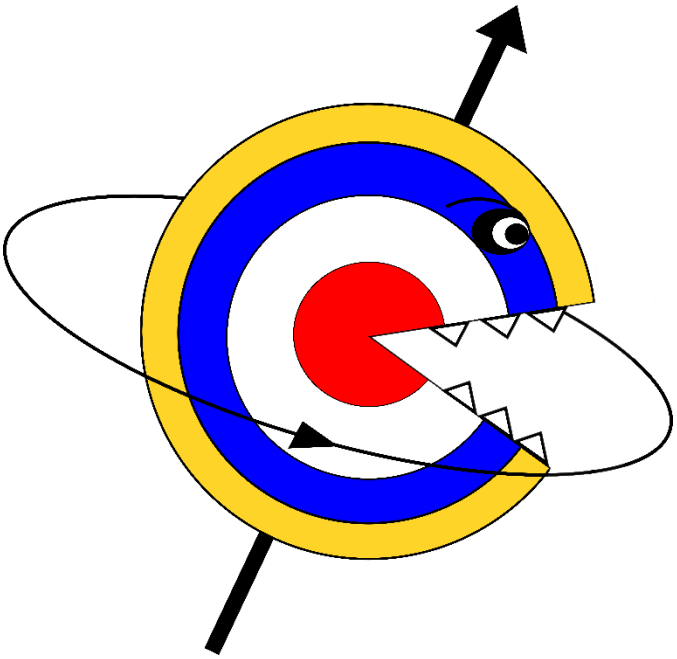
MADByTE Quick Start Tutorial

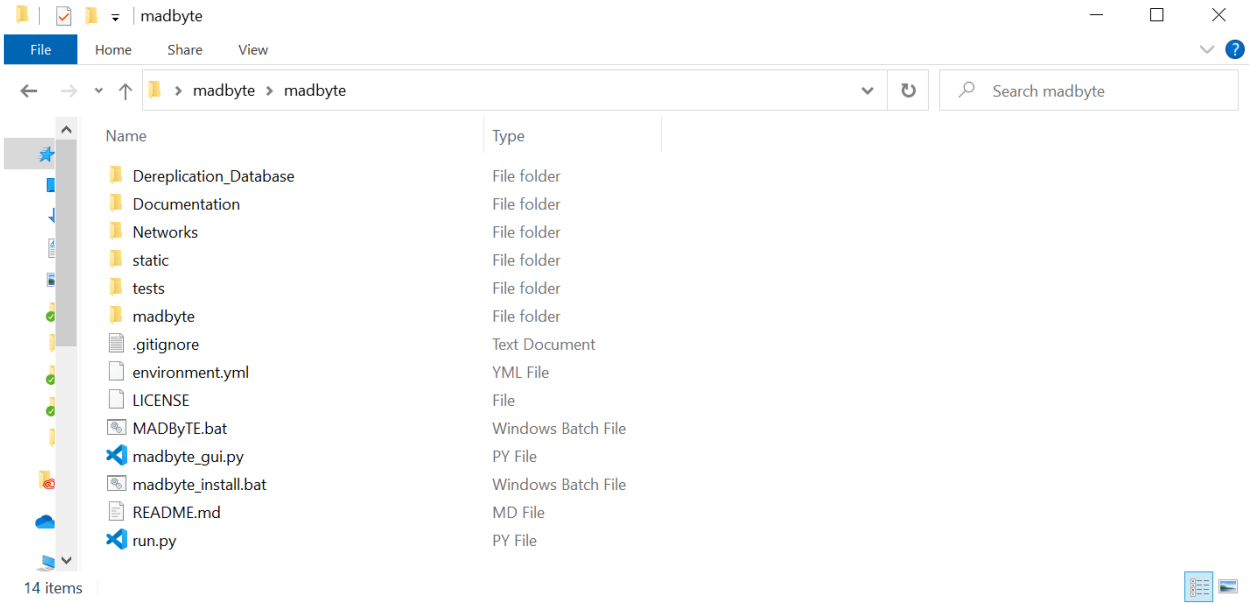


Step 1: Gather Data

MADByTE requires processed and peak picked NMR data to perform analysis. For this example, these data can be found and downloaded at https://zenodo.org/record/3825107. To use your own data, please see the User Manual for detailed requirements.

