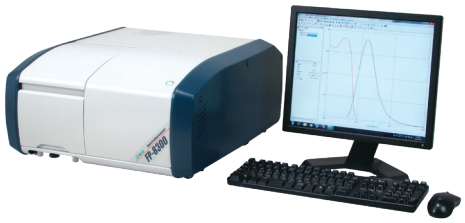
Application Note
FP-0020

Component Analysis of an Excitation-Emission Matrix of Water Samples Using PARAFAC Analysis

Introduction

Excitation-Emission Matrix (EEM) can be used in a wide variety of applications, especially in the analysis of environmental water. EEM provides the following information; (1) determining of the origin of environmental water and chromophoric dissolved organic matter (CDOM), (2) monitoring of the component variation from influences such as climate patterns or local weather.



FP-8300
Spectrofluorometer

Environmental water typically contains a variety of fluorescent materials (humic acid, fulvic acid, protein, amino acid, chlorophyll, synthetic compounds etc.) and analysis using EEM includes several fluorescence peaks, resulting in very complicated data which may be difficult to interpret.

Parallel Factor Analysis (PARAFAC) is a type of multivariable analysis, which can be used to extract the components from mixed 3D fluorescence data. JASCO has developed an advanced solution using PARAFAC, which can help to interpret the complicated data found in the EEM.

As an example of component analysis by PARAFAC, this application note shows the 3D fluorescence measurement and component analysis results of a mixed sample (Tryptophan, humic acid and fulvic acid).

Keywords

FP-8300, Fluorescence, PARAFAC (Parallel Factor Analysis), EEM (Excitation-Emission Matrix), CDOM (Chromophoric Dissolved Organic Matter), IFE (Inner Filter Effect)

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Experimental

Measurement Conditions			
Excitation Bandwidth	5 nm	Emission Bandwidth	10 nm
Response Time	50 msec	Scan Speed	500 nm/min
Sensitivity	High	Data Interval	1 nm

Solutions of tryptophan (0.0175 mg/L), humic acid (0.5 mg/L) and fulvic acid (1 mg/L) were prepared in the following mixture ratios (tryptophan: humic acid: fulvic acid): 6:2:2, 5:5:0, 5:0:5, 4:4:2, 4:2:4, 2:6:2, 2:4:4, 2:2:6, 0:5:5.

The excitation and emission spectra were obtained and corrected for using calibrated light sources (WI and D_2).

Results

The 3D fluorescence spectra of ultra pure water and sample were obtained and corrected for using the calibrated excitation emission spectra. The ultra pure water spectra were then subtracted from the sample spectra to remove the water Raman peaks. The subtracted sample spectra are shown in Figure 1.

