Chenomx NMR Suite V9 New Features

GENERAL

• Enhanced **drag-n-drop support** through-out the entire suite
• Complete native support for the **Apple M1 chip**
• **Enhanced Preferences settings** [“Default Compound Sets” and “Concentration Fitting” are new and allow for better control of the software]

PROCESSOR

• Improved **Automatic Phasing:** *Automatic:* Click the **Auto** button to have Processor automatically calculate phase angles. Review the spectrum after automatic phase correction to ensure that the results are acceptable. If necessary, you can use the manual controls to adjust the phase angles before accepting them.

• **Batch import of sample pH information** from excel workbook

• **Automatic concentration fitting:** Once peak clusters have been positioned, compound concentrations can be fit and optimized using constrained penalized linear least squares, according to: $\min_{l \le x \le u} \|W(Ax - b)\|_2$

• **Export of statistical standard deviation** errors on concentrations, for the calculation of confidence intervals on concentration values. Exported as a second Excel tab when exporting concentrations.

• *Compound Specific* **Profile Importing** as well as **Batch MetaProfile importing** added. Spectral profiling can be accelerated by importing, partially or entirely, profiled data of spectra that have already been fit. This is particularly efficient when dealing with large series of similar spectra.

• **Multiple spectral region searches**: Right-click on the spectrum, and click "Search for Compounds Near x.xx ppm" to initiate a single location search, or "*Add x.xx ppm to search locations*" to append the current location to the existing search location(s).