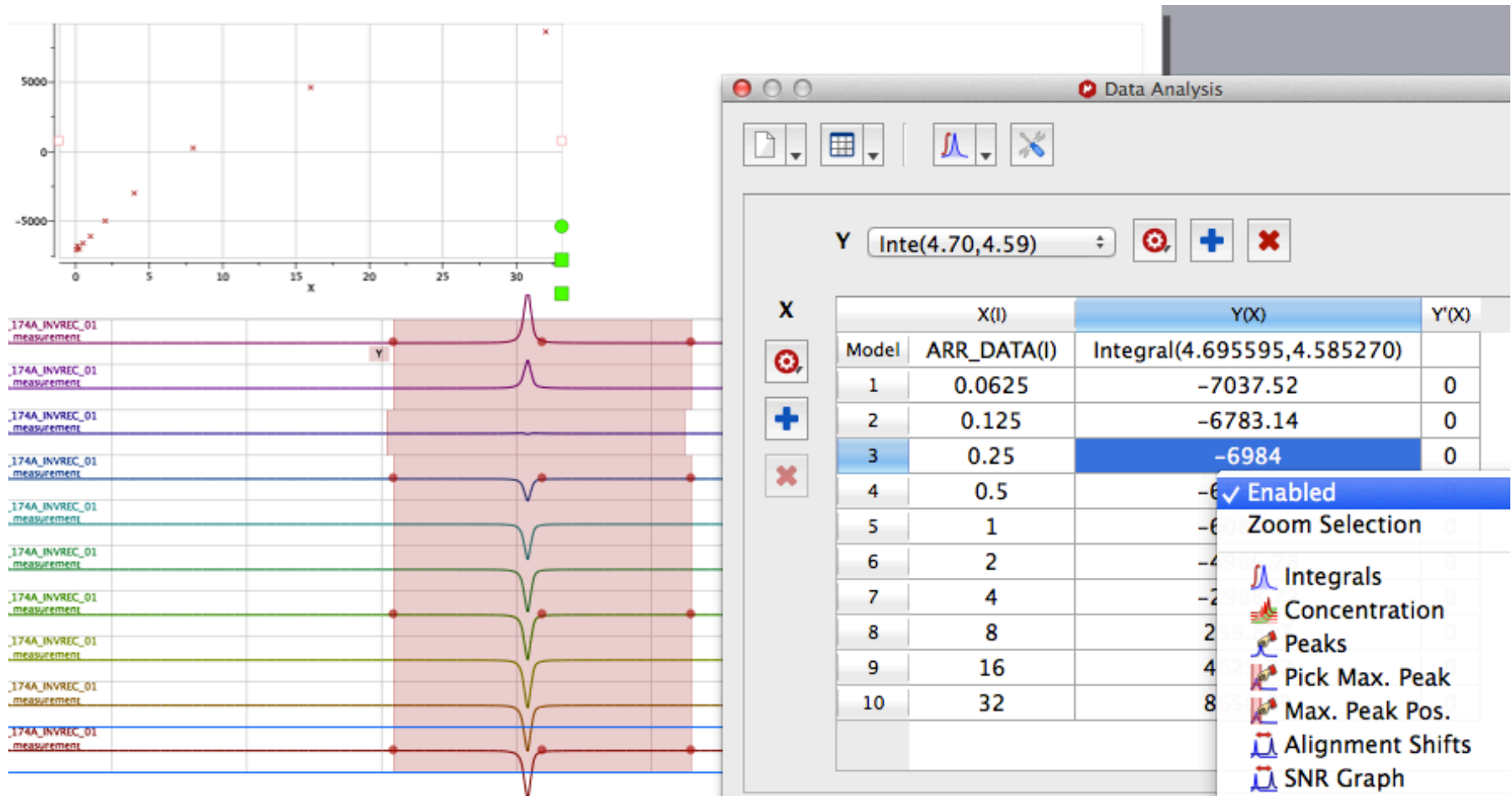



To do T1 analysis

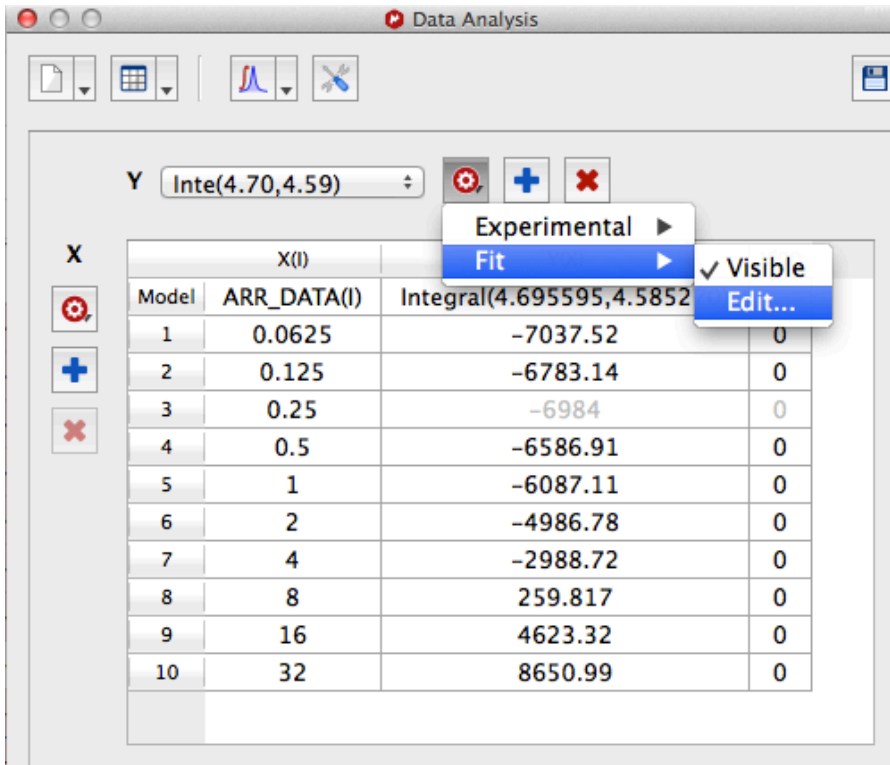
First click **File, Open** to open the T1 array dataset. If the signal-to-noise is low, apply apodization with some line broadening (e.g. 0.5 Hz). Next, highlight the spectrum at the very top, then click the icon  and choose **Active Spectrum**. It will then display the last spectrum for which complete T1 relaxation is usually achieved and all peaks should flip upwards. Next, phase the spectrum if needed and apply baseline correction as described before. To go back to the stacked display mode, simply click the icon  and then click **Stacked**.



Next, click **Analysis, Integration, Options**, choose **Sum** as the **Calculation Method** in the pop-up window. If you choose Peaks as the Calculation Method, the fitted T1 values could be way off. After that, click **Advanced, Data Analysis, Create, Integrals Graph**, then drag the mouse to select the peak of interest for integration. The peak integrals will be listed in the Data Analysis window, as shown below. If some integral value is abnormal (e.g. the 3rd integral value in the picture below), you can highlight that value and then right click to uncheck **Enabled** to discard that value.