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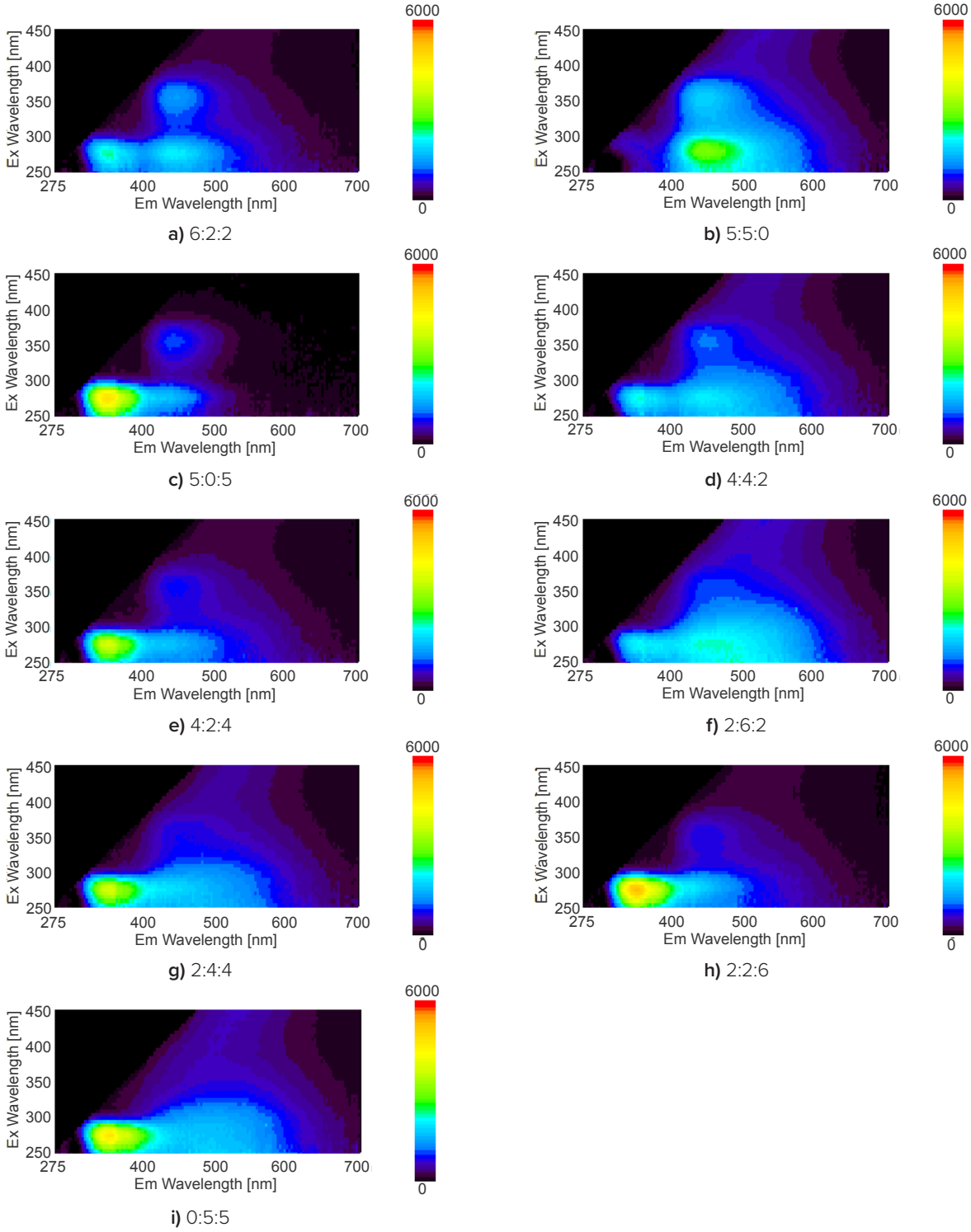

Figure 1. 3D fluorescence spectra of the different mixture ratios (tryptophan: humic acid: fulvic acid).

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Component analysis using PARAFAC analysis was performed on the 3D fluorescence data and the number of component spectra was set as 3. Figure 2, left shows the component spectra calculated by PARAFAC, and Figure 2, right shows the 3D fluorescence data of the pure sample (tryptophan, humic acid and fulvic acid). As shown in Figure 2, the component spectra are closely similar to the 3D fluorescence data of the pure sample.

