



Data Collection and Data Processing for the NMReady Benchtop NMR Spectrometer

Data Collection

The user interface is surprisingly easy to use; it is not cluttered with 2 letter commands that are confusing to beginners but are familiar to expert NMR users. For novice users, such as undergraduate students, spectral parameters can be presented so that when the correct solvent is chosen, students need only press "Go" to collect data. Changes to other basic parameters, such as number of scans, are possible to enhance the learning experience.

For more advanced users, seeking optimized spectra, the default data acquisition parameters can be manipulated prior to data collection. These include both the basic parameters - spectral width, recycle delay - and more advanced parameters - e.g., number of points, zero filling.

Data Processing

Once the data is collected, it can processed directly on the touchscreen. As is shown for this isopropanol spectrum, the data can be manipulated manually or automatically for proper 1) baseline correction, 2) phasing, and 3) referencing. Spectra can also be 4) integrated and 5) have the appropriate peaks picked. These operations use a standard threshold method as is shown for this spectrum of 4'-hydroxypropiophenone.

Post-Processing

Additional post-processing parameters such as line broadening and zero-filling can also be accessed directly from the processing window.

Data Accessibility

The NMReady is network capable through an Ethernet port so it offers a number of options for a user to access data. From the processing window it can easily be:

- 1) Saved to the NMReady as a .jdx file so it can be further manipulated later
- 2) Printed to a network printer
- 3) Saved to the NMReady as a .png file so it can be viewed later
- 4) Saved to a LAN location

Saved spectra are easily re-accessible through the results window. To re-load a previous spectrum it select the correct file name and hit "Load".









