Technical Note: 52151

Multi-component Analysis with the Evolution Array Spectrophotometer and VISION*collect* Software

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Key Words

- Evolution Array UV-Visible Spectrophotometer
- VISION*collect* Software
- MCA
- Multi-component Analysis

Introduction

Many analytical methods require the analyst to quantitatively determine a specific component within a mixture. This type of analysis is often possible only after time consuming sample preparation, which may require the extraction, separation, chemical transformation and purification of each component of interest. However, a multi-component sample can be analyzed using UV-Visible spectroscopic data collected with Thermo Scientific VISION*collect* MCA software and a Thermo Scientific Evolution Array UV-Visible spectrophotometer. This method requires the measured absorbance response of each component to be linear with respect to concentration and that all possible components of the mixture are known.

Principle

According to Beer's law, the absorbance of a particular component in a mixture is proportional to the concentration of the component. This proportionality holds for each absorbing species. Multi-component quantitative methods are based on the principle that the absorbance of a mixture at a particular wavelength is equal to the sum of the absorbances of each component in the mixture at that wavelength. Thus, the absorbance of the mixture depends on both the concentration and the molar absorptivity[1] of each component.

For the two components x and y, we can then say that:

$$A'_{(x+y)} = A'_x + A'_y = e'_x bc_x + e'_y bc_y$$

$$A''_{(x+y)} = A''_x + A''_y = e''_x bc_x + e''_y bc_y$$

Where,

A' is absorbance at wavelength,

A" is absorbance at wavelength,

e' is molar absorptivity at wavelength,

e" is molar absorptivity at wavelength,

c is concentration

b is path length

[1] *Also known as extinction coefficient*

Experiment

In this experiment composite solutions consist of two components, A and B, where A is Red dye and B is Blue dye. Pure forms of each dye were used as standards. Five test samples were prepared according to Table 1.

	Sample 1	Sample 2	Sample 3	Sample 4	Sample 5
Standard A	2.7	2.1	1.5	0.9	0.3
Standard B	0.3	0.9	1.5	2.1	2.7

Table 1: Volumes for preparing 2-component mixtures in mL

To accommodate a variety of applications, VISION*collect*™ MCA software allows the user to select from three data calculation methods:

- Selected Wavelength: *Enter individual wavelengths to be used*
- Range Wavelength: *Enter wavelength range to be used*
- All Range Wavelength: *Complete spectrum is used*

In this experiment, the absorbance spectra of the dye standard solutions and sample mixtures were collected using the MCA mode of VISION*collect* software with the method parameters shown in Figure 1. The spectra are displayed in Figures 2 and 3.

