VERSION 8.6 RELEASE NOTES

Processor

- Improved, more accurate and faster automatic phasing (in proton spectra when TSP or DSS is used as CSI)
- Introduction of a new automatic baseline algorithm (BXR).
- Addition of two additional settings in the number of baseline points (Very High and Extreme)
- The number of baseline points is no longer static. It is automatically adjusted based on the spectral sweep width.
- Implementation of a box-tool for selecting and deleting several baseline breakpoints at once
- Clusters transforms automatically readjust to keep their fit location following change of CSI that is pH-dependent and/or following a pH change.
- Introduction of a peak reference tool: (Right-Click) Brings up an interface to specified at desired frequency at the clicked location. Cluster transforms will be automatically modified to reflect the change so that cluster fit locations won't be altered.

Profiler

- Introduction of an automatic Compound/Cluster Snapper tool to automatically get the best cluster fit location (fully based on global cluster shapes). The procedure can operate on both the original spectral line, or the subtraction line to take into account what's been fit already.

- Introduction of a pH tool. Analyses the fit position of clusters that are pH sensitive and that have been transformed in the current fit, and reports the pH that would best explain the location of each. An optimized pH value is proposed. The pH can be now be changed right from Profiler instead of having to go back to the Processor module. Upon pH change, the transforms are automatically recalculated so that the positions of the clusters do not change. If cluster(s) are selected, the pH tool does the analysis on those. If compounds are selected in the compound table, then it uses those. If no compounds are selected, then it analyses the entire list of profiled compounds.

- Batch Import Profile: Transfer a profile (i.e a fit) from a source CNX file to several other CNX files automatically. In both Import Profile (individual) and Batch Import Profile, the peak cluster transforms are automatically adjusted according to the pH of the spectrum it is imported to versus the pH of the spectrum the profile is from.

- Addition of two overlay modes: Overlay Sum Line and Overlay Subtraction Line. Instead of the just the original spectra you can now overlay their sum or subtraction lines

- Reintroduction of Clear Transforms and Clear Concentrations commands on selected clusters/compounds.
- Improvement of Autofitting
- Ghost line: now without transforms

Compound Builder

- Addition of Overlay Subtraction Line. This is particularly useful to model compounds/unknown resonances on the residual line.

Spin Simulator

- Support for negative coupling constants.