SiREM Fitting Python Code Quickstart Guide

Step 1: Download Anaconda

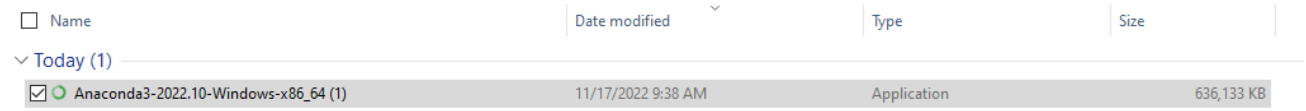
1. Follow the link to: https://docs.anaconda.com/anaconda/install/index.html

2. Click **Installing on Windows**

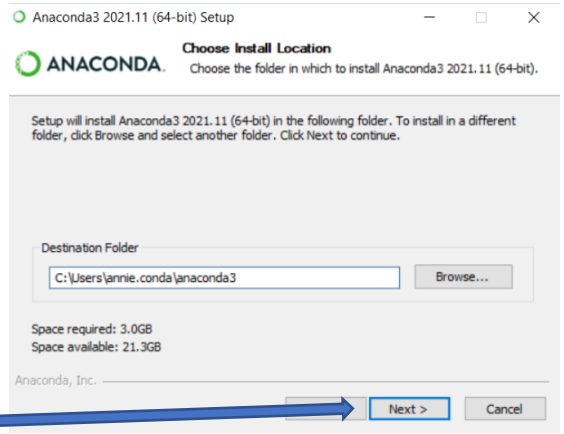
3. Click **Download the Anaconda Installer**

4. Click **Download**

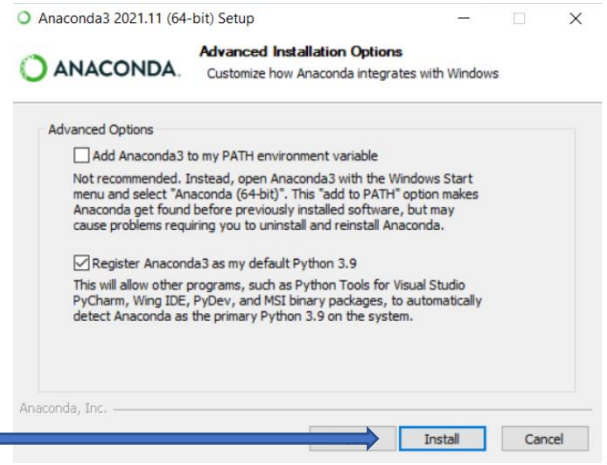
Step 2: Install Anaconda



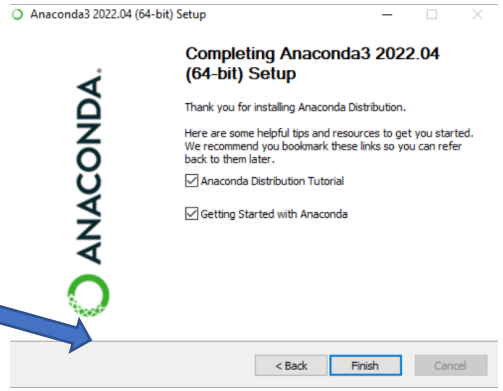
1. Once the download is complete, navigate to your downloads folder and double-click the installer to launch



2. Install for **Just Me**
3. Click **Next**
4. Confirm that the destination folder matches this format:
   C:\Users\{your username}\anaconda3
5. Click **Next**



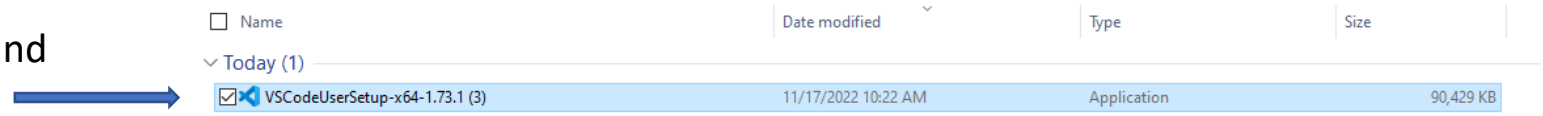
6. Accept default advanced options and click **Install**
7. Click **Next**
8. After installation (may take a few minutes) click **Next** twice. You will the see the following dialogue box. Select **Finish**



