



Arithmetic

MestReNova: NMR plugin

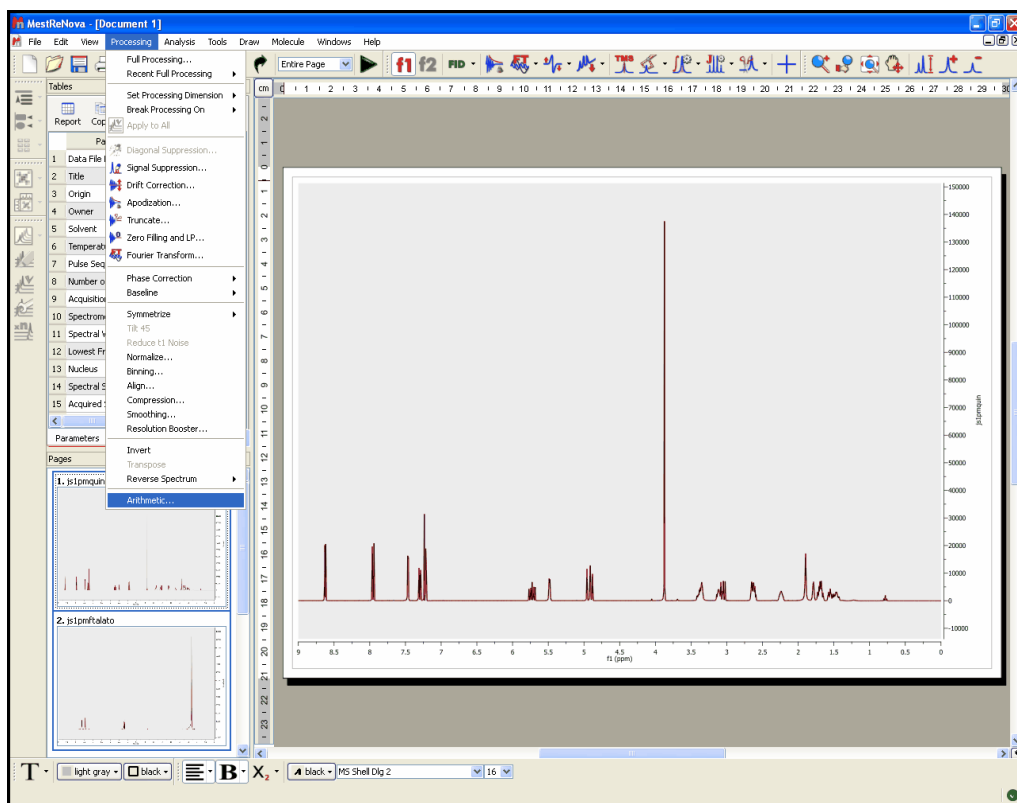
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This feature is used to carry out arithmetic operations with 'fid's or processed spectra. Typically, you will use the arithmetic module implemented in MestReNova to sum 'fid's' acquired under the same measurement conditions in order to improve the signal-to-noise ratio.

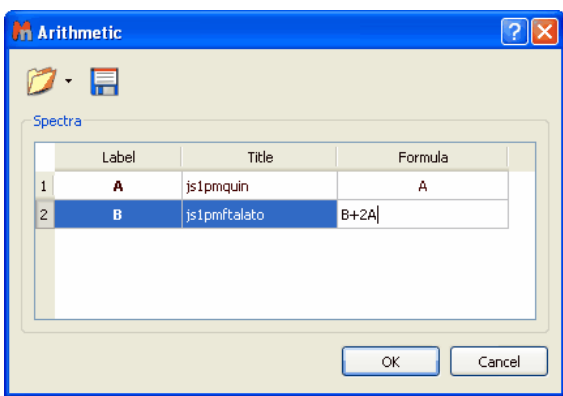
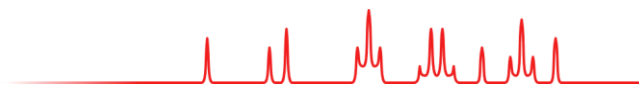
This tool is also very useful to **remove impurities** or solvent signals from a spectrum, to **analyze DEPT experiments** and also to **subtract FIDs of Selective Experiments** (such as NOE or ROE)



How to sum or subtract spectra?

