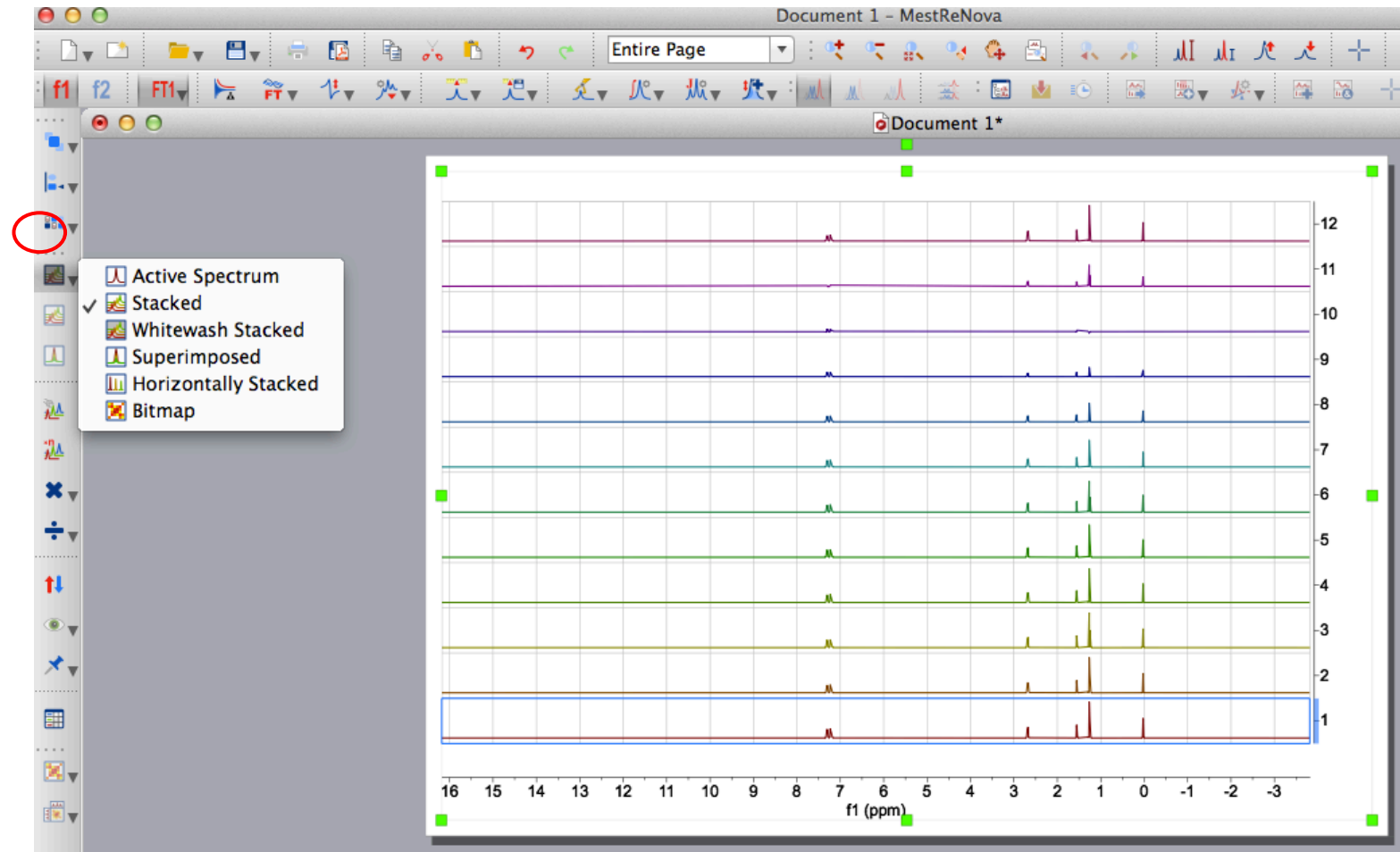


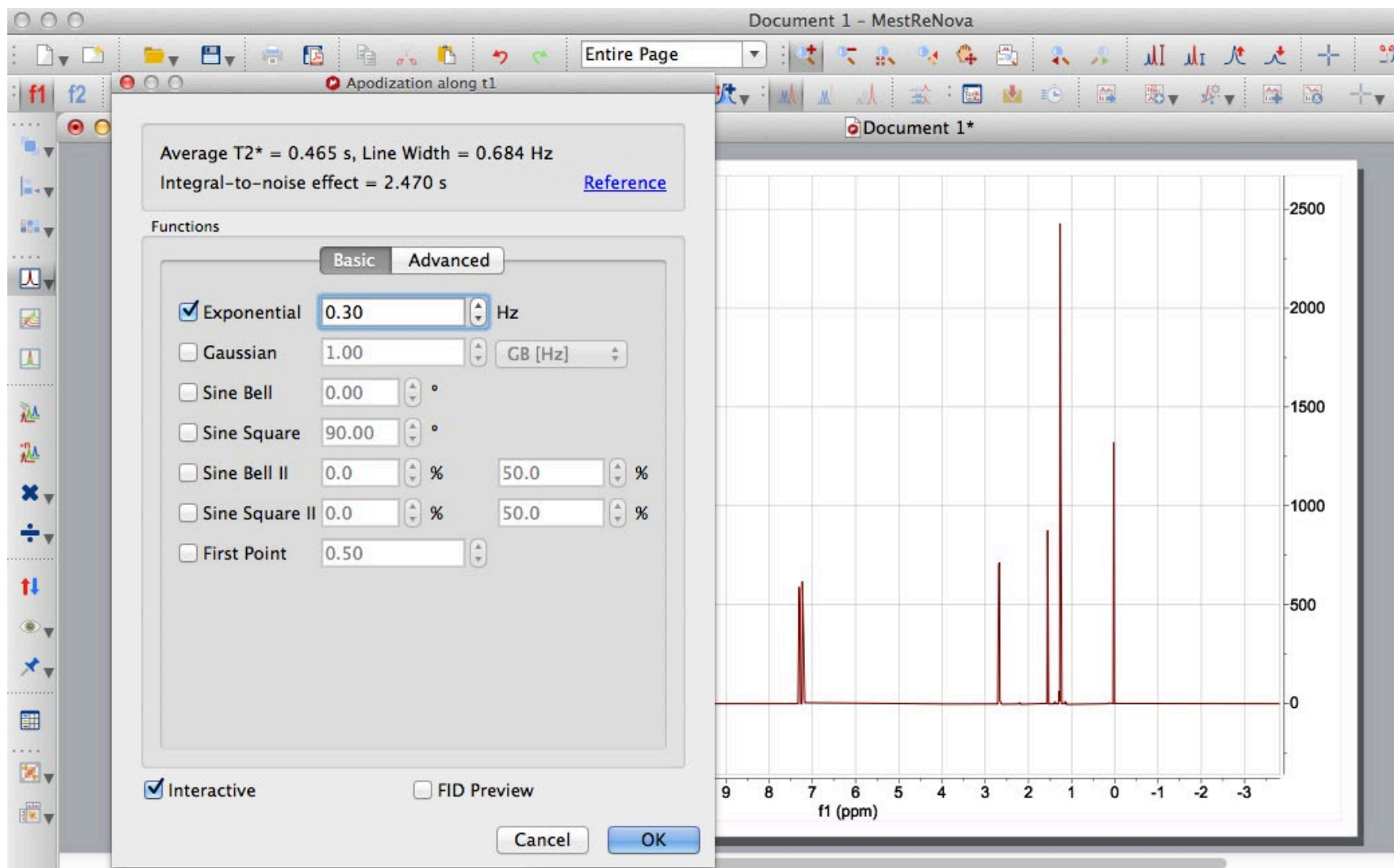
Data Analysis For T1 Measurements Using Mnova (classic mode)

To analyze T1 NMR data in Mnova, please follow the procedure as below.