Step 2: Launch MADByTE

Launching MADByTE can be done by opening a terminal window in the directory where the MADByTE code base is located. That directory will look like this:



In the terminal, navigate to this directory.

- One method (although not the only one) is to open anaconda prompt and change directory by using ‘cd’. An example is shown below.

```
(base) C:\Users\Jmegan>cd desktop

(base) C:\Users\Jmegan\Desktop>cd madbyte

(base) C:\Users\Jmegan\Desktop\madbyte>cd madbyte

(base) C:\Users\Jmegan\Desktop\madbyte\madbyte>
```

Then, activate the madbyte environment by using the command ‘conda activate madbyte’. This will ensure we are using the anaconda environment set up by the install script. Then, launch MADByTE by using the command ‘python madbyte_gui.py’.

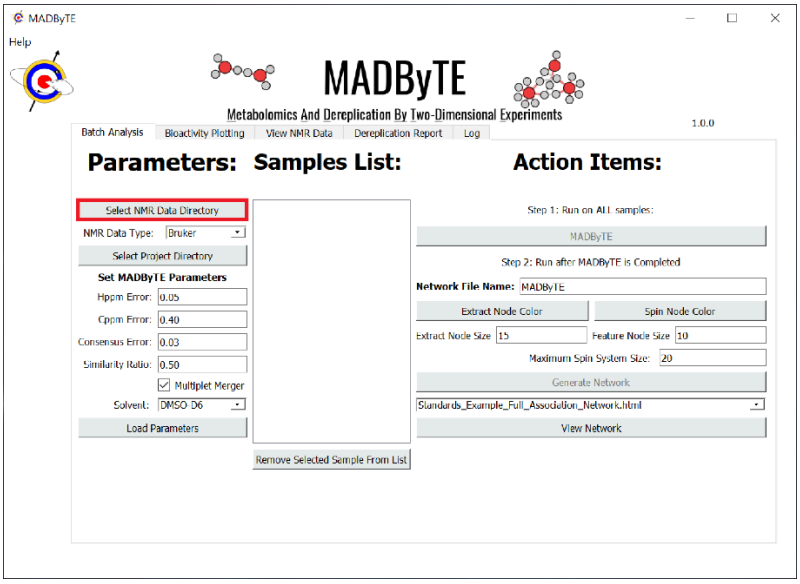
```
(base) C:\Users\Jmegan\Desktop\madbyte\madbyte> conda activate madbyte

(madbyte) C:\Users\Jmegan\Desktop\madbyte\madbyte>python madbyte_gui.py
MADByTE is loading...
Multithreading with maximum 8 threads
```

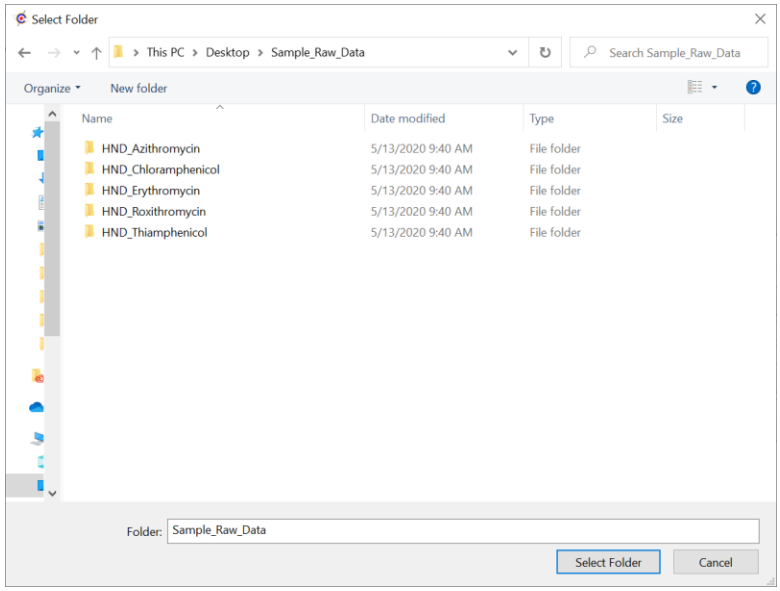
On windows, you can launch MADByTE by using the “MADByTE.bat” file. This script will check to ensure anaconda and the dependencies are properly installed before launching.

