NMR Data Analysis Program

1. In Top Spin, record peaks of Surfactant, Counter Ion and TMS to be analyzed for every pH.
   1. rser 1, ef, apk
2. Make a file on desktop named **NMR\_Files** if it doesn’t already exist. This is where a macro in Top Spin will output the data files.
3. In Top Spin, open up the folder of the first pH to be analyzed and open the first trial. Use commands in step one. Then type` xmac analysis` to have a macro begin outputting the data files. Make sure the ranges are in terms of ppm ‘LEFT = 14.721240043640137 ppm. RIGHT = -5.304302936942399 ppm’. If not, redo step 1 before executing the macro.
4. Files 1.txt – 18.txt (or however many gradients were run) should be created in the NMR\_Files folder. Moves these into the corresponding trial folder within the pH. Directory must be in the form of (see “https://github.com/rileybusche/nmr\_data\_analysis” README for a visual example) :
   * 1. Surfactant Name
        1. pH7.60
           1. Trial1
           2. Trial2
           3. Trial3
        2. pH8.00
5. Repeat steps 3 and 4 for the following trials and pH’s, putting the files in to corresponding folders.
6. Move **Surfactant Name** folder into the folder on the Desktop titled **NMR\_Analysis** for easier path specification later. (Otherwise you must specify the full path in step )
7. Confirm that the file from the spectrometer, Difframp – which contains the gradients, is in the **Surfactant Name** folder. If it is not there, obtain the file and place it there.
8. Confirm that the **NMR\_Analysis** folder also contains the files: **main.py**, **build\_csv.py** and **functions.py**. These files are necessary for the program to run. If they are not there, ask your professor. The files can also be found in the github repo linked above.
9. On windows, run the program Power Shell
10. To navigate to the folder containing the script, type the command: **cd Desktop\NMR\_Analysis**
11. From here you can execute the python script. In the script you must specify the directory name to be analyzed. This is the **Surfactant Name** folder. In Power Shell type:

python main.py --path “**Surfactant Name**”

1. The script will prompt you to enter in frequencies to be analyzed at each pH. Enter them separated by space. Example:

2.918 -0.1212 5.675

1. Once the script finishes, open the **NMR\_Analysis** folder on the desktop and confirm that there is are csv files for all pHs analyzed. One will be the raw data, the other is has tables containing all the values and the gradients.