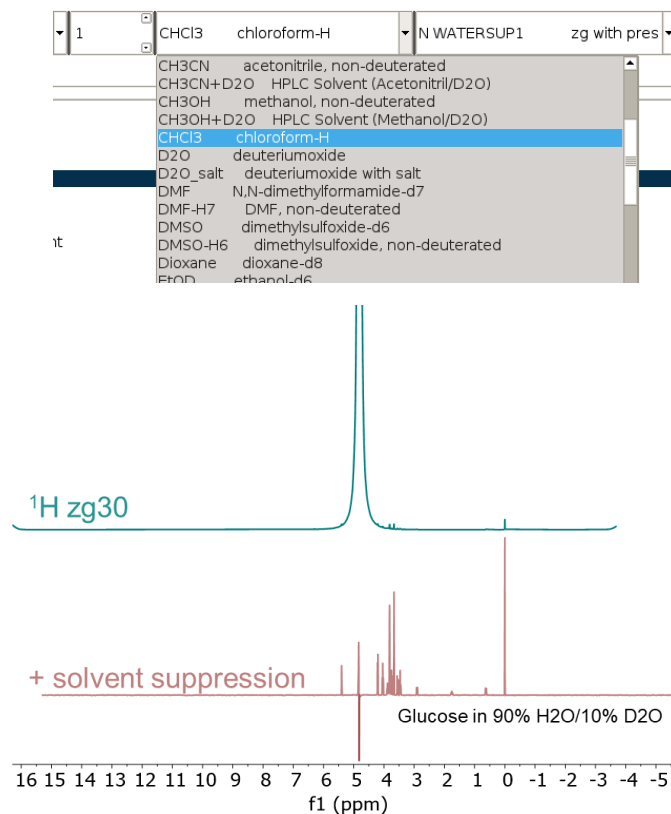


Using Non-Deuterated Solvents

- Collecting data from samples in non-deuterated solvents is very easy on our systems– there are just two caveats:
 - For ^1H -observe spectra, peaks near the solvent signals may be overlapped and/or suppressed
 - The field may possibly fluctuate or drift, leading to multiple copies of peaks. This is very uncommon.

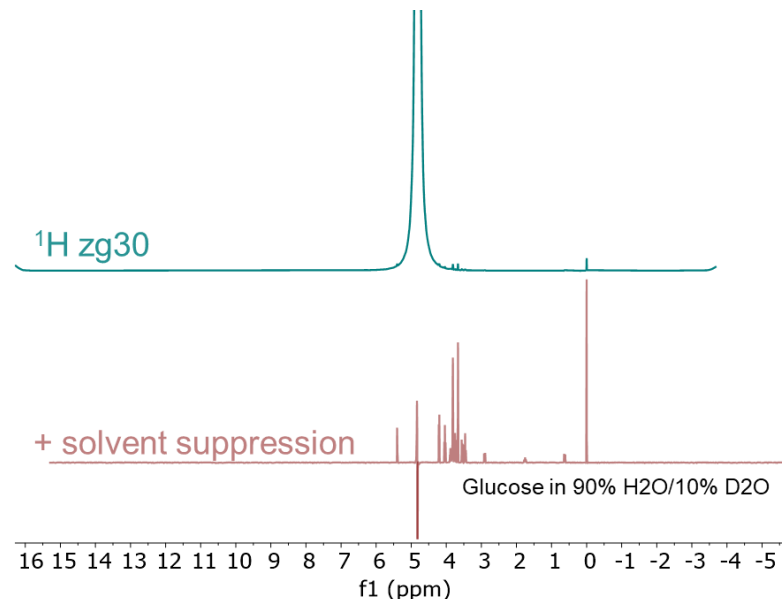
Using Non-Deuterated Solvents

- Step 1: Select the appropriate (non-deuterated) solvent from the drop-down list in ICON-NMR:
 - A macro will adjust the field and shim on the ^1H signal
- Step 2: For the best possible ^1H -observe data, select a solvent suppression experiment such as WaterSup1. Non- ^1H spectra can be run as usual.