Step 3: Set up MADByTE Parameters

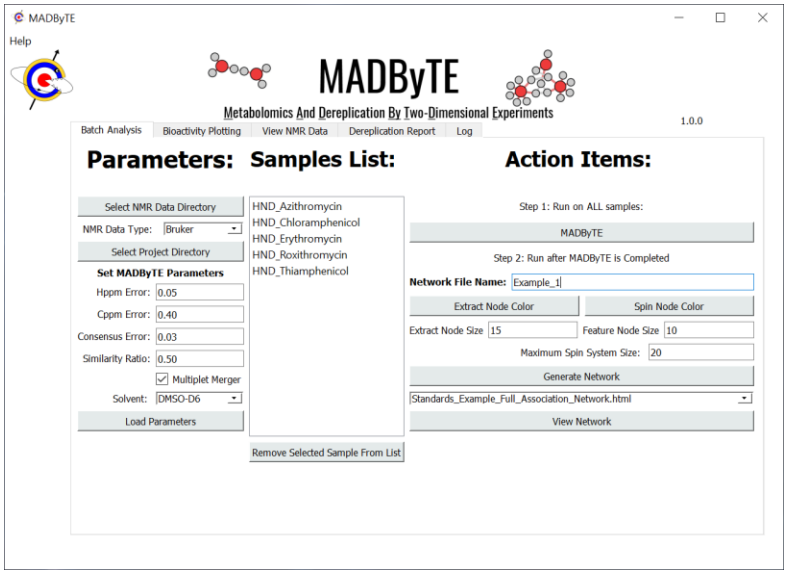
Users are required to select an NMR directory and a project directory before MADByTE can be run. To do this:



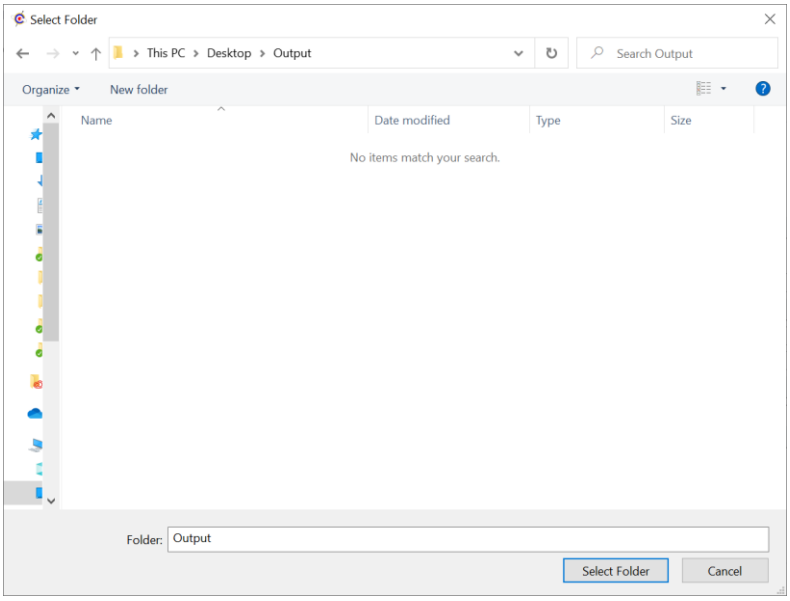
This will open a file dialog which allows you to navigate to the directory where your NMR data is stored.



