日本化学会 第102春季年会 (2022)

Detection method for blue colorants in food samples by applying multivariate curve resolution alternating least squares to second derivative of UV-Vis spectra

(*Division of Hygienic Chemistry, Osaka Institute of Public Health*) ○Hiroshi Matsui
Keywords: Food Additives; Food Colorants; MCR-ALS;

Food colorants are widely used in various foods to enhance characteristics of food products. In terms of public health, it is important to monitor their appropriate use. Nowadays, liquid chromatography and thin layer chromatography techniques are mainly adopted to analyze colorants in food samples. However, these techniques require complicated pretreatments of the samples. To overcome this disadvantage, the multivariate curve resolution alternating least squares (MCR-ALS) has been studied as a prospective alternative because it enables to decompose measured signal of mixture into the individual contribution of each compound in the sample.[1] Though these previous studies have succeeded simultaneous determination of several colorants, methods for more components are desired for practical use.

In this study, a detection method for six blue colorants, Brilliant Blue FCF (BB), Patent Blue V (PBV), Patent Blue VF (PBVF), Fast Green FCF (FG), Green S (GS) and indigo carmine (IC), was developed by applying MCR-ALS to second derivative of UV-Vis spectra. The UV-Vis spectra were measured in citrate buffer (pH = 5.5) and carbonate buffer (pH = 10.0). MCR-ALS was applied to the augmented matrix composed of second derivative spectra in both buffers under the nonