

MY Baseline Corrector: Tutorial

Introduction:

MY Baseline Corrector application allows performing automatic and reproducible baseline correction of 1D NMR spectra. It is especially adapted for large bandwidth, single pulse acquisition which suffers from important baseline distortions due to time domain truncation of the first points of the FID. Baseline corrector has been proved versatile enough to correct a wide range of baseline deformation on diverse nuclei and experimental conditions. The application support Bruker raw and ASCII format.

Tutorial:

MY Baseline Corrector is developed in Matlab® but shared as a standalone application which doesn't need any license to be used. It is available for Windows, Mac and Centos 5 or 7. It can be launched from Topspin through a python macro (myBC) included in the zip installation file.

1. Main windows

The first window of the application is presented here:

The screenshot shows the MY Baseline Corrector application window. On the left, there is a control panel with several sections: 'Open NMR file' (with buttons for 'Open *.1 File', 'Open ASCII File', and 'Reload File'), 'Truncation parameters' (with fields for 'DE' set to 10 and 'DW' set to 0.3, and a checked 'Truncation limit' checkbox), 'Sinus cardinal fit' (with a 'Number of truncated points' field set to 34), 'Sinus cardinal Fit' (with 'Frequency Guess' at 0.001979 and a 'Cardinal Sinus Fit' button), 'Smoothing spline Fit' (with 'Smoothing' set to 10 and a 'Smoothing spline Fit' button), 'Manual Modification' (with a 'Start Point modification' button and 'Number of points' set to 100), and 'Save NMR file' (with 'Save *.1 File' and 'Save ASCII File' buttons). The main window area contains two plots: an upper plot showing the inverse Fourier transform of the real part of the spectrum with a red line indicating the dead time zone, and a lower plot showing the original spectrum (in blue) and the proposed baseline correction (in red). Callout boxes on the left point to 'Open Bruker 1D NMR file or ASCII file.', 'Acquisition and correction main parameters', 'Sinus cardinal fit', 'iterative smoothing spline', 'Manual correction', and 'Save file'. Callout boxes on the right point to 'Display of the inverse Fourier transform of the real part of the spectrum showing the dead time zone which is usually characterized by a very low signal intensity.' and 'Display of the spectrum (in blue) and the proposed baseline correction in red.'

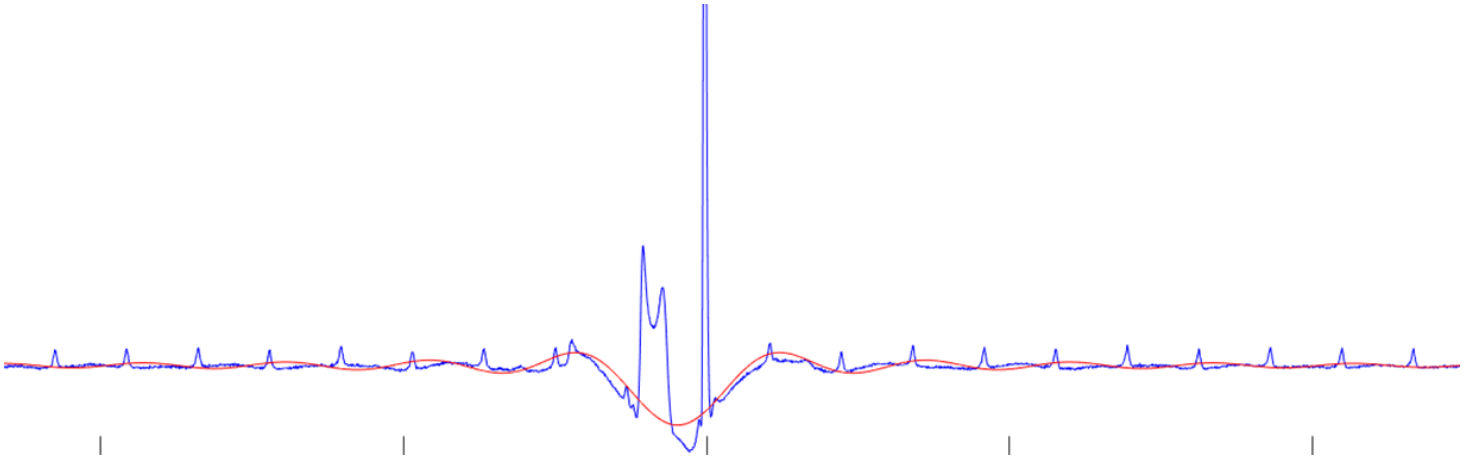
2. Time domain plot and number of truncated points