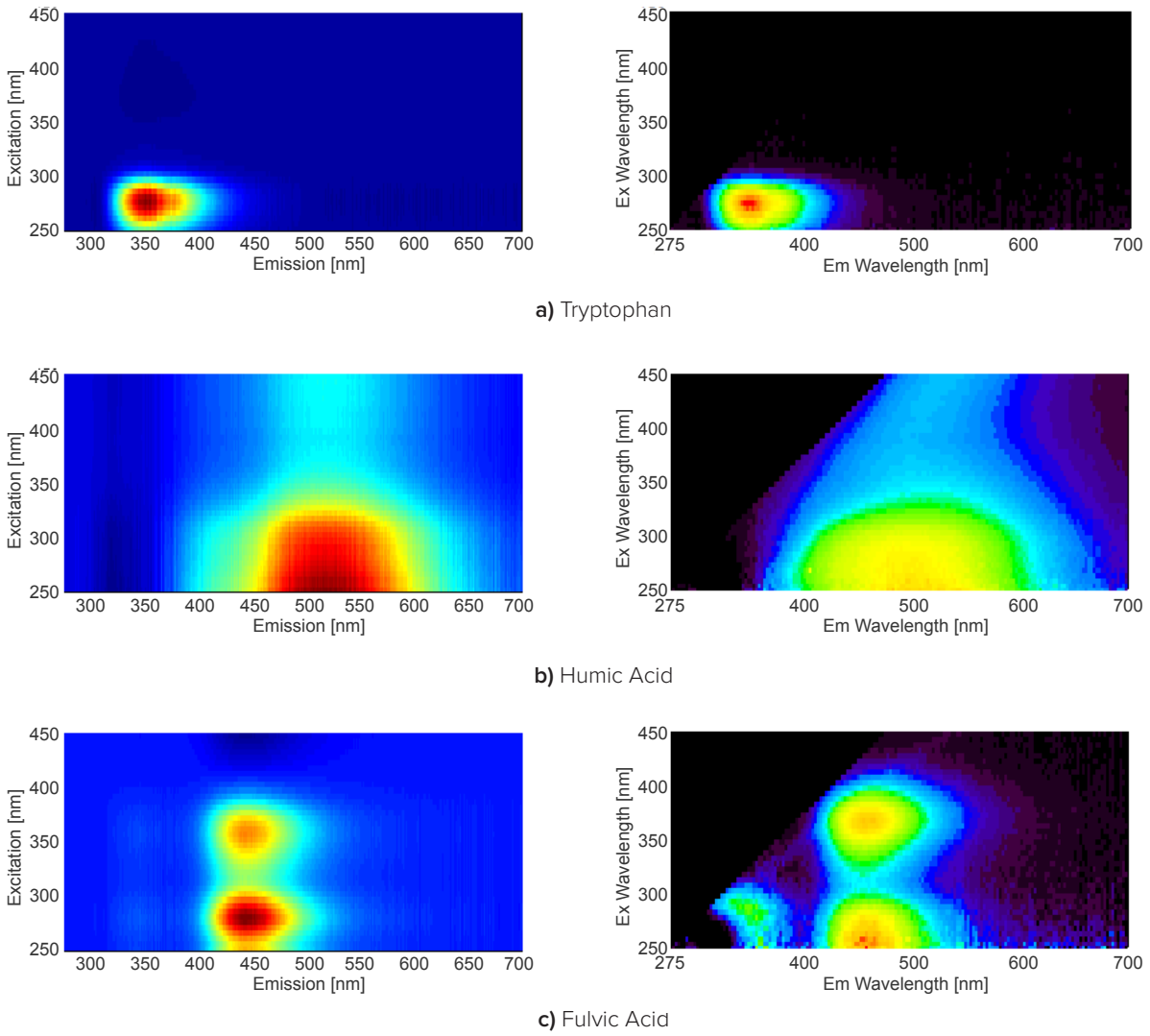

Figure 2. 3D fluorescence spectra of the pure samples (right) and component spectra by PARAFAC (left).

Figure 3 shows the score plot of the first component (tryptophan) and the second component (humic acid) as calculated by PARAFAC. The ratio of the components calculated by PARAFAC is similar to the mixture ratio of tryptophan and humic acid.

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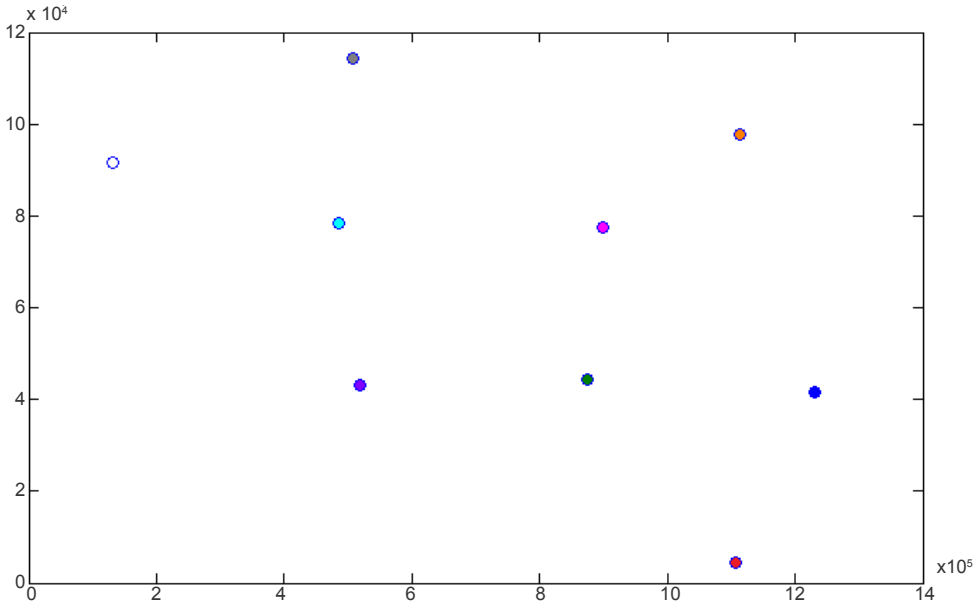

Marker	Tryptophan	Humic acid	Folic acid
●	6	2	2
●	5	5	0
●	5	0	5
●	4	4	2
●	4	2	4
●	2	6	2
●	2	4	4
●	2	2	6
○	0	5	5

Figure 3. Score plot of tryptophan and humic acid.

Conclusion

These results demonstrate that PARAFAC analysis is a useful method to identify a component spectrum in a mixed spectrum, and can be used to determine the components in a mixed solution from the peak information of each component spectrum. PARAFAC can also be used to provide quantitative analysis for each component in the mixture.

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