Application of Linear Combinations (sums, subtraction and multiplication) to spectra in the MestRe Nova interface is extremely simple. Just select the desired spectra on the Page Navigator (by holding down 'CTRL key' or 'Cmd key' while clicking on each spectrum) and follow the menu 'Processing/Arithmetic':

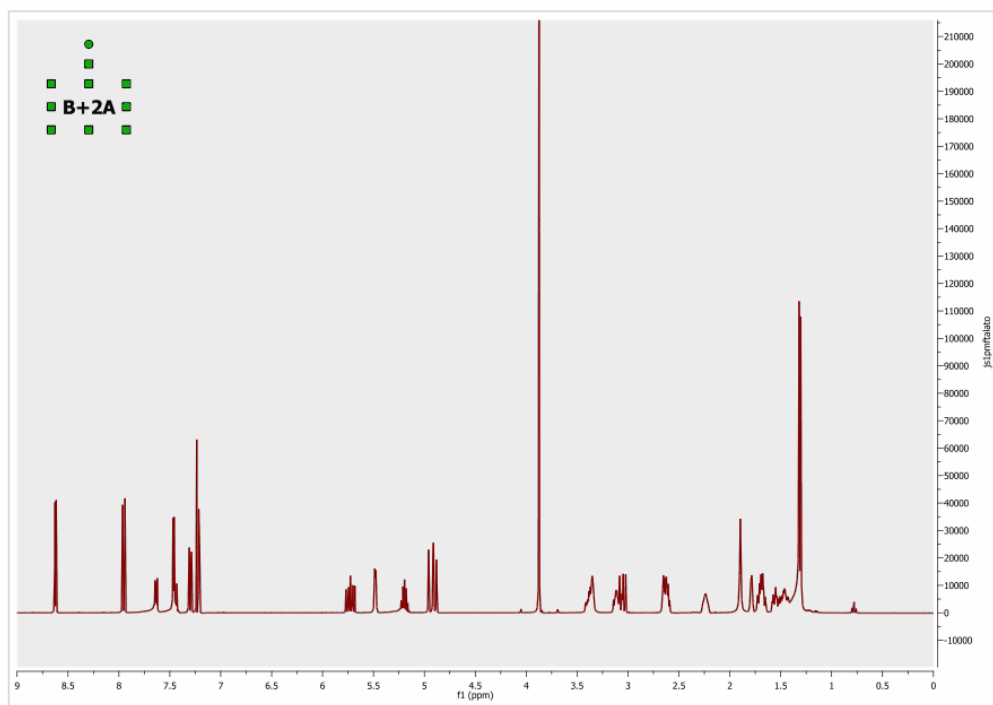


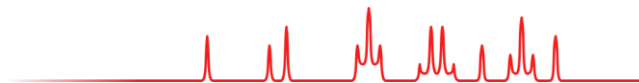
This will display the 'Arithmetic' dialog box on screen. In this example, we want to add two times spectrum A to spectrum B, so we shall type the formula 'B+2A' in the corresponding cell.



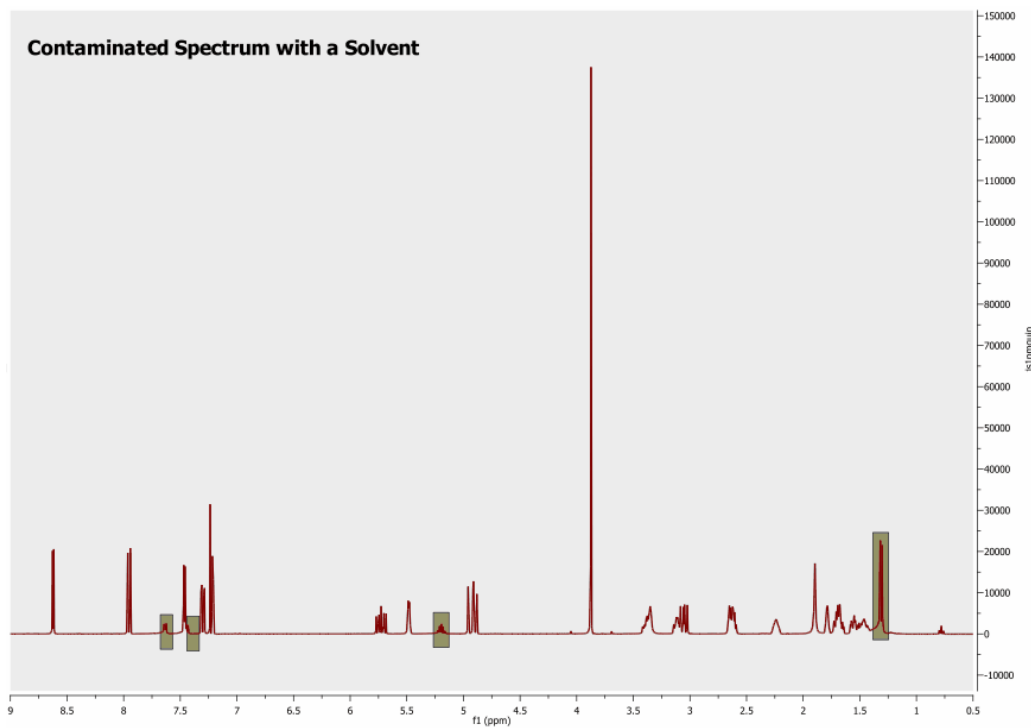
The 'Save Formulas' icon  will allow the user to save formulas, which can then be loaded by using the 'Load Formulas' icon .