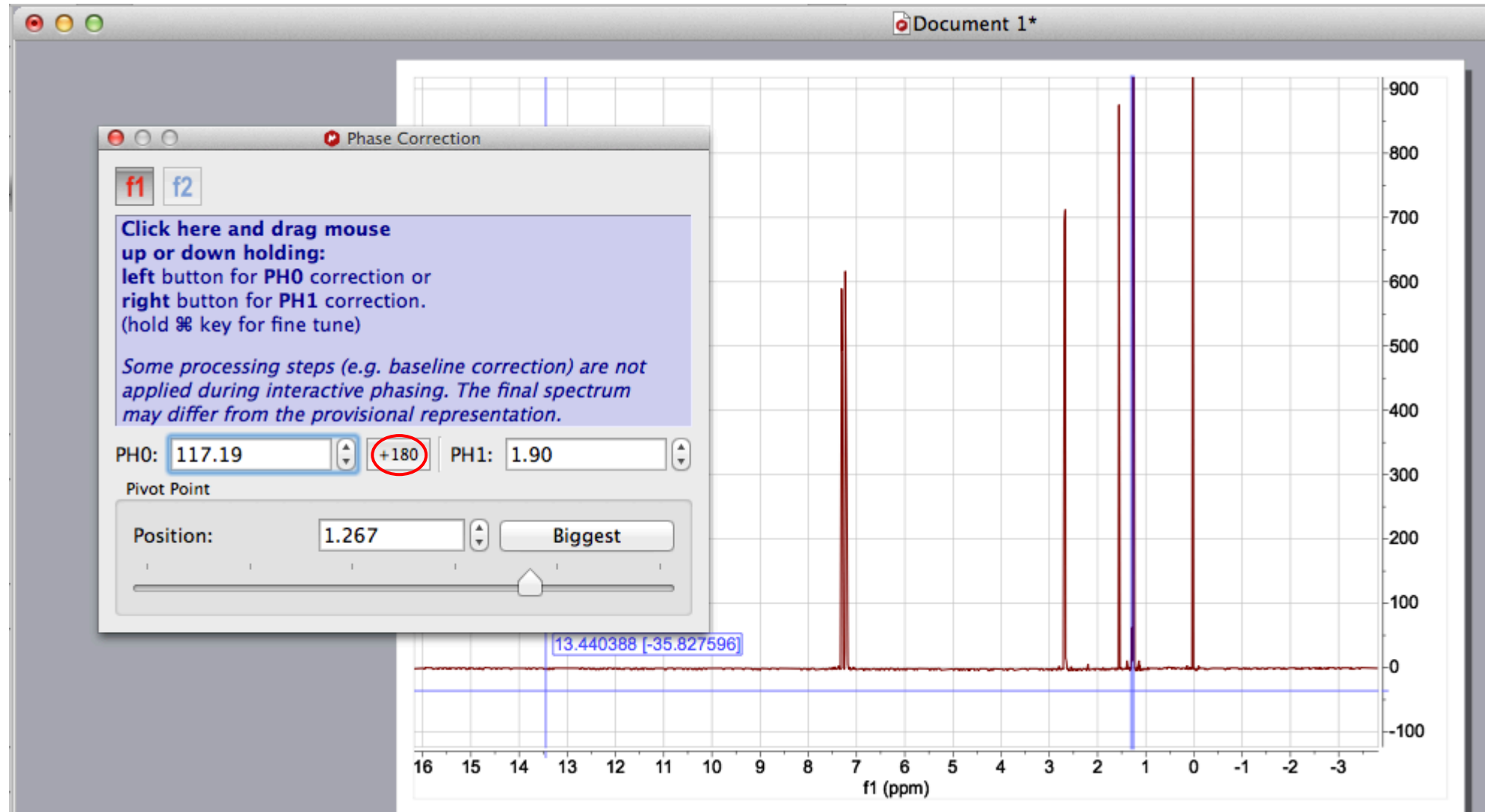
(1) Drag the zip file or data folder containing NMR raw data into Mnova. The arrayed dataset will be displayed in Mnova, as shown in the picture below, there are 12 spectra where spectrum 1 has the shortest inversion recovery delay and spectrum 12 has the longest inversion recovery delay. Next, click the stacked spectra icon (circled in red) and select **Active Spectrum** to display spectrum 1. The **Active Spectrum** is the one highlighted in a blue rectangle.