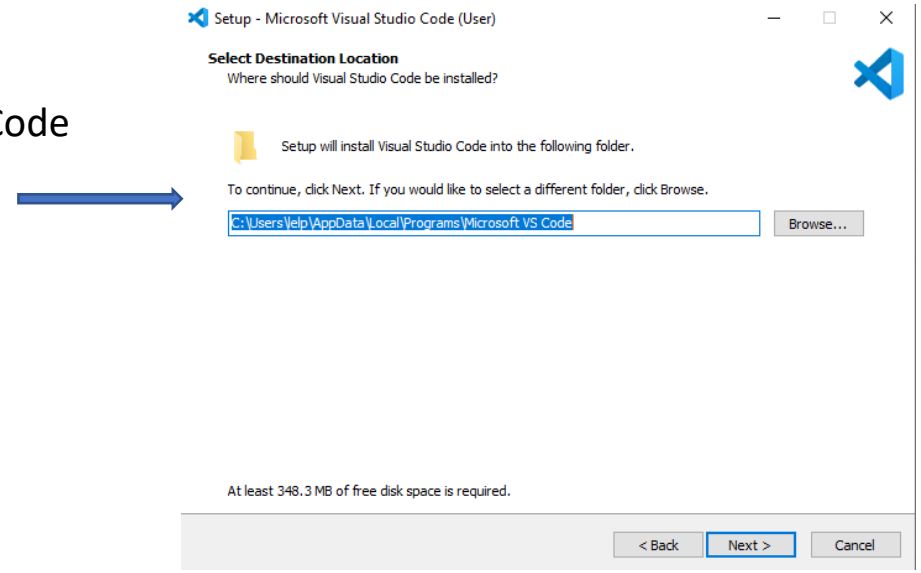
Anaconda is now installed! Move to Step 3

Step 3: Download and Install Visual Studio Code

1. Follow the link to: https://code.visualstudio.com/docs/setup/windows
2. Click **Visual Studio Code installer**
3. Navigate to your downloads folder and double-click the installer to launch



4. Accept the agreement and click **Next**
5. Accept default installation path C:\Users\{yourusername}\AppData\Local\Programs\Microsoft VS Code and click **Next**



6. Accept default Start Menu Folder setup and click **Next**
7. Accept default Additional Tasks and click **Next**
8. Click **Install**
9. Click **Finish**
10. Visual Studio Code may open automatically after installation. We will return to this in Step 5

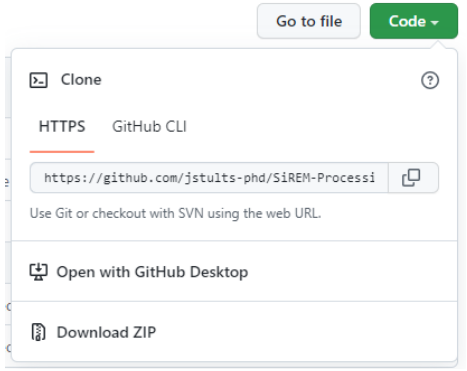
Step 4: Download and Extract SiremFitting Code