When opened from Topspin, the application retrieves two key acquisition parameters which are the dead time and the dwell time of the acquisition. These two parameters are used to define the "number of truncated points" which is one of the more important parameters of the correction. As this number might not be exactly equal to the dead time divided by the dwell time due to the application of filters, the user can change the value of the "number of truncated points". In order to help the user in this decision, the upper plot shows the inverse Fourier transform of the real part of the spectrum presenting the equivalent dead time (dead time plus filter time) which is usually characterized by a very low signal intensity. In the figure above this zone is perfectly defined as the red lines framed the time domain zone of "zero" intensity which corresponds to the dead time.

The "number of truncated points" parameter is used to limit the time domain expression of the baseline if the parameter "Truncation limit" is checked. This allows obtaining a baseline correction which does not modify the acquired points of the FID which is the main disadvantage of the baseline correction through model-free smooth fitting of the baseline. This option is relevant only if the baseline deformation is due to time domain truncation.

3. First recommended step: sinus cardinal fit

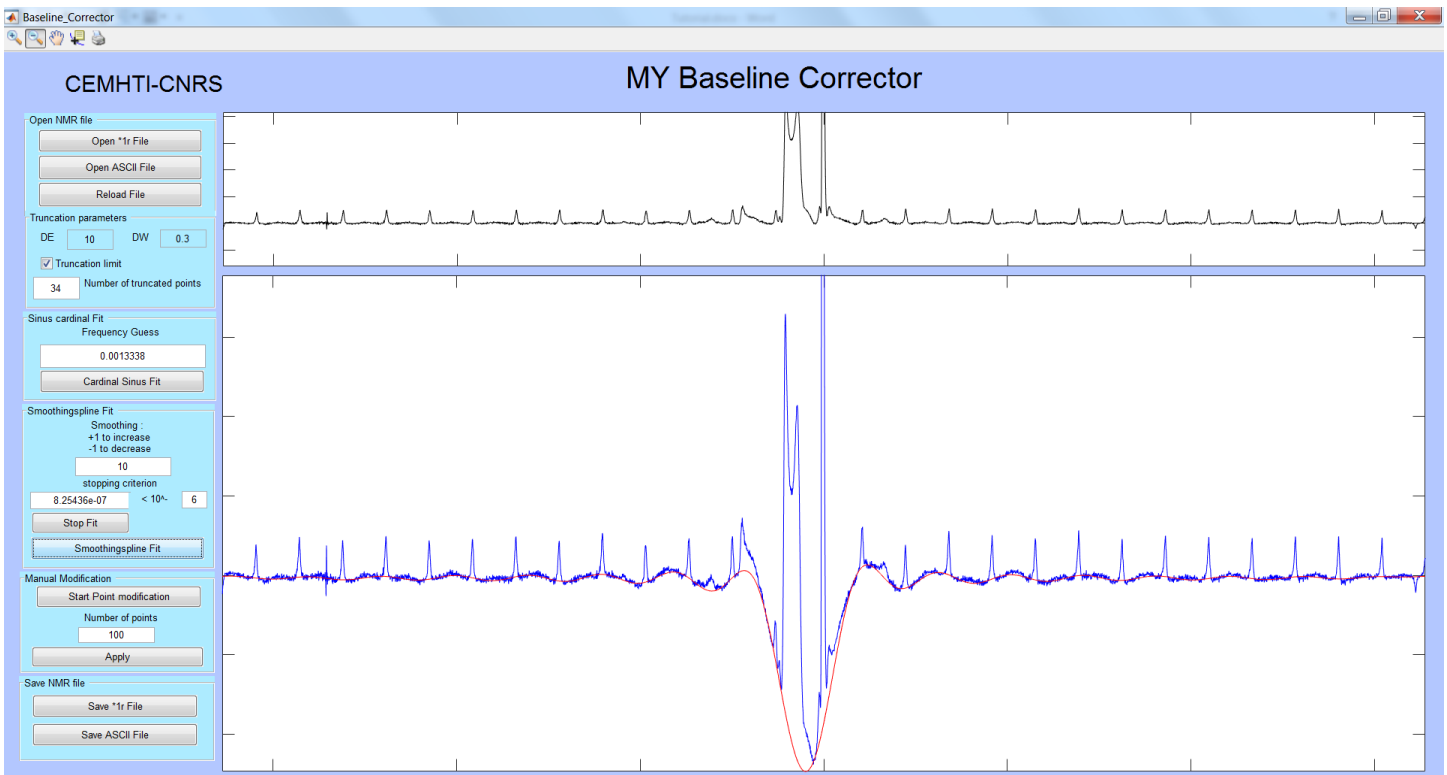
In the majority of the cases, the user is advised to start the correction with a simple sinus cardinal fit to correct the major distortions of the baseline. This correction will usually not give a good enough correction (as shown in the next picture) but will improve the selectivity of the baseline points histogram filter used in the second algorithm.



