MADByTE Example

For this example, please download the sample data from https://zenodo.org/record/3825107. Next, unzip the data into a location you feel works well. Remember, the raw data and processed data should be kept separate. These data are already processed and peak picked, allowing us to skip the spectrometer side of things.

Next, launch MADByTE.

Under Parameters, select the *NMR Data Directory* (folder with the sample data in it) and a *Project Directory*. You can create a project directory with any name, so for this, we're simply going to create a directory called "Example_1". You'll notice that by selecting the NMR data folder, we can see the experiment directories of each of the compounds, if you wish to remove one, simply highlight it and select remove sample.

Under parameters, we can see some adjustable tolerances. We are going to leave these at default, except that we will adjust the *Similarity Ratio* to 0.51 (This means there must be >50% similarity to network).

Next, under action items, select MADByTE to run the analysis. If you have the terminal visible, you should be able to see the process working in the background.

Once completed a popup will appear saying the process has completed. At this point, all comparison is done between the samples, but we don't have a visual result. Let's fill out *Network File Name* to be "Example_1", and you may select node colors for both the extract and spin nodes, or you can leave them default if you wish. For this dataset, the prefix "HND_" signals to the system that these data are standards, so color assignments for the central node are re-written to teal. Once you are satisfied, simply click *Generate Network* and your data will be processed into the three network styles.

If you hover over the nodes, you can see exactly what resonances are in each spin system, and if that spin system is connected to any other spin system in your sample list. If you wanted to adjust the similarity cutoff, you can simply enter a new similarity cutoff and hit *Load Parameters* to read in the new values. You are not required to run a new MADByTE analysis to create a new network, but you are required to re-run if you adjust the Hppm or Cppm cutoff values, as these are used for multiple backend calculations.