1. Follow the link to: https://github.com/jstults-phd/SiREM-Processing

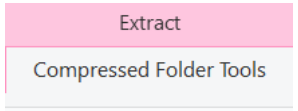
2. Click the green 

button

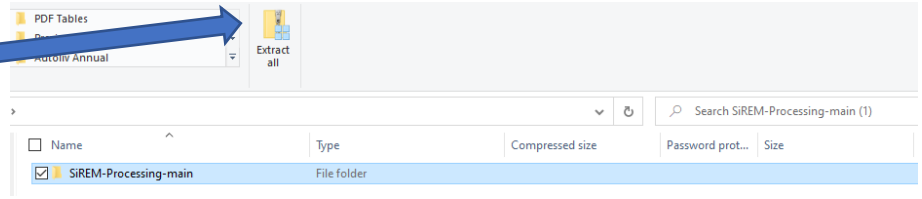
3. Click **Download ZIP**



4. Navigate to your downloads folder, select SiREM-Processing-main, click **Extract**

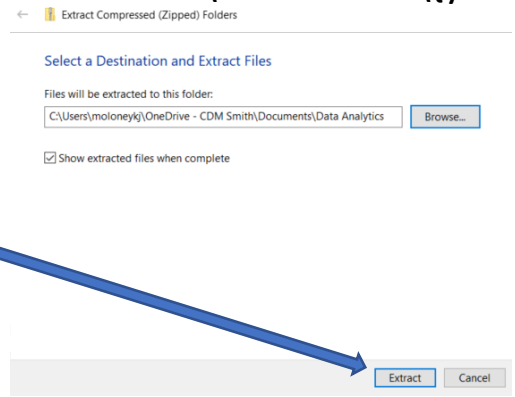


5. Click **Extract all**



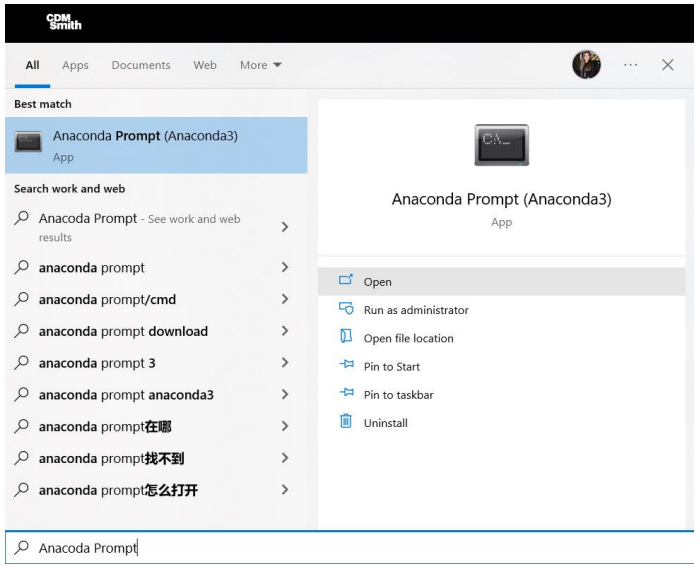
6. The default setting is to extract to your downloads. DO NOT select this. Instead, select the following folder destination C:\Users\{your username}\OneDrive – CDM Smith\Documents\{your folder name}