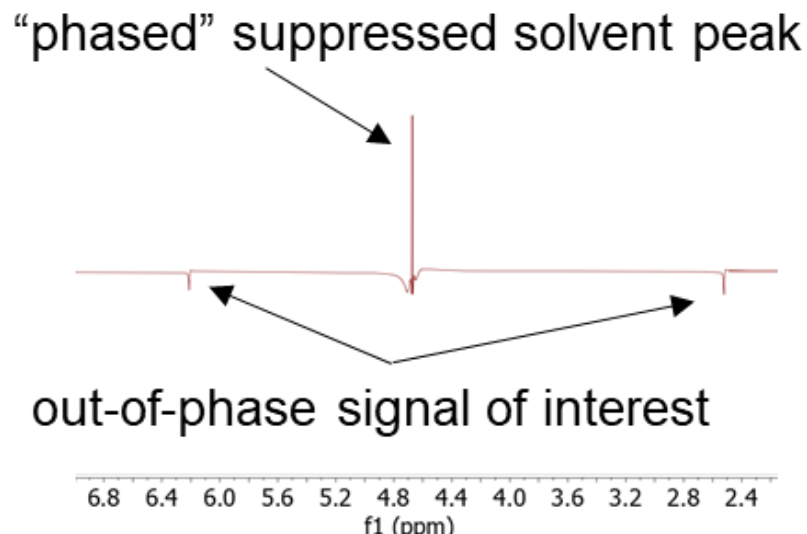


Solvent Suppression

- Use WaterSup1, PROTON_1HSOLV, or various WET parameter sets.
- Completely automated— a macro identifies the single highest peak and suppresses it.
- Can be used for large undesired peaks even if you are using a deuterated solvent!
- NOTE: WaterSup1 works for all solvents with a single signal, not just H₂O.
- Contact Alex if you want to suppress multiple peaks, as for a solvent like Ethanol-H6 or DMF-H7. We can set up a WET parameter set for this purpose.



Phasing Solvent-Suppressed Spectra

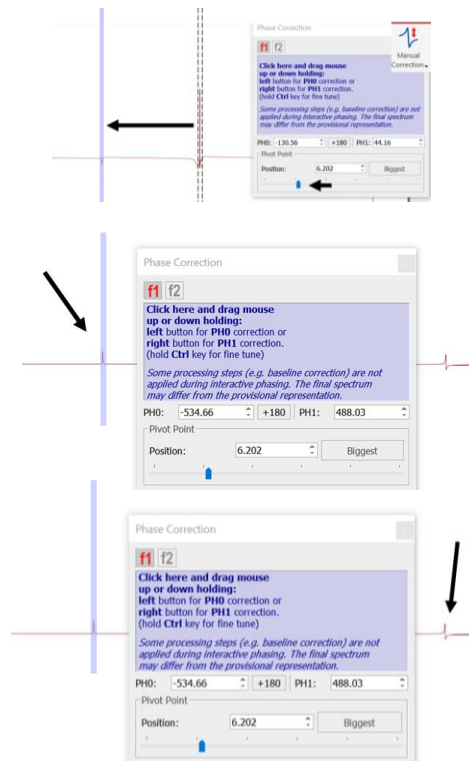


Autophasing routines may prioritize your residual solvent signal! In that case, you will need to apply manual phasing!



Phasing Solvent-Suppressed Spectra

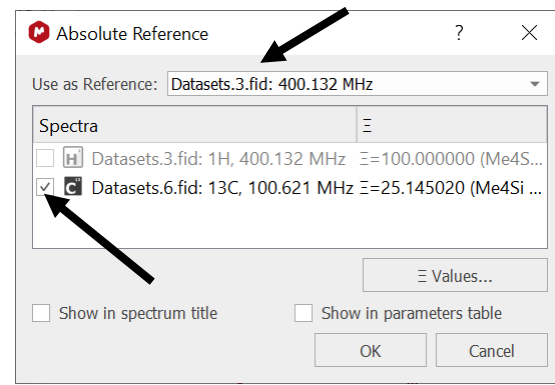
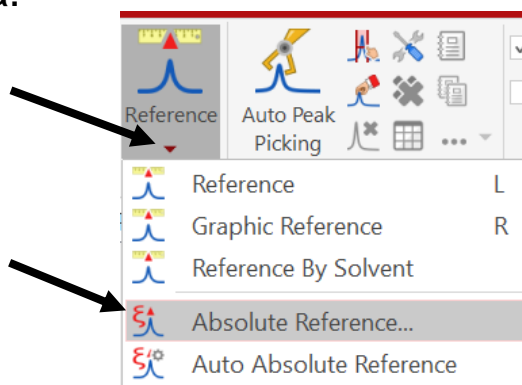
- 1) Click on **Manual Correction** under **Processing**. Use the slider to move the purple bar from the solvent peak to a peaks of interest
- 2) Holding your left mouse button in the purple window, drag the mouse vertically until the peak you selected is in-phase (positive and symmetric). This is “0th order” phasing and applies to all peaks equally.
- 3) Holding your right mouse button in the purple window, drag the mouse vertically until (non-solvent) peaks far from the earlier peak are also in-phase. This is “1st order” phase correction which is linearly dependent on frequency.