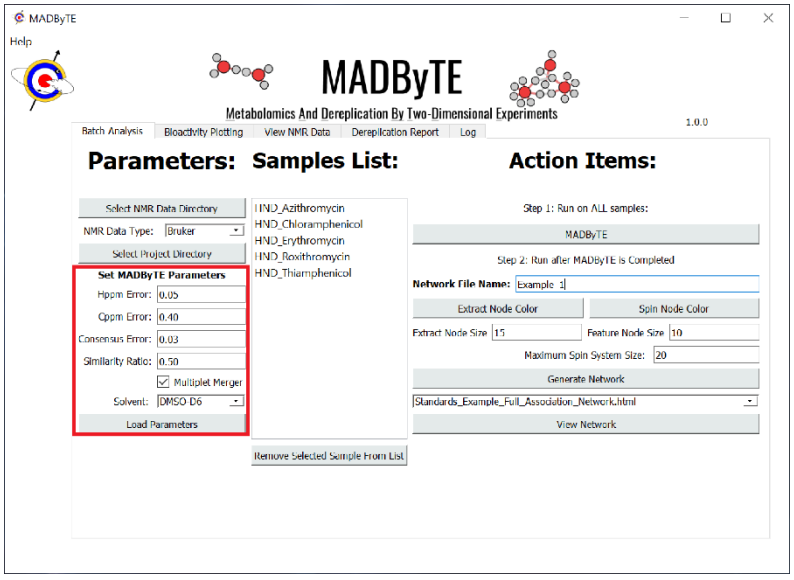
Here, you simply want to select the directory containing your samples, not each sample file folder. After selecting the folder, you will see the samples list populate with the samples from the directory.



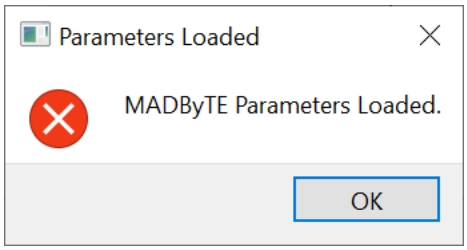
Repeat this step for the Project Directory – This is where the output files will be stored. There will not be any change to the Main GUI when a project directory is selected.



Next, the user can adjust the settings in the space below. This allows for users to adjust the Hppm Error, Cppm Error, the Consensus Error, and Similarity Ratios. Detailed information on what each of these does to the processing can be found in the main user manual.

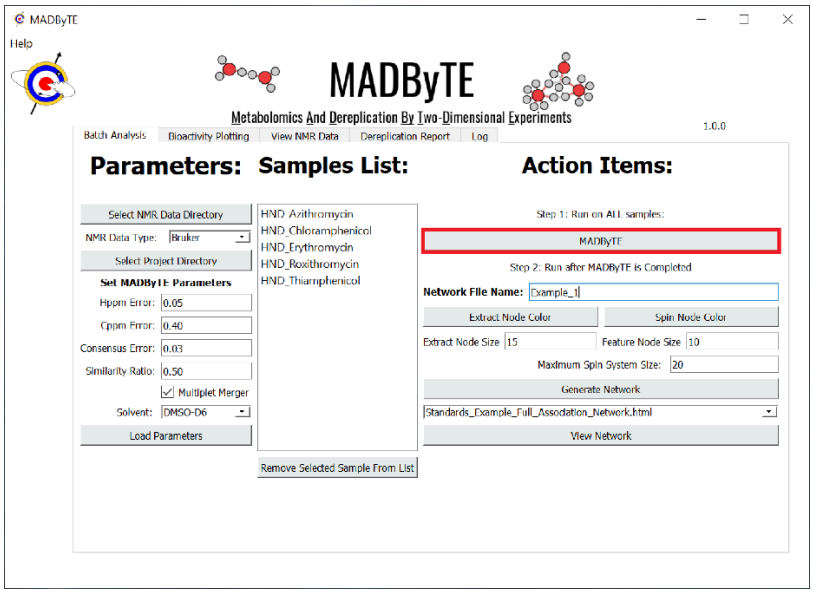


After adjusting these parameters, select “Load Parameters” and a message will display showing the parameters have been loaded.