If the fitting correction doesn't correspond to the baseline, the user is invited to modify the value of the "Frequency guess" parameter and redo the fit.

4. Main algorithm: iterative smoothing spline fitting

To refine the correction the user can use the "Smoothing spline fit" which consists of an iterative smoothing spline fit of baseline points of the real part of the spectrum. This iterative algorithm should allow obtaining the finale baseline correction presented in the next figure. The upper plot is now showing the spectrum after baseline correction.



If the baseline distortion is only caused by time domain truncation, the algorithm should lead to a good correction with the parameter "Truncation limit" checked. The correction is then non-parametric and does not modify the points of the FID acquired after the equivalent dead time. If not, the baseline distortion is probably also due to other factors such as acoustic ringing or low-quality filters. The user is then invited to uncheck the "Truncation limit" and play with the parameter "smoothing" to obtain the desired baseline correction. In this case, the time domain expression of the baseline correction will not be limited to the dead time anymore. An increase of the parameter "smoothing" reduce the freedom of the fit and a reduction will increase it.

The user can interrupt the fit at any time by clicking on the "stop fit" button without losing the correction. Indeed, the stopping criterion might be too low for some spectra.

5. Manual correction

If these two algorithms didn't enable a perfect correction, the user can define the baseline points manually with the "manual correction" option. Even at this stage, if the "Truncation limit" is checked the baseline expression will be limited in the time domain to the equivalent dead time.

6. Saving the data

When a satisfying correction has been obtained the user can save the resulting spectrum in the format in which it has been opened. Both real and imaginary parts of the spectrum are then corrected and saved to allow further operation such as phase correction or fitting.

Conclusion:

My Baseline corrector does not aim at calculating the mathematically exact baseline modulation but to allow an easy, rapid, and reproducible baseline correction. As such, the quality and the interpretation of the baseline correction remain at the judgment of the user.

A video tutorial summarizing this example and more can be found at:

<https://www.youtube.com/watch?v=SRp6quKLbBM&t=4s>

More information about the algorithm can be found in the corresponding article which you can also cite if you used this program for your research: *Automatic iterative baseline correction of single pulse one-dimensional solid-state MAS NMR spectra.*

Wishing you a reproducible research.

Maxime Yon