7. Click **Extract**



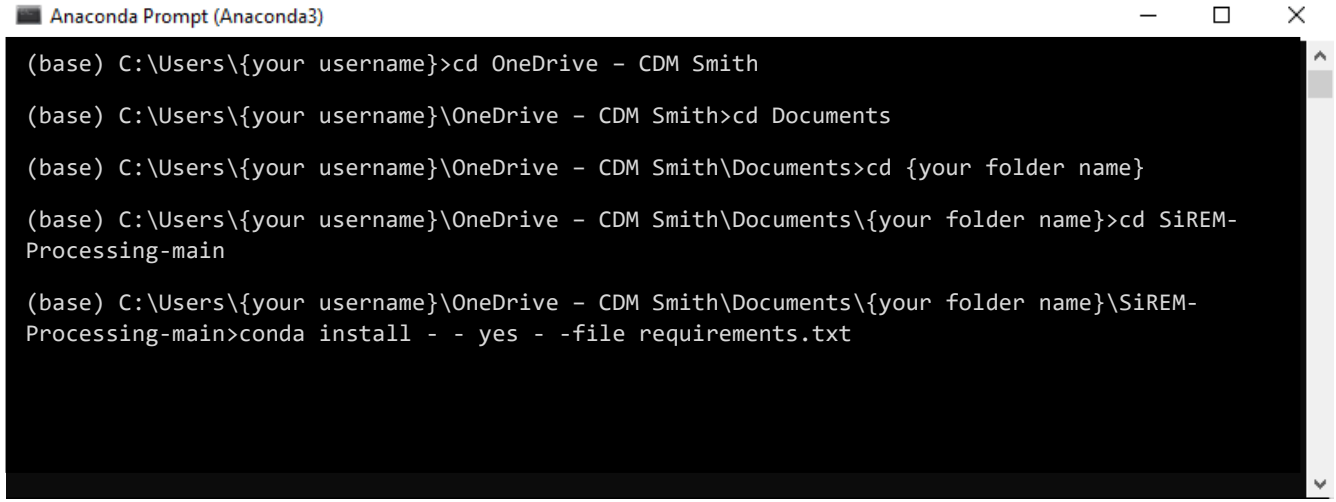
Step 5. Install Required Packages

1. Open Anaconda Prompt by searching in taskbar and clicking **Open**



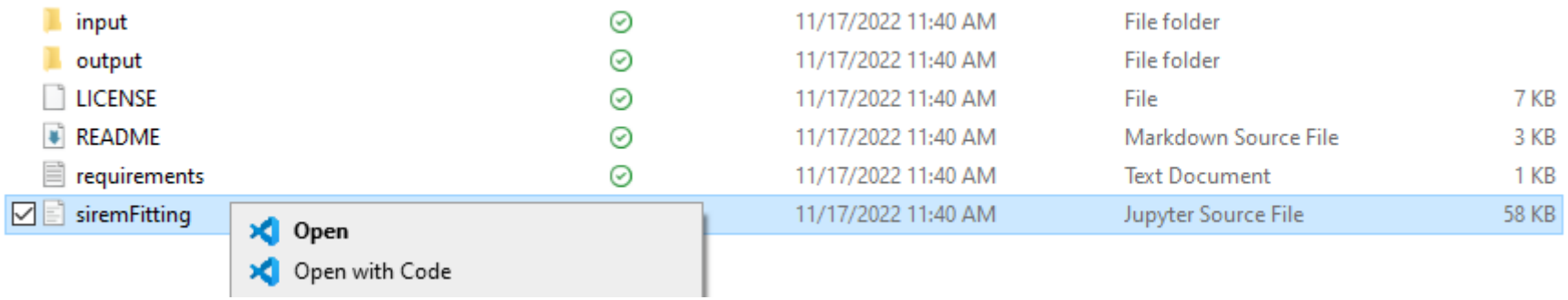
   The following line of code will appear: (base) C:\Users\{your username}

2. Type “>cd OneDrive – CDM Smith” and press enter
3. Type “>cd Documents” and press enter
4. Type “>cd {your folder name}” and press enter
5. Type “>cd SiREM-Processing-main” and press enter
6. Type >conda install - - yes - - file requirements.txt to install packages

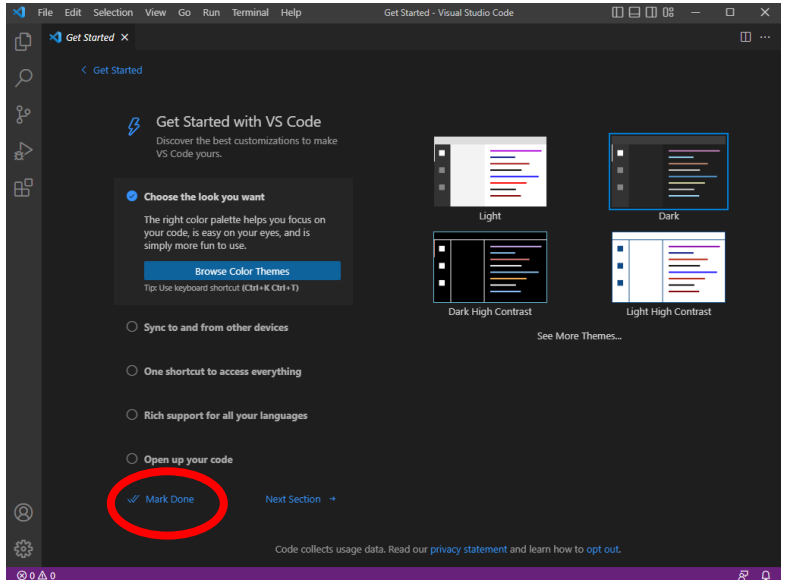


Step 6. Open SiREM Fitting Code in Visual Studio Code

1. In file explorer, navigate to C:\Users\{your username}\OneDrive – CDM Smith\Documents\{your folder name}\SiREM-Processing-main
2. Click siremFitting Jupyter Source File and click Open