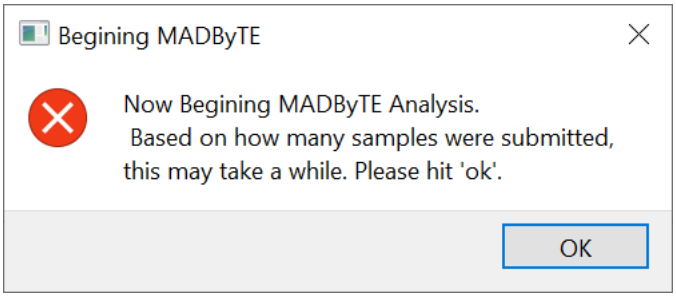


Step 4: Run MADByTE

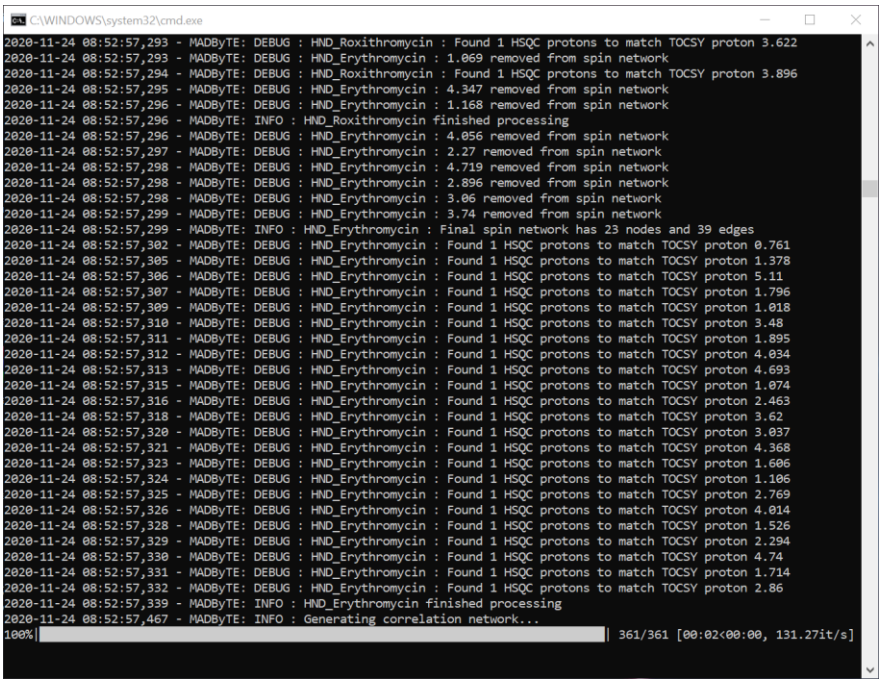
Once parameters have been set, run MADByTE analysis using the MADByTE button.



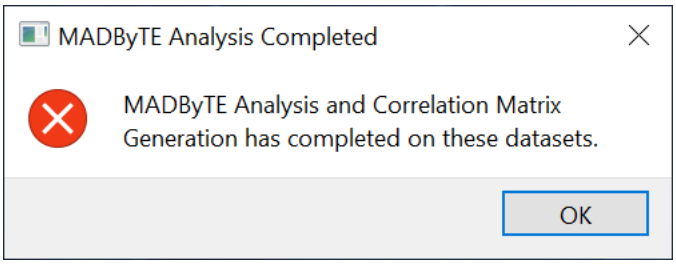
Users will get the following message to show that MADByTE analysis has begun. Select OK to begin processing.



