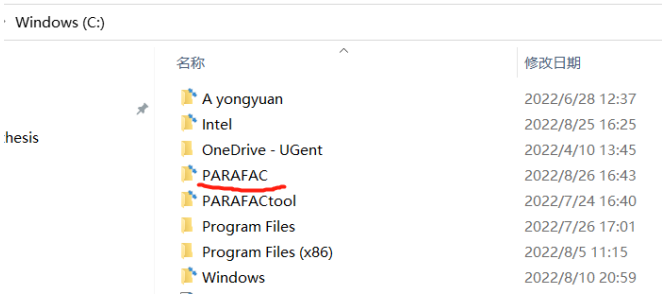
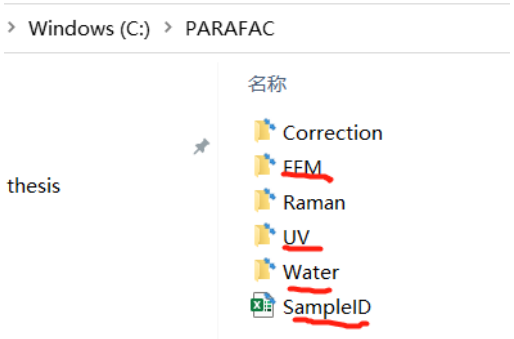
Manual of PAFAFAC analysis using the PARAFAC.mlapp in MATLAB

Step 1: Prepare data files in demo **PARAFAC**, located in C disk.
%You need to replace/change the csv files of EEM, UV, Water and Sample ID based on your samples. But do not change the name and location of any folders.
If the location is change, for example you don't want to put the PARAFAC in C disk, the code of **PARAFAC.mlapp** should be adapted. You can use the MATLAB to open the **PARAFAC.mlapp** and adapt the code. %





Step 2: Load the **drEEM** folder into the path of your MATLAB:

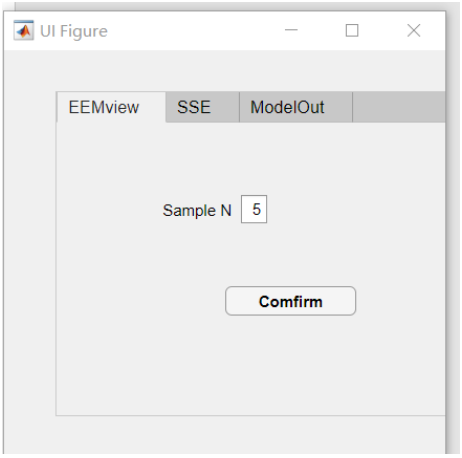
Step 3: Double click the PARAFAC.mlapp, which including the functions of **EEMview**, **SSE**, and **Modelout**.

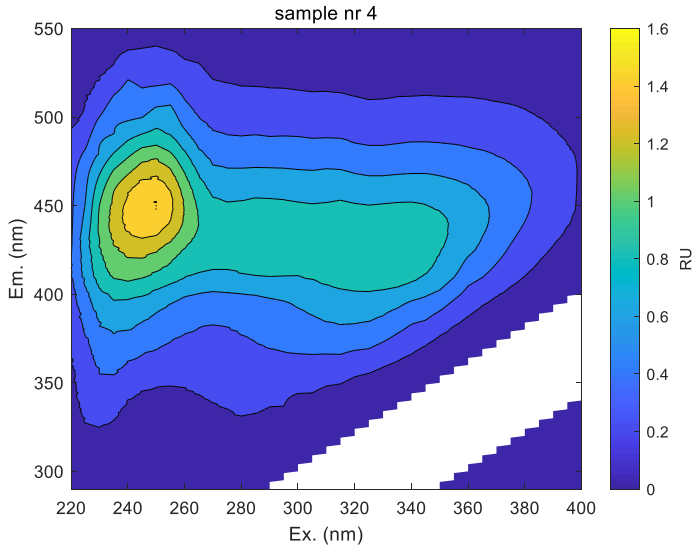
% PARAFAC.mlapp is an APP (application) working on MATLAB. You can add more function or do the individualized design using the APP designer in MATLAB%

EEMview: Enter Sample N (e.g., **5**) and **confirm.**

%Here we can obtain the EEM image of sample N with all necessary correction%

% It takes several mins, depending on the status of your laptop%.

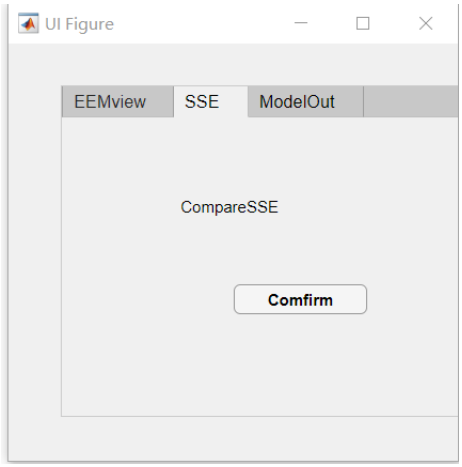




SSE: **Confirm.**

%Here we are doing the PARAFAC modeling based on the component numbers from 3 to 7. You can get the output consists of a series of Figures. You can just look at **Figure 11** and determine which component number for modeling is suitable. As can be seen, the 3-component modeling appears high error, while 4 to 7 component modeling are comparable. Thus 4-component is suitable. More component modeling, e.g., 5 leading to a pair of components which could be highly correlated. %

% It takes several mins, depending on the status of your laptop%.



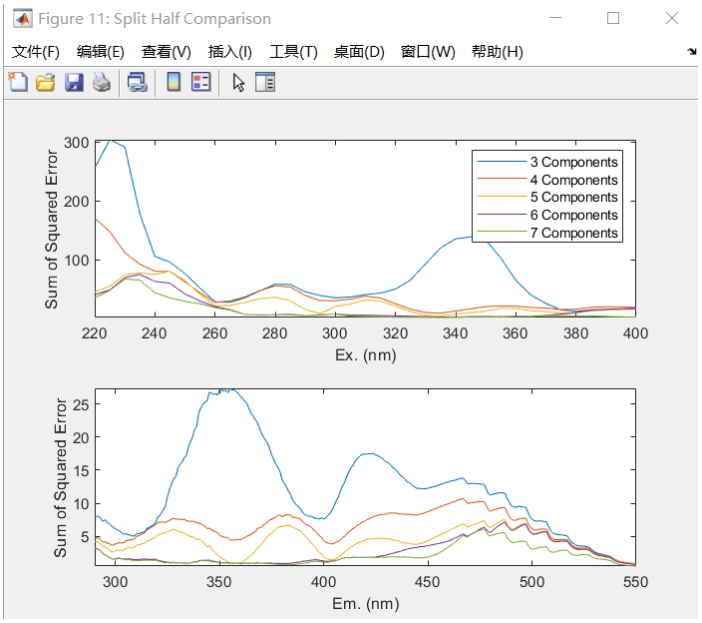
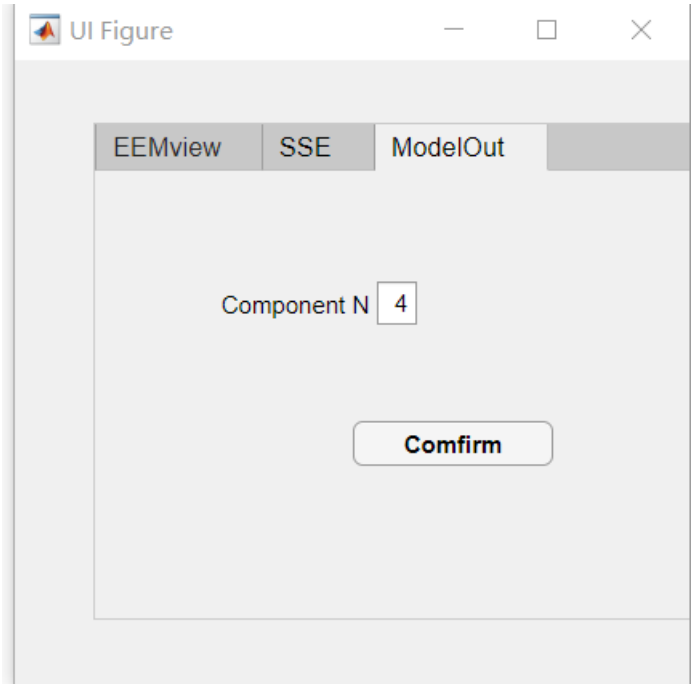


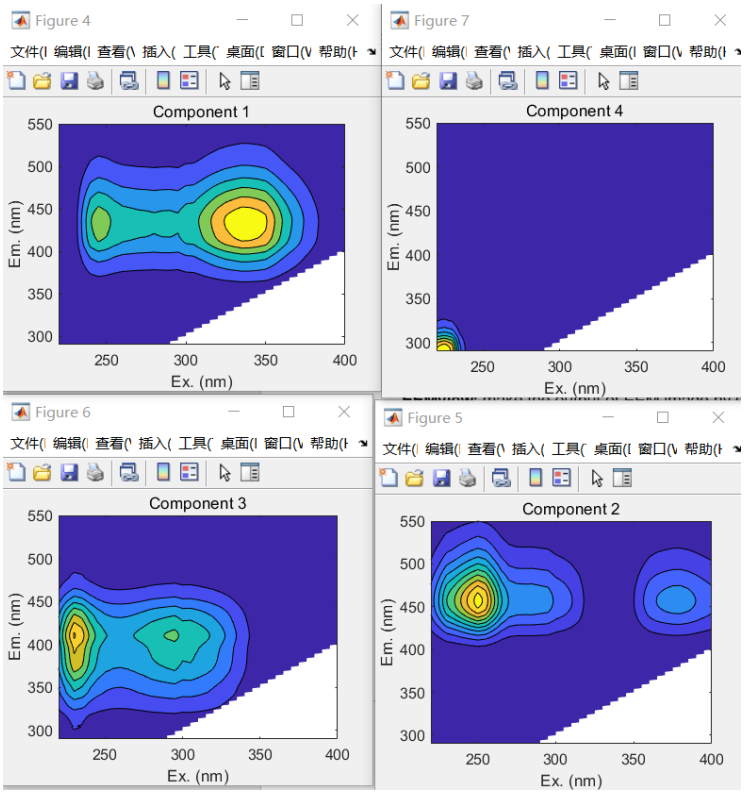
Figure 11. Sum of Squared Errors for the PARAFAC modeling by different component number (3: 7).