On pressing 'OK', the result is a new spectrum which will consist of the sum of spectrum B plus two times spectrum A.

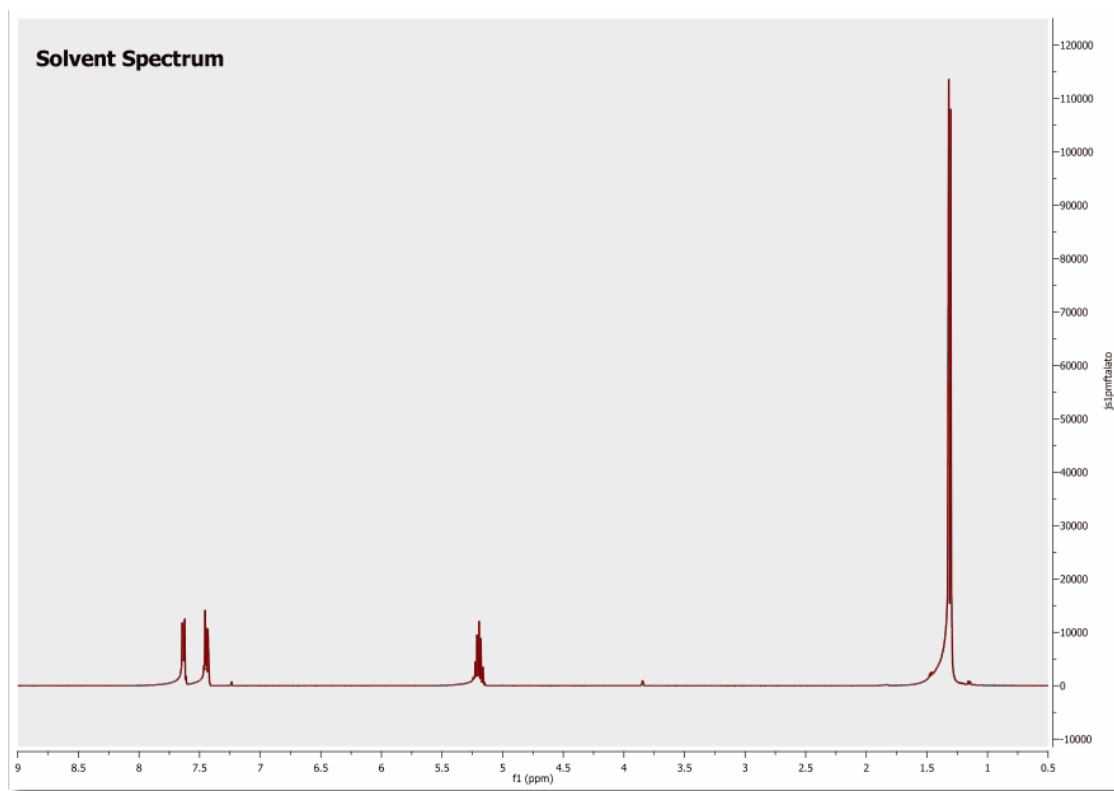
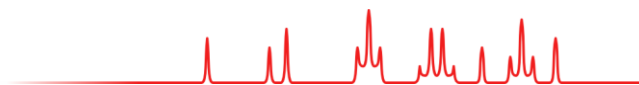




It is also possible to subtract spectra, but in this case it is important that the user calculates the intensity ratio of both spectra. For example, in this spectrum we have a sample contaminated with a solvent.



Whilst the spectrum below corresponds to the solvent which we need to eliminate from the sample.



To successfully carry out the subtraction, we need to calculate the intensity ratio between the contaminated spectrum and the solvent spectrum. To obtain this ratio we can measure the intensity of a signal present in both spectra (by applying the command 'Peak by peak' and getting the result on the corresponding table). For example, we measure the intensity of the singlet which appears at 1.32 ppm. For the first spectrum, we obtain an intensity of 22617 and for the second, 115031, indicating the the intensity ratio to be 1/5, or 0.2.

Typing the formula '**A-0.2B**' (or 'A-0.2*B') in the 'Arithmetic' dialog box, we shall obtain the spectrum below, where the solvent signals have been removed:

