Data Processing in MNova NMR

Below is a series of video tutorials covering different topics of MNova NMR processing. It is advisable to watch them in a sequence as they refer to previously discussed tools.

Episode 1. Which MNova do I need?

Removed.

Episode 2. Creating MNova Document

This video covers basic toolbars and menus of the MNova window. We create a new document with a title page and save it.

Summary

- Make a title page with the basic sample info for each document
- Save with the original NMR data
- Save the MNova document frequently as you progress through your project

Episode 3. Load data and move around with zoom tools

This episode demonstrates how to load NMR data into MNova document and explore the NMR spectrum using zoom tools.

Summary

- Load NMR data through drag-and-drop or Data Browser
- Update the spectrum Comment field and adjust its fonts size for display
- Add a title to the page itself to be able to find it easier in the Pages view
- Save frequently! (Cmd-S or Ctrl-S)

- Zoom intensity with a mouse wheel
- Zoom with 'Z', unzoom with Shift-'Z'; repeat a keystroke to switch the zooming direction
- Scale up with 'H' and 'F'. Pan with P.
- Navigate a spectrum with Shift-Z-Z-Z mode: click to zoom out, drag a box to zoom in
- Hit ESC on a keyboard to exit a zoom mode (or any other MNova tool)

Episode 4. Manual Phase and Baseline Correction

This episode demonstrates a brief workflow for manual phase correction in a full version of MNova NMR.

Spectral Resolution

This section discusses how you can control resolution in you spectrum after it has been acquired.

First, I must mention that the best approaches to make your peaks more narrow and better resolved are

1. to use an instrument with the highest magnetic field available to you and
2. pay attention to sample shimming step: the better it is shimmed the narrower the peaks. The next section **Reference Deconvolution** can help remove residual distortions from shimming procedure.

Once the dataset has been acquired, it is possible to further increase resolution by giving away some of spectral quality. The peaks may be made more narrow by using **apodization window function** such as **gaussian** or **sin-squared**. The caveat is that you “pay” with spectral quality for any resolution improvement you get in this step. In particular, spectral noise and artifacts around peaks become stronger.

Our goal is to strike a balance between resolution (improved enough for your purposes) and sensitivity (degraded to yet a tolerable degree).

Here are resources you can follow:

1. MNova manual section on Apodization
2. A great tutorial paper: **Resolution Enhancement in 1D NMR Spectroscopy: A Guide to Using This Underappreciated Tactic** by Orr JC, Toll KB, Hoye TR, //J. Org. Chem.// 2026, 91, 20, 6967–6973

1D NMR Processing: Reference Deconvolution

This episode introduces a way to improve peak shapes in the spectrum if they were distorted by imperfect shimming. The tutorial focuses on basic concepts and a practical workflow. For more background on reference deconvolution, see this blog post

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Work in progress! Future episodes are coming…