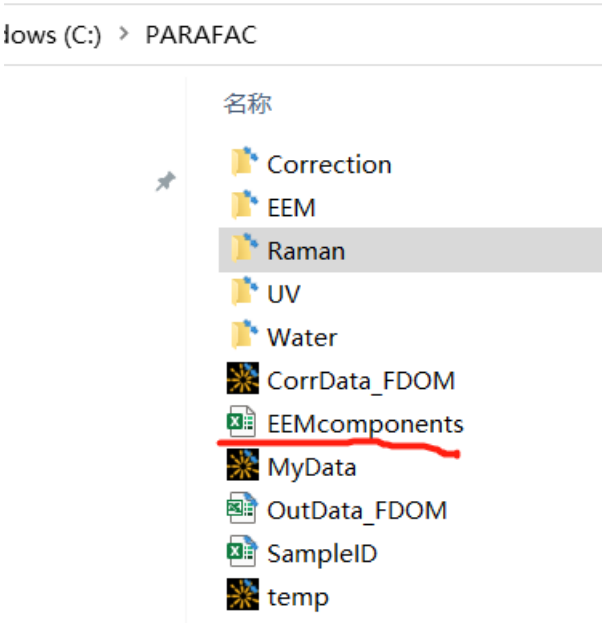
ModelOut: enter **Component N** of modeling (based on SSE, here is 4) and **confirm.**

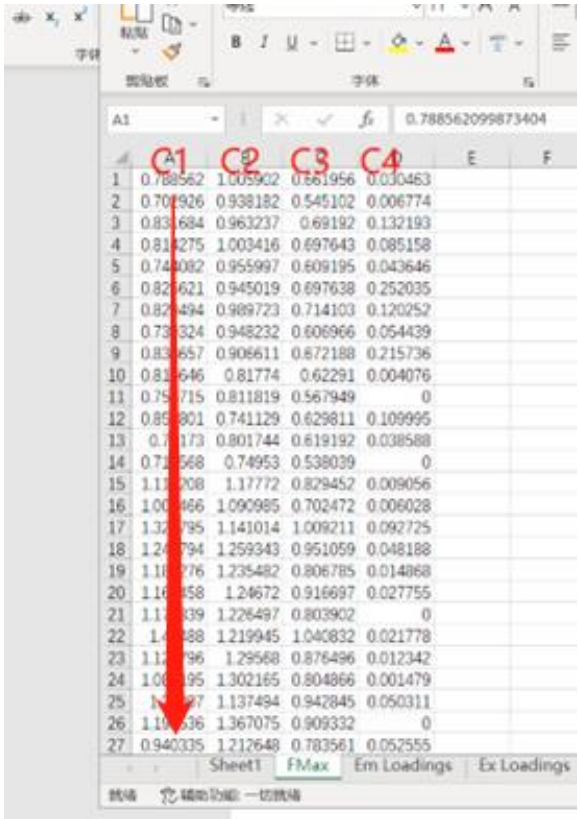
%Here we can get the results of 4-component modeling, including the component Figures, and data of Fmax (see EEMcomponents.xlsx in C:\PARAFAC). Fmax data at the column 1 (1:4) is the Fmax of component 1 (1:4) for all samples%

% It takes several mins, depending on the status of your laptop%.



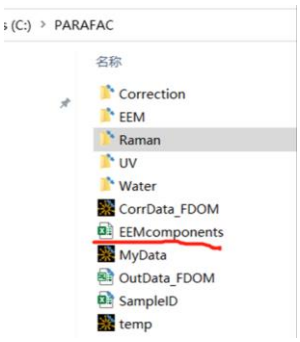


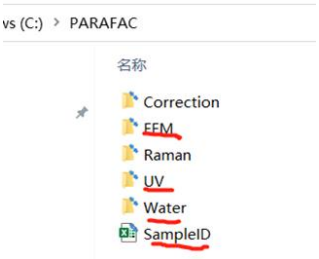

lows (C:) > PARAFAC
名称
Correction
EEM
Raman
UV
Water
CorrData_FDOM
EEMcomponents
MyData
OutData_FDOM
SampleID
temp


C1
C2
C3
C4
Sheet1
FMax
Em Loadings
Ex Loadings

Cleaning the PARAFAC folder.

%After finish, it is suggested to clean the folder as follows%





Reference:

Murphy, K. R., Stedmon, C. A., Graeber, D., & Bro, R. (2013). Fluorescence spectroscopy and multi-way techniques. PARAFAC. Analytical Methods, 5(23), 6557-6566.