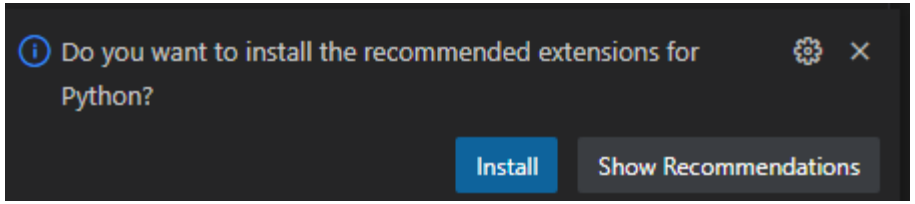
Step 7: Set up Visual Studio Code



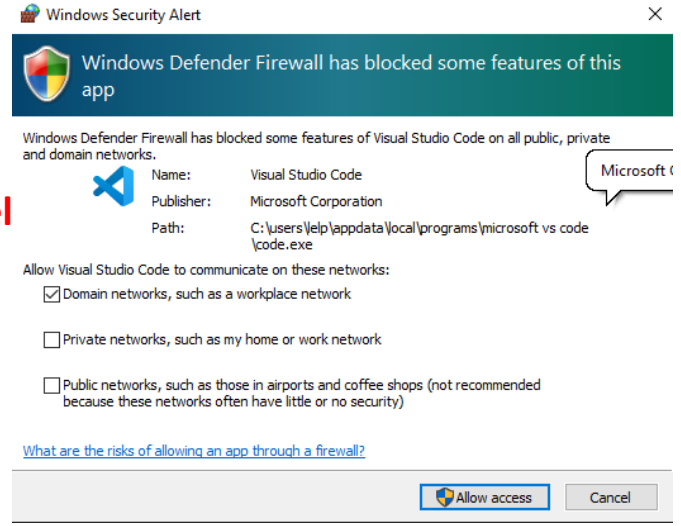
1. Visual Studio Code should open automatically

2. Complete “Get Started with VS Code” walkthrough and click **Mark Done**

3. A pop-up will appear asking to install the recommended extensions for Python. Click **Install**

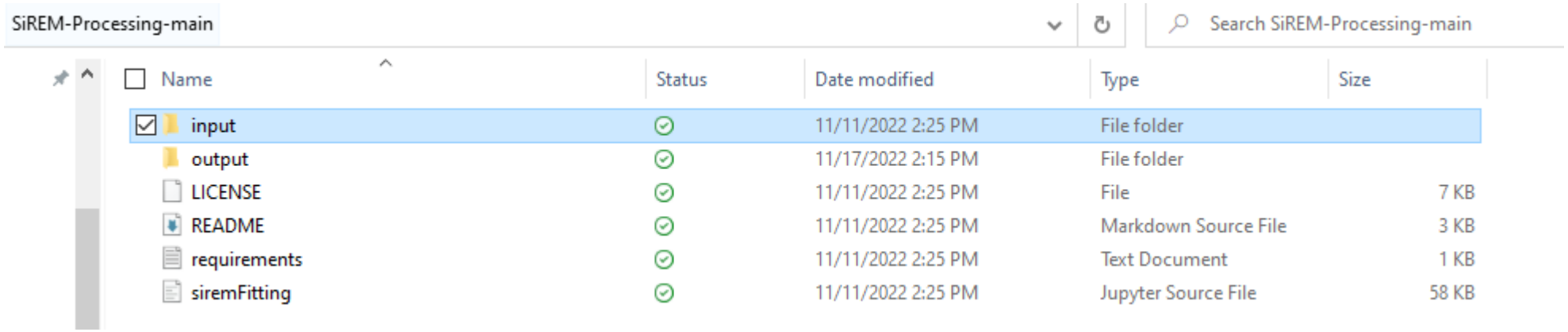


4. **A Windows Defender Firewall pop-up may appear. If so, click Cancel**



Step 8. Check input folder files

1. Check input folder for test Data excel file
2. If using different data, save input data into the input folder as an .xlsx excel file at file path C:\Users\{your username}\OneDrive – CDM Smith\Documents\{your folder name}\SiREM-Processing-main\input



