## Instructions for Metabolomics QC Report Generator

Instructions:

1. Upload workbook with sheet containing data with peak heights. The data should display on the right side of the UI if the upload was a success. Important notes about the format for the input file:
   1. Files **MUST** be in .xlsx format (the file upload will fail if .csv or .txt files are used). Uploading as a .xlsx ensures the original metabolite and column names are retained.
   2. The sheet containing peak heights **MUST** contain the 3 following metadata columns ( **sampleType, time, and label**), which are case-sensitive. These columns distinguish between experimental samples and quality control samples, indicate the injection order, and include individual sample names, respectively. Additionally, experimental samples in the **sampleType** column must be labelled as **Sample**, which is also case-sensitive. See “example\_file.xlsx” for precise formatting guidelines.
   3. Include a second sheet in the same workbook to assign MSI levels and class annotation numbers. If this information is not available, include a second sheet in the same workbook but leave blank. This sheet may include columns with any number of identifiers so long as the following columns are present within the sheet: **Class, MSMS match, mzrt match, Similar MSMS match,** and **Similar mzrt match**. The **Class** column consists of user-provided metabolite classes assigned to each annotation. It is recommended that these be obtained using Classyfire or a similar software tool that supports automatic metabolite class assignments. The remaining columns correspond to criteria used during data curation to identify each annotation in the dataset. The MSI levels are automatically assigned to each metabolite based on these criteria.
   4. Include a second sheet If annotation and match criteria are available, include this information as a separate sheet within the same workbook. Upload this information below the data sheet upload box and select the same file used in the previous upload, which will now read the 2nd sheet of the file. **IMPORTANT:** All instruments, chromatography platforms, and ionization modes are acceptable for data files as long as data are expressed as integers (i.e. values such as “1.5 ppm” entered in the data sheet will cause an error, but “1.5” will not).
   5. Max file upload size is 50 MB.
2. Complete the Study Information fields. Any values can be provided in these fields as these are not used in calculations within the report. Required data fields are indicated by red asterisks.
3. Complete the data processing and QC information fields. Any values are acceptable, except the quality control sample names provided must match the names of these samples within the uploaded data sheet (ex. QC1 must be named “QC1” within the **sampleType** column and is case-sensitive).
4. Click on **Generate Report** after all fields have been completed. A progress bar will be displayed in the bottom-right side of the UI.
5. If desired, download plots and tables from the report. Please note that plots and tables will not be available for download until a report has been generated.

Notes:

* App testing was only performed on untargeted metabolomics data. However, targeted metabolomics data should also be compatible with the app.
* The default output is a .html file that can be opened in a web browser. If .pdf format is desired for the report, open the file in a web browser, right-click and select **Print**, then save the file as a PDF. Minor edits to the PDF may be required as the .html file contains elements that will not display properly in PDF format.
* Address inquiries/issues with the app to Chase Stevens at ncstevens@ucdavis.edu.