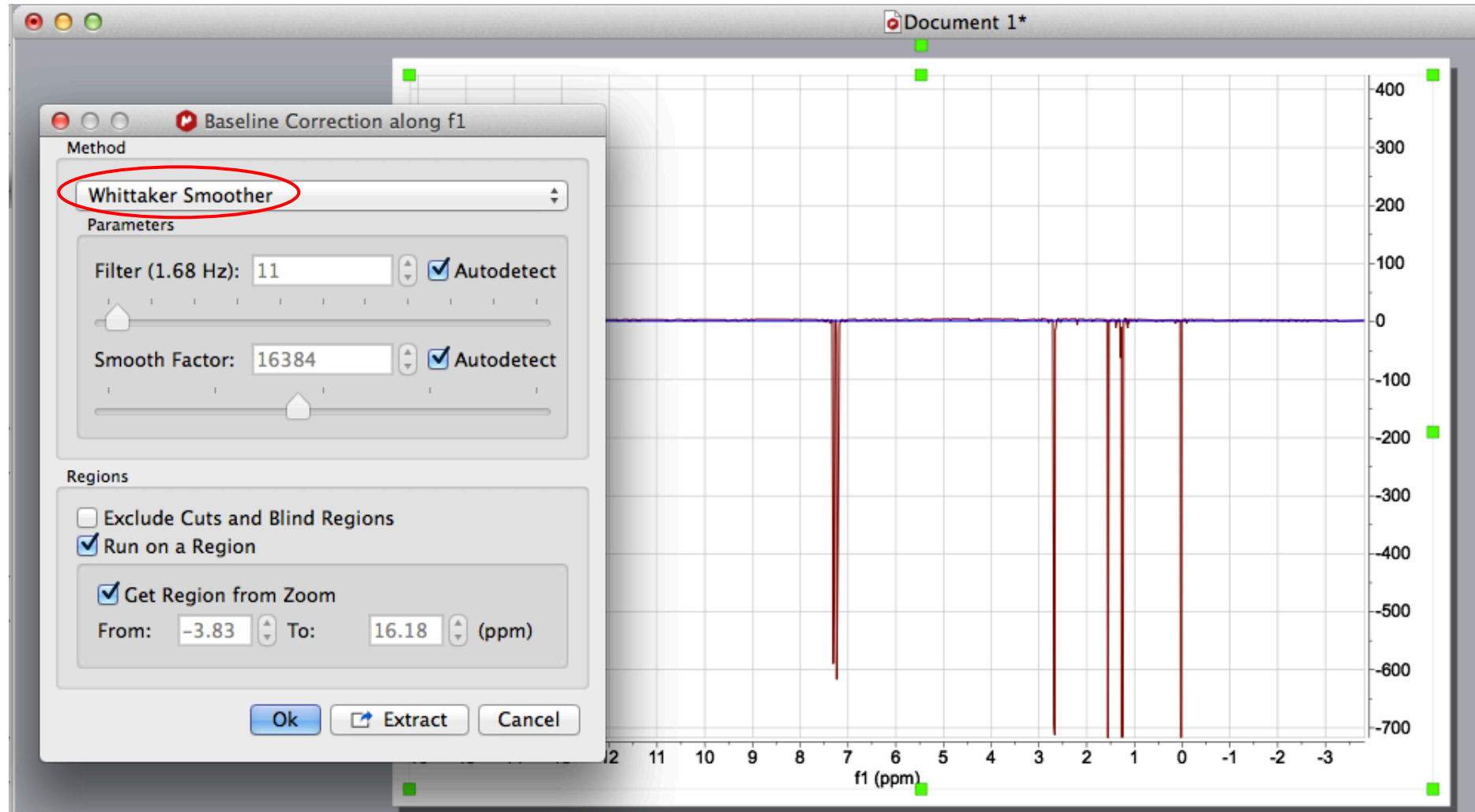
(2) To improve the signal-to-noise of the spectra, exponential line broadening can be applied. To do that, click **Processing**, **Apodization**, in the pop-up window (shown below), enter the line broadening value (0.3-1 Hz is recommended) and click OK.



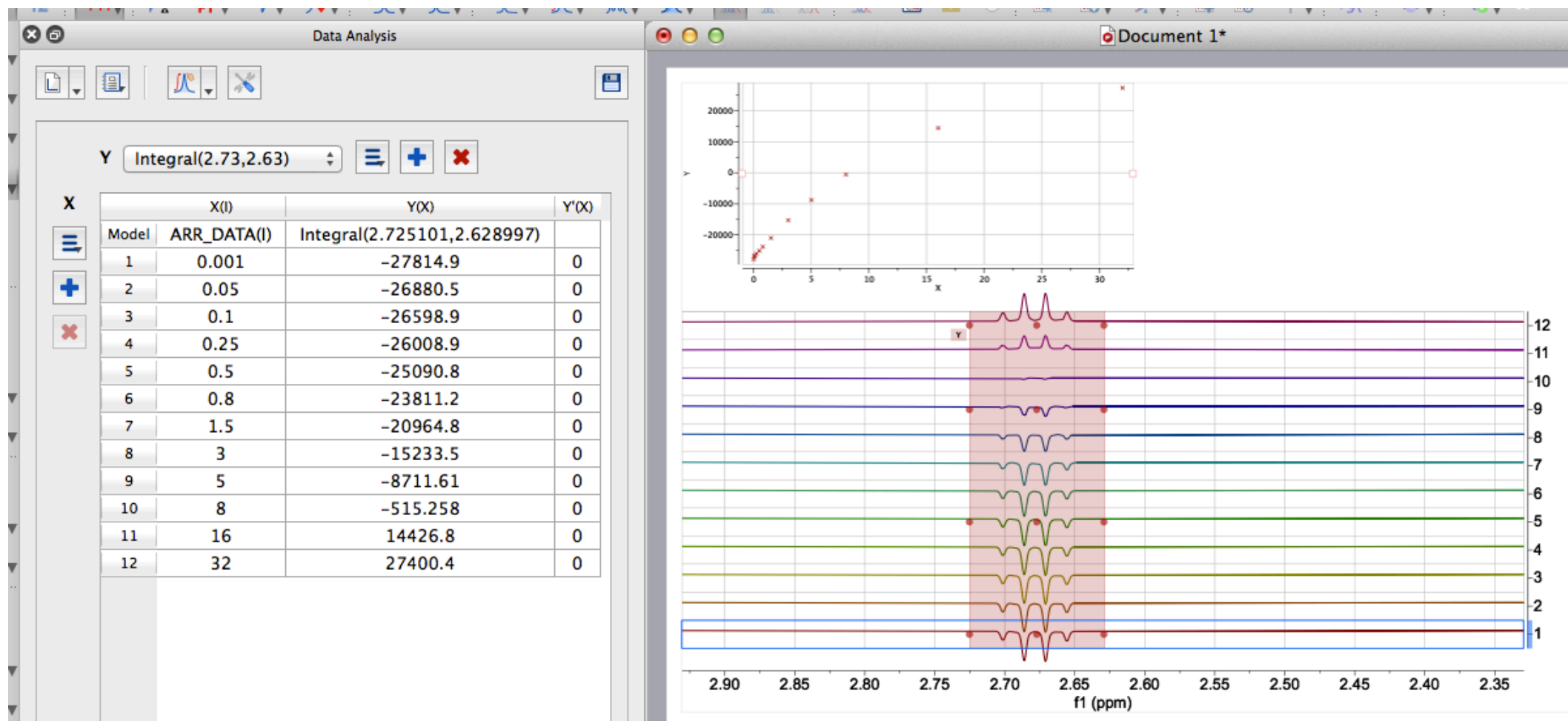
(3) Next, spectrum 1 needs to be properly phased such that all peaks are inverted. To phase the spectrum, first click **Processing, Phase Correction, Automatic**. At this point, all peaks will be phased up. Next, click **Processing, Phase Correction, Manual Correction**, a window will pop up, simply click the 180 button (circled in red) to invert the spectrum. Once spectrum 1 is properly phased, the same phasing parameters will be automatically applied to the rest of the spectra.