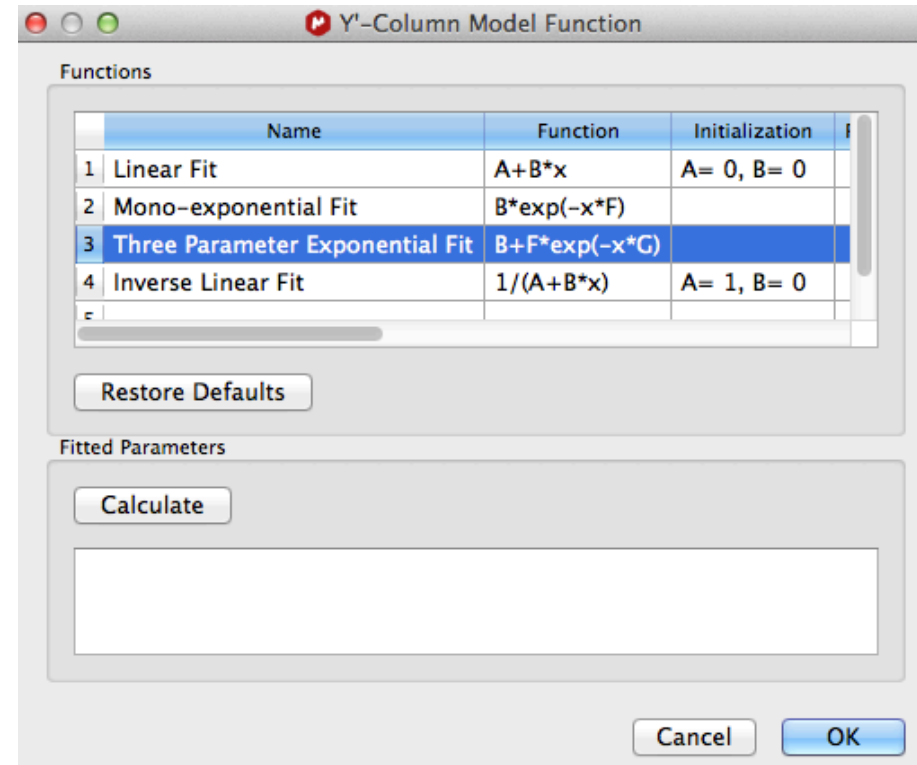
Next, in the **Data Analysis** window, click the icon  and then click **Fit, Edit**. In the pop-up window, choose **Three-Parameter Exponential Fit** and then click the **Calculate** button.



The **Data Analysis** window displays a table with the following data:

Model	ARR_DATA(I)	Integral(4.695595,4.5852	
1	0.0625	-7037.52	0
2	0.125	-6783.14	0
3	0.25	-6984	0
4	0.5	-6586.91	0
5	1	-6087.11	0
6	2	-4986.78	0
7	4	-2988.72	0
8	8	259.817	0
9	16	4623.32	0
10	32	8650.99	0

A context menu is open over the table, showing options: **Experimental**, **Fit**, **Visible** (checked), and **Edit...**.



The **Y'-Column Model Function** window displays a list of functions:

	Name	Function	Initialization
1	Linear Fit	$A+B*x$	$A= 0, B= 0$
2	Mono-exponential Fit	$B*\exp(-x*F)$	
3	Three Parameter Exponential Fit	$B+F*\exp(-x*G)$	
4	Inverse Linear Fit	$1/(A+B*x)$	$A= 1, B= 0$

Below the list is a **Restore Defaults** button. Under the **Fitted Parameters** section, there is a **Calculate** button and a large empty text area. At the bottom right are **Cancel** and **OK** buttons.

Eventually, Mnova will fit the peak integral as a function of the inversion recovery delay time and report the fitting result in the Data Analysis window. A fitting curve will be also displayed. Note that the T1 value is defined by $1/G$. For example, the fitting in the picture below shows $G=0.0656 \text{ s}^{-1}$ for the water peak at $\sim 4.65 \text{ ppm}$, therefore, the T1 value of the water ^1H should be $1/G=15.2 \text{ s}$. Note that Mnova will also report the uncertainty of the fitted G as rError. For example, if $G=0.0656 \text{ s}^{-1}$ and $\text{rError}=0.0012$, the uncertainty of the T1 value = $G^{-2} * \text{rError} = 0.0656^{-2} * 0.0012 = 0.28 \text{ s}$.