Step 9. Check input/output files

1. Check second block of code, change folder or file names as needed to match your input naming scheme

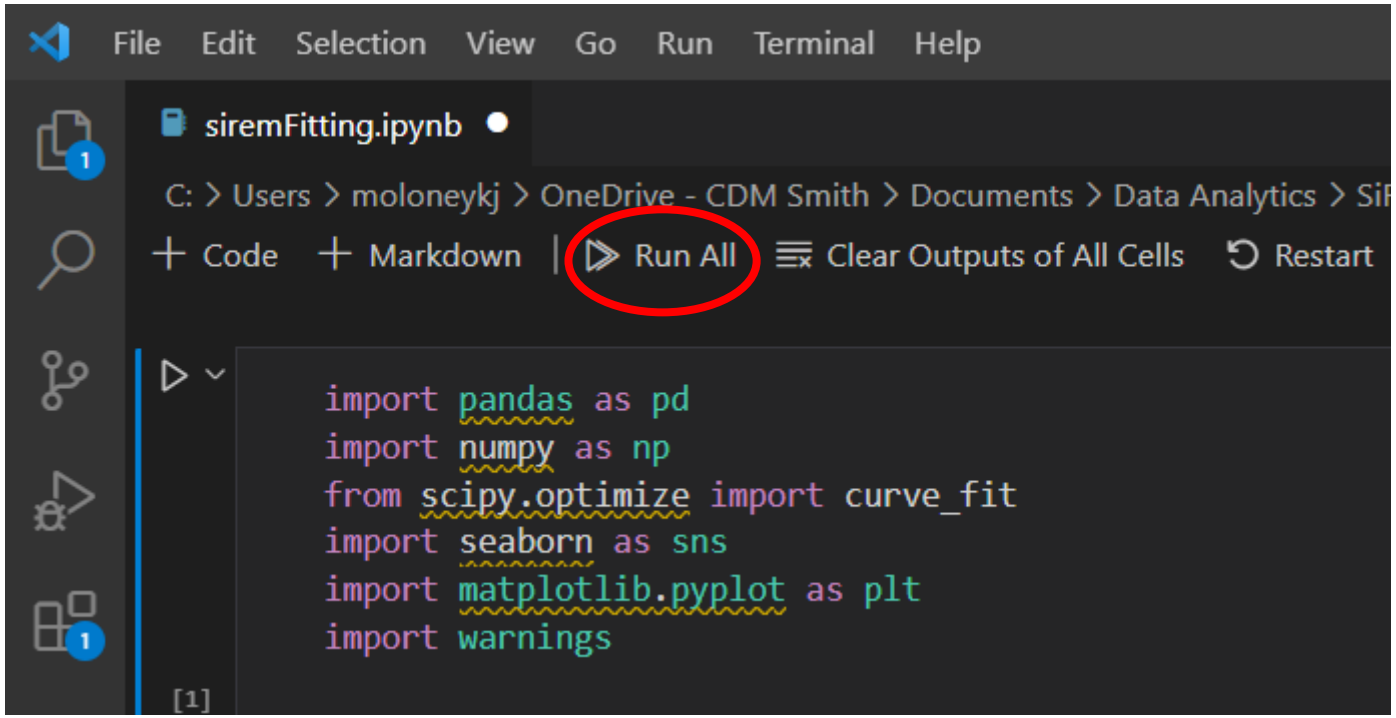
```
# *** Specify directories files for input and output *** #
openDir = 'input'
saveDir = 'output\\'

saveCal = 'testCalCurve.xlsx'
saveStds = 'testStandardsCalc.xlsx'
saveSam = 'testSamplesCalc.xlsx'
# *** End directories /files for input and output *** #
```

2. Check excel file names in third block of code, change file or sheet names as needed to match your input data .xlsx file

```
# *** Specify excel for input *** #
refs = pd.read_excel(openDir + '\\testInputData.xlsx', sheet_name='sampleRef')
stds = pd.read_excel(openDir + '\\testInputData.xlsx', sheet_name='standards')
samples = pd.read_excel(openDir + '\\testInputData.xlsx', sheet_name='samples')
chemRef = pd.read_excel(openDir + '\\testInputData.xlsx', sheet_name='chemRef')
# *** End Specify excel for input *** #
```

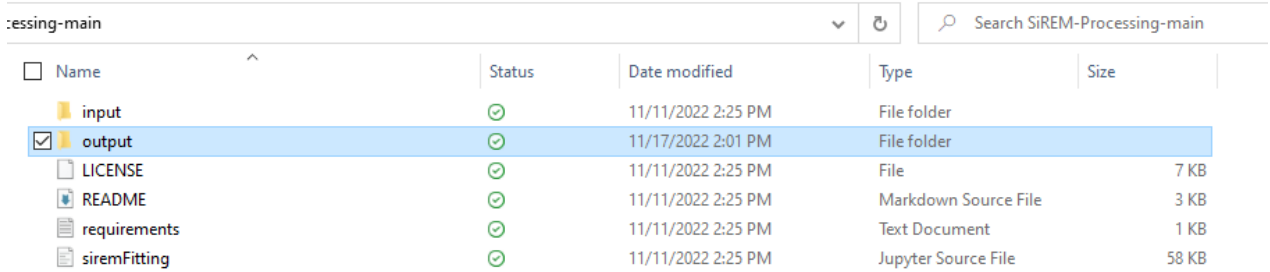
Step 10. Run Code

1. Click **Run All** at top left of screen
2. This will take a few seconds to process



Step 11. Check output folder for results

1. In file explorer, navigate to C:\Users\{your username}\OneDrive – CDM Smith\Documents\{your folder name}\SiREM-Processing-main\output



2. Click output subfolder
3. See results as shown below