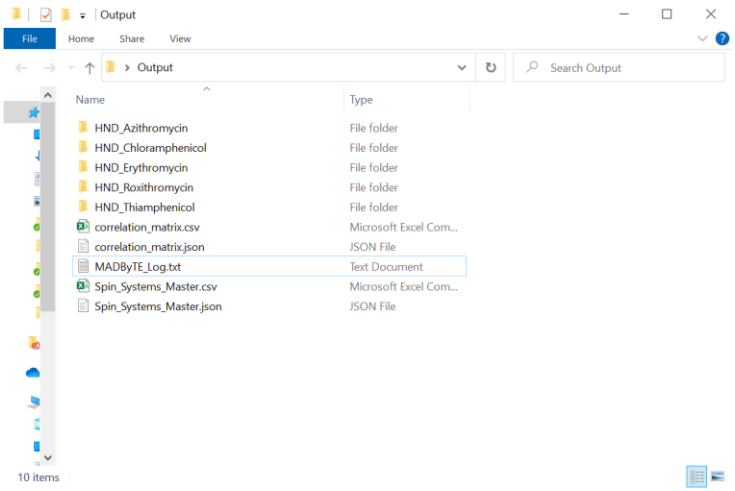
During this process, detailed information will be displayed in the terminal window. This information is also stored in the log file.



Once MADByTE has completed analysis, the following message will be displayed:

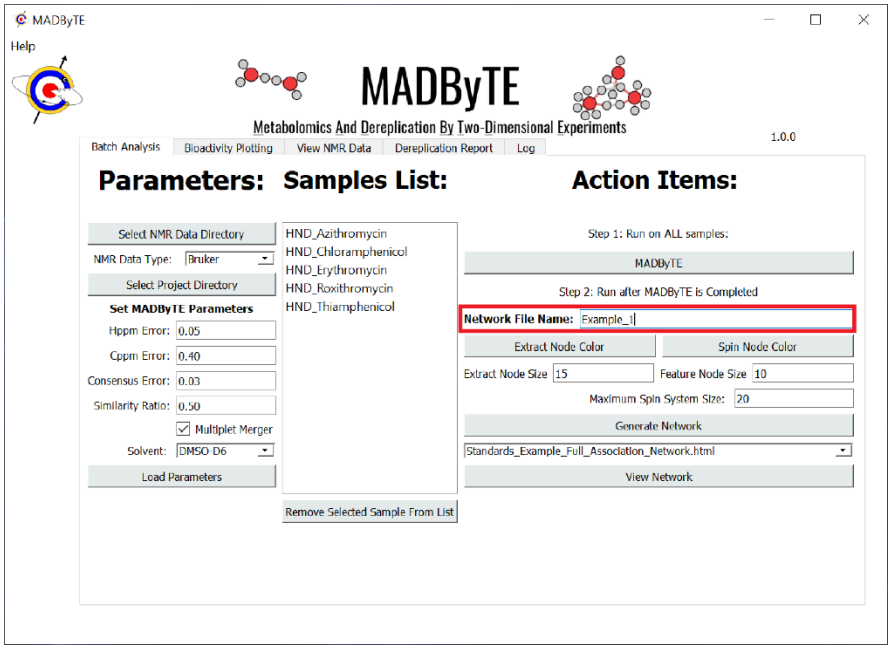


Once this has completed, the Project Directory will now have a suite of new files in it. These are used to construct the MADByTE network.



