The basic idea of running the workflow is as follows:

1. Add all the NMR spectra into: Data / NmrData
2. Add all the MS spectra into: Data / MsData
3. Run the featureGeneration.py script:
   1. This generates a hash table of features for all reagents. This will be saved as a pickle file.
   2. It then iterates through all the possible reactions and uses the hashtable to create features from the reagents in the reaction. This will be saved as a pickle file.
4. Run the lableGeneration.py script to read NMR and MS and label the reaction as failed or pass. This is also stored in the pickle file generated in step 3b. This script also sees to optimize several parameters done by decision maker.