**POSSUMS Flow Injection Analysis**

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Run the MATLAB scripts in the following order (see diagram for workflow).

Important notes:

* Raw FabGuard data should be exported as .dat files and saved with the following filename convention: “yy\_MM\_dd-HH\_mm”. They should be saved in a folder called "RawData\FabGuard".
* The porewater sampling log data are automatically saved as .txt files with the following filename convention: “PWSampler\_MM\_dd\_yyyy hh\_mm”. They should be saved in a folder called "RawData\PWLog".
* In addition, you should create the following four subfolders: "ProcessedData\FabGuard", "ProcessedData\PWLog", "Output\Timepts", and "Output\PeakAreas".

# Step 1: Data Processing

This step only has to be run once for all gases.

## LoadMIMSData.m

**Function**: Transforms raw FabGuard text file into MATLAB table

**Input folder**: “RawData\FabGuard” (contains FabGuard .dat files)

**Output folder**: “ProcessedData\FabGuard” (saves .mat file)

## LoadPWData.m

**Function**: Transforms raw porewater sampler data log into MATLAB table

**Input folder**: “RawData\PWLog” (contains porewater log .txt files)

**Output folder**: “ProcessedData\PWLog” (saves .mat file)

# Step 2: Peak Finding

This step must be run for each gas of interest. The current scripts are able to analyze *m/z* 15, 28, 32, 40, and 44 (CH4, N2, O2, Ar, and CO2); for other gases, they need to be modified.

## FindMIMSTimepts.m

**Function**: Finds the start and stop indices for the peaks and the baseline intervals. The peak start index is based on the switch to Position B, plus a user-defined delay period; you will be prompted to set this offset, as well as the peak width. This will require some experimenting, as these parameters will be unique to the data set (the offset depends on factors such as the flow rate, and the peak width depends on factors such as the analyte concentration).

**Input folders**: “ProcessedData\FabGuard” and “ProcessedData\PWLog”

**Output folder**: “ProcessedData\Timepts\GAS” (GAS = CH4, N2, Or, Ar, or CO2)

# Step 3: Peak Analysis

## PeakIntegration.m

**Function**: Baseline-corrects the peaks and integrates them

**Input folder**:“ProcessedData\FabGuard” and“ProcessedData\Timepts\GAS” (GAS = CH4, N2, Or, Ar, or CO2)

**Output folder**: “Output\PeakAreas\GAS”

