SECIM NMR Data polishing workflow
in MATLAB
USER GUIDE for Version 1.0

Preliminary Steps:

1) Clone the MATLABworkflow from secim's git repository. To do that make sure Git is installed in your system, execute the following command on the command line:

>>> cd “where ever you'd like to deposit the MATLAB workflow”
>>> git clone secim@git.hpc.ufl.edu:MATLABworkflow.git
>>> cd MATLABworkflow

and make sure you have a v1 folder inside and a projectExample folder in there.

2) Run MATLAB. Under the “home” tab, in the environment section, click on the “Set Path”. Click on “Add folder”. Then browse to the MATLABworkflow, choose v1 folder and hit save.

3) Next, click on “open” again under “home” tab. Choose “secim_workflow_GUI.m” in v1 folder.

4) open up the “path_for_ft_files.csv” file which contains two columns dir and filename. Edit it to have it point to the ft files you'd like to analyze.

In the projectExample folder there is a test set called proton_ft you could use.

Ideally you would want to have a project folder somewhere and have this “path_for_ft_files.csv” in it and set the path as your working directory in MATLAB so that all the parameters and associated files gets saved in there.

Workflow:

Execute (control+Enter while you are on the line) the secim_workflow_GUI.m step by step.

1)loading a template of parameter table and setting up our parameters table

2)loading all ft files based on their path

```
loadStudyFTdata('path_for_ft_files.csv');
```

if you create a different file with a different name, do not forget to modify the above line accordingly (change the name of path_for_ft_files.csv to the other file name you have created.)

3) Finding region for referencing GUI

This GUI helps you to choose a range that contains the peak for internal standard for all samples to be used in the next step where you reference all spectra.

You would only need to choose appropriate parameters inside GUIs and and at the end your parameter table is saved as “chosen_workflow_parameters.csv” along with the polished files in your working directory.