Remember to always perform a baseline subtraction after phasing, especially if you want to integrate peaks!

Referencing Spectra for Samples in Protonated Solvents

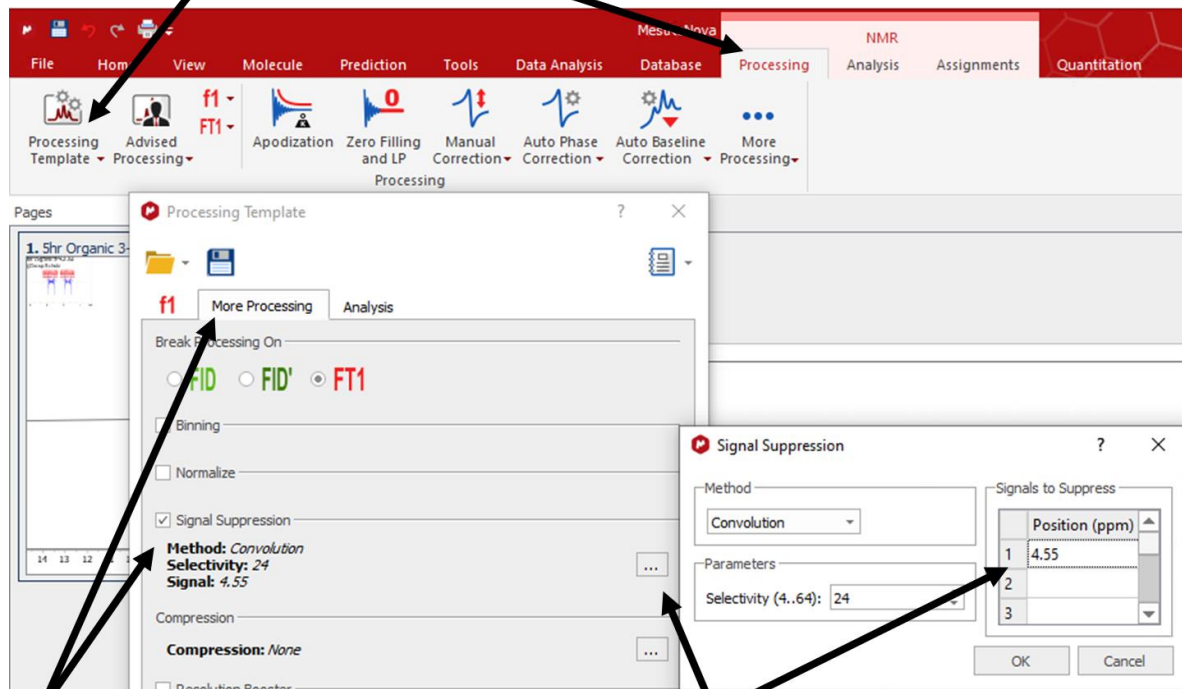
- 1) Load all spectra collected for your sample into an Mnova document. There will be ^1H experiments starting with expno **901** that are collected automatically— load these in as well. Spectrum 901 would have been collected prior to collection of spectrum 1, etc.
- 2) With the ^1H spectrum (901 or higher) shown, click on **Reference** under **Analysis**. Select your TMS/DSS peak if available and set to 0 (this is the ideal approach). Otherwise, select your solvent peak and set it to its expected shift.
- 3) Select **Absolute Reference** under **Reference** and select the now-referenced ^1H spectrum in the drop-down for **Use as Reference**.
- 4) Check the rest of the spectra that correspond to the sample and click **OK**. This will reference the other spectra.



Removing Solvent Peaks in MNova

If desired, solvent peaks can be removed by signal suppression in MNova. This is mostly “cosmetic” and other signals near the solvent peak will also be removed.

- 1) Processing tab
- 2) Processing template



- 3) “More processing”/ Select “Signal Suppression”

- 4) Open up options, confirm there is an entry near solvent peak