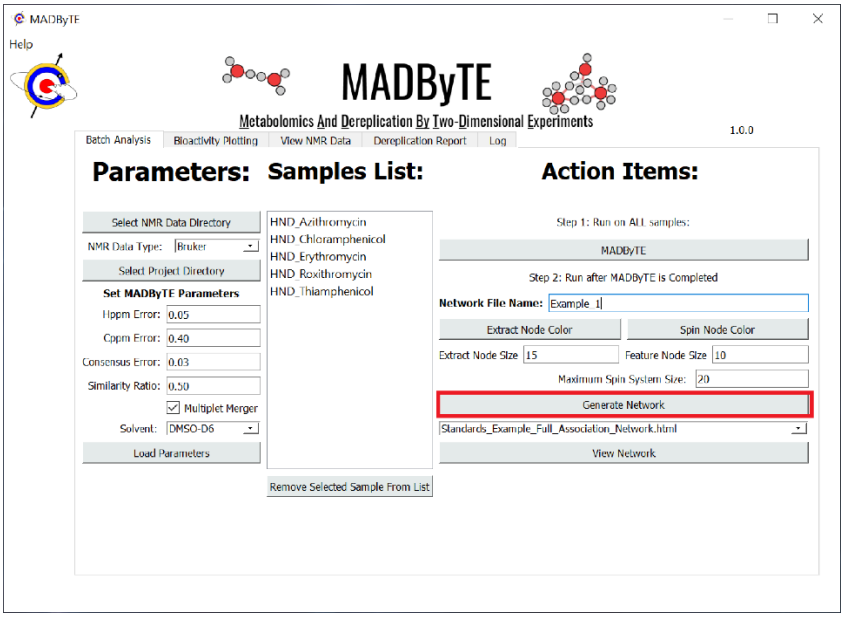
Step 5: Generate Networks

Once MADByTE has completed, the network generation will take the spin system information and the correlation matrix information and construct a network. To give the network a customized name, fill in the "Network File Name" field.

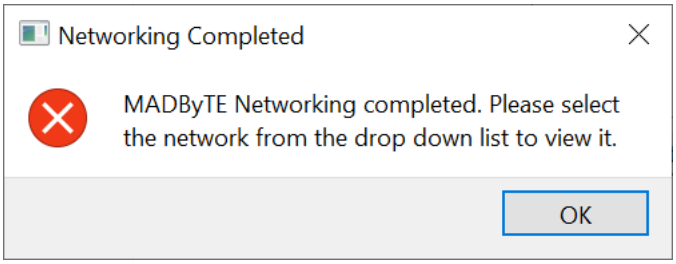


Users can customize the look of the finished network by altering the Extract Node Color and Size, the Spin Node Color and Size, and the Maximum Spin System Size values. Detailed information on these can be found in the user manual. For this example, we will use the default values.

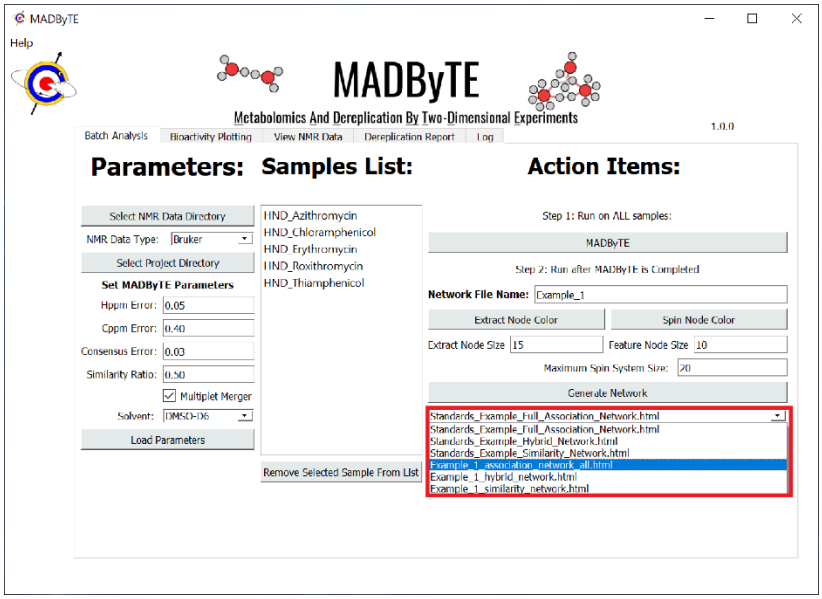
To generate the network, click the Generate Network Button.



Upon completion, the following message will be displayed:



To view the resulting network, select it in the dropdown list and click View Network.



This opens the Network Viewer Plugin and displays the selected network. Users can interact with the network by hovering over nodes to see membership of each spin system as well as the identity of the spin system feature.