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INSTRUCTIONS → Annotated instructions on how to prepare absorbance and EEM scans to run the DOM indicator script

Cary\_EEM\_Abs\_Code.R → The DOM indicator script

NutrientProtocols\_CJW.doc → A protocol for running DOM scans and information on the DOM indices calculated with relevant papers cited, written by Clayton Williams (former lab member).

AbsData.csv, ChangLog.csv, MILLIQBLANK06DEC19, THESIS30106DEC19.csv → Example files to refer to when compiling your own data. Explanations in the instructions below.

EEMinstrumentCorrectionMatrix.csv → Correction file needed for running the Cary\_EEM\_Abs\_Code.R script. See instructions below.

Steps to correct Abs/EEM data for PARAFAC analysis and to compute common DOM indices using the Cary\_EEM\_Abs\_Code.R:

1. Compile and organize all your absorbance and EEM .csv files into a folder that will function as your working directory
2. In this folder add the **EEMInsturmentCorrectionMatrix.csv** file
3. Create a **ChangeLog.csv** file with four column headings
   1. SEM -- ‘name of the EEM sample’.csv
   2. BEM -- ‘name of associated EEM blank’.csv. This is the blank you ran on the day that you ran the sample.
   3. Abs.Sample -- The name of the associated absorbance scan
   4. Abs.Blank -- the name of the associated absorbance blank
4. Check each EEM file to make sure they are formatted like the example I uploaded in the drive “**THESIS30106DEC19.csv”**
5. Compile all of the absorbance data into one file **“AbsData.csv”** following the example I uploaded.

Steps 3-5 can take a long time if you have many samples from different days, like I did.

1. Now you should have 1 folder with:
   1. ChangeLog.csv
   2. AbsData.csv
   3. EEMInsturmentCorrectionMatrix.csv
   4. All of your EEM.csv samples
   5. All of your EEM.csv MilliQ blanks
2. Open the R script and set the working directory
3. Run the entire code. Hopefully, it runs smoothly. After the script runs it will produce an **output.csv** that includes the calculations for various peaks and indices. Briefly:
   1. A254 -- used to calculate SUVA (specific absorbance at 254nm); indication of aromaticity
   2. SR -- spectral slope ratio; indicator of molecular weight
   3. BA -- beta:alpha ratio; indicator of ratio of autochthonous:allochthonous or bacterial:terrestrial signature of organic matter. Sometimes referred to as “freshness index”
   4. FI -- fluorescence index
   5. HIX.ohno -- Humification index calculated based on Ohno, 2002 (if I recall correctly). We use this version of HIX.
4. If the code runs into an error, still check to see the output.csv to see if any samples were calculated. This way you’ll be able to deduce which one it ran into a problem with and can investigate.
5. For each sample, the script will also produce a simple graphic of the emission spectrum, as well as a corrected version of the sample in your working directory. These corrected versions are used for the PARAFAC analysis.

If you run into an error I find it is often due to a spelling mistake or mismatch between the right blanks associated with the samples. There have been times where I just could not figure out how to get specific samples to run. I will gladly help troubleshoot as best I can.