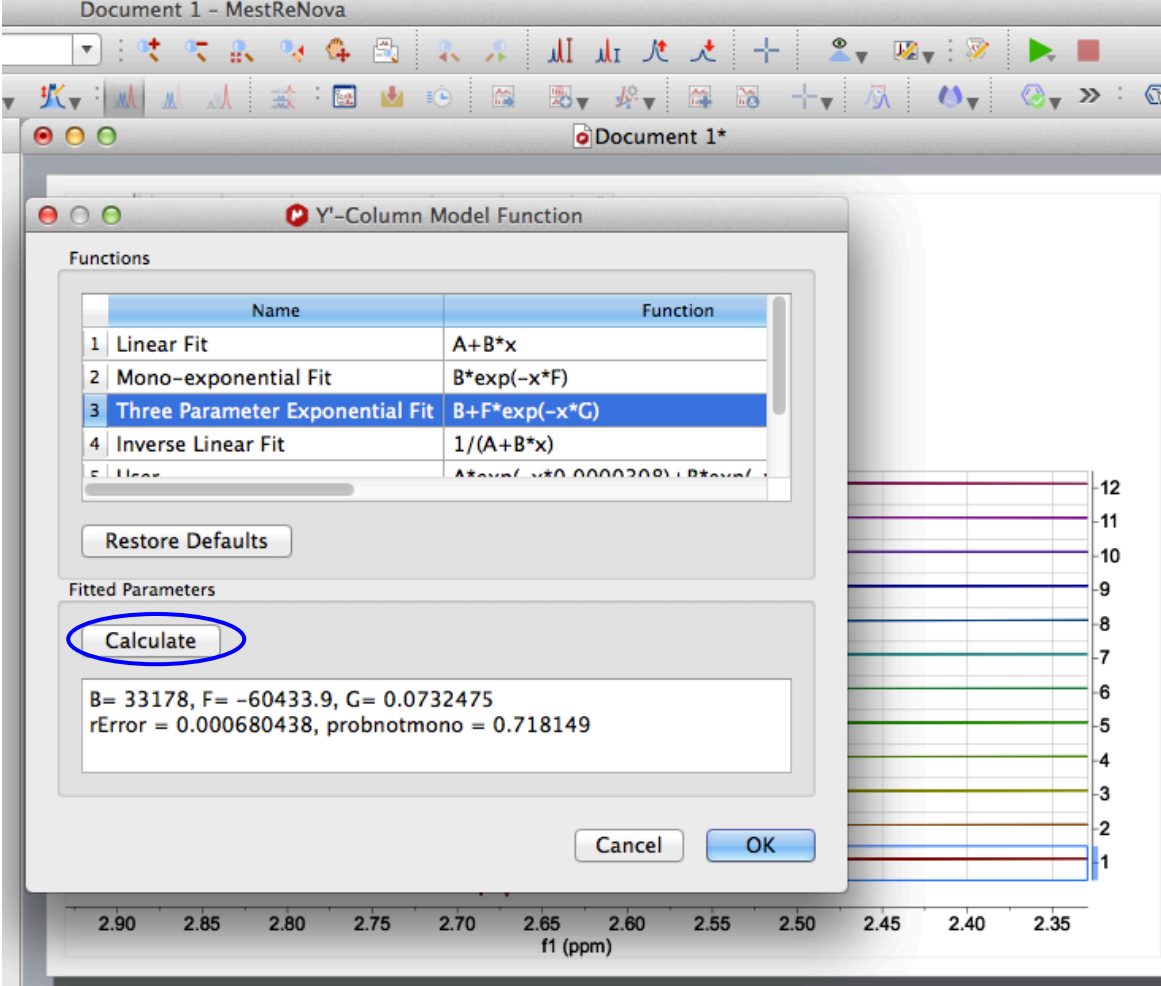
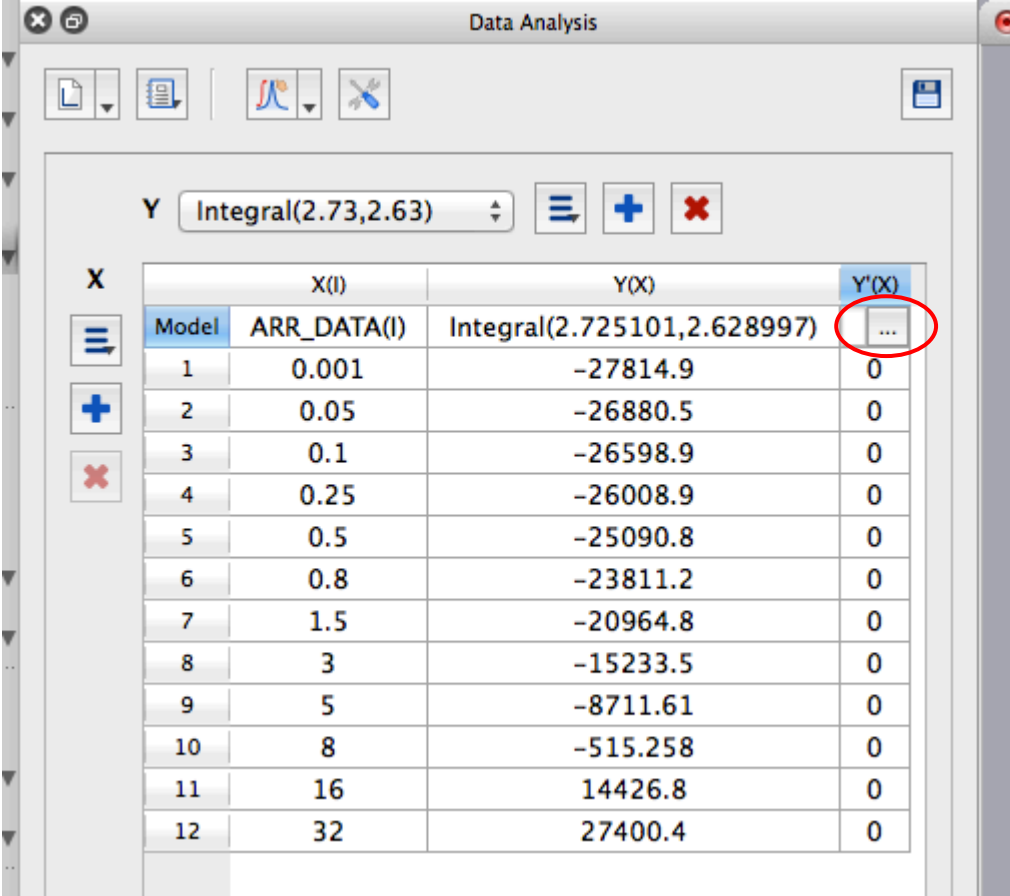
(4) To make peak integration accurate, proper baseline correction needs to be applied to make the baseline as flat as possible. To do that, click **Processing, Baseline, Baseline Correction**. In the pop-up window, you can choose a method that gives the best baseline correction, e.g. Whittaker Smoother (circled in red). As shown in the picture below, the blue line refers to the background to be subtracted from the spectrum. Similar to phasing, once spectrum 1 is baseline corrected, the rest of the spectra will be also automatically baseline corrected.



(5) Next, click the stacked spectra icon (refer to step 1) and select **Stacked** to display the stacked spectra, then left click and drag to expand the peak of interest, e.g. the peak at 2.68 ppm. Next, click **Advanced, Data Analysis, Create, Integrals Graph**. Then left click and drag to select the peak region of interest to generate the integral graph, as shown below.



(6) Next, in the Data Analysis window (see picture on the left side), double click the box right beneath $Y'(X)$ and click the button with three dots (circled in red). A window will pop up showing the fitting functions to be used (see picture on the right side). For T1 data fitting, a three parameter exponential fit of $B+F*\exp(-x*G)$ is employed since the signal $M(t)$ is defined by the equation of $M(t)=M_o(1-2e^{-t/T1})$, where t is the inversion recovery delay and M_o is the signal at thermal equilibrium state. After selecting the three parameter exponential fit equation, click **Calculate** (circled in blue) to perform the T1 data fitting. The T1 value is equal to $1/G$, in the current fit, G is 0.073 and thus T1 is 13.7 s.



(7) To determine the T1 of another peak, first click the icon circled in red in the Data Analysis window shown below and choose Integrals, then select another peak in the spectrum. The new integral data points will be added to the original integral graph and another two columns of Y1(X) and Y1'(X) will be added to the Data Analysis window. To calculate the T1 of the new peak, repeat step 6 but in the Y1'(X) column. Please note that the longest T1 in your compound is from the peak which is the last to flip back up in the arrayed spectra and you should set the recycle delay (D1) to 5x longest T1 to obtain quantitative NMR data. Also note that one can determine all T1's in Excel. To do that, first select each individual peak to generate the integrals in the Data Analysis window. The inversion recovery delays in seconds are listed in column X(I) and the integrals are listed in column Y(X), Y1(X), etc. Do the calculations on all the peaks as described in Step 6. Next, click the icon circled in blue in the Data Analysis window and choose Report Table to Clipboard and then paste the data in Excel. You can then easily get the inverse of G.