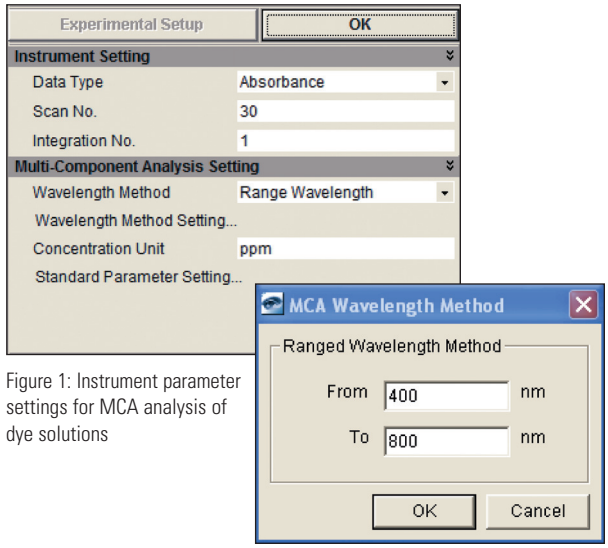

Figure 1: Instrument parameter settings for MCA analysis of dye solutions

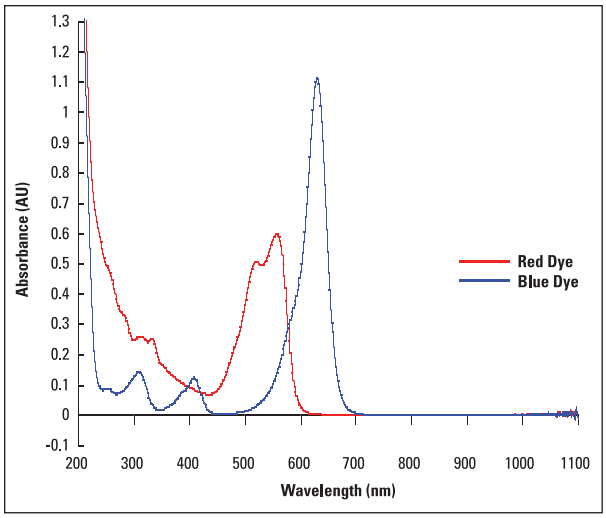

Figure 2: Spectra of dye standard solutions

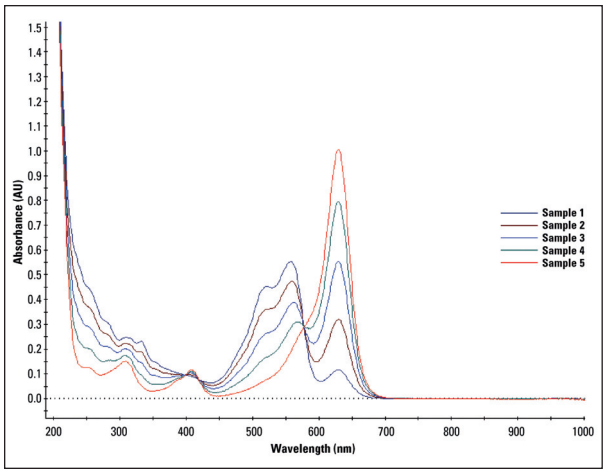

Figure 3: Overlaid spectra of dye standard solutions and sample mixtures

The sample mixtures were analyzed to determine the individual concentrations of each component. These calculated concentrations were then compared to the expected concentrations. A comparison of the expected and calculated values, shown in Table 2, confirms that the VISION*collect* MCA software can be used to quantitatively measure multi-component mixtures quickly and accurately.

	Sample 1	Sample 2	Sample 3	Sample 4	Sample 5
Expected Ratio	9:1	7:3	5:5	3:7	1:9
Standard A (ppm)	89.54	71.08	50.69	29.91	10.01
Standard B (ppm)	10.07	28.46	49.49	71.30	90.24

Table 2: Results of calculated component concentrations

For ease of analysis, VISION*collect* MCA software allows the user to display both a sample spectrum and a pie chart of the sample components. The results for Sample 4 are 29.91 ppm for component A (Red dye) and 71.30 ppm for component B (Blue dye) as shown in Figures 4 and 5.

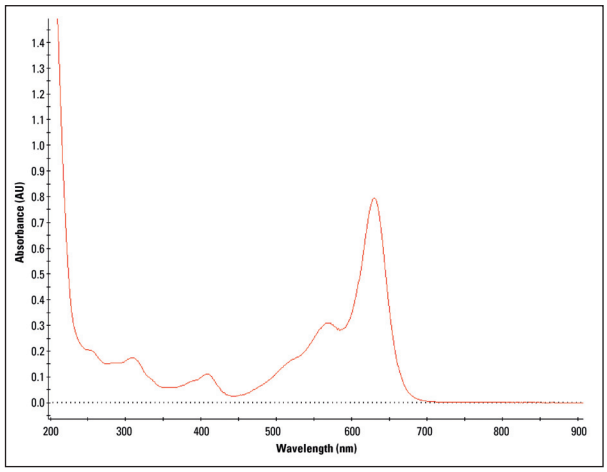

Figure 4: Spectrum result for Sample 4

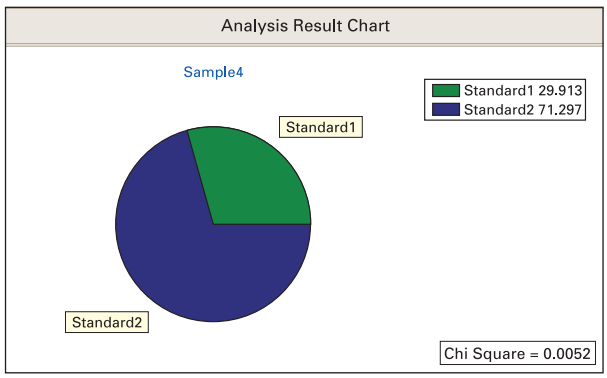

Figure 5: Pie chart result for Sample 4

Conclusion

Quantitative analyses of multi-component mixtures can be performed quickly and accurately with the Evolution™ Array™ UV-Visible spectrophotometer and VISION*collect* MCA software. Three data calculation method options provide added flexibility to accommodate a variety of applications.

Ordering Information

Product Name	Part Number
Evolution Array UV-Visible Spectrophotometer	222-26200
VISION*collect* MCA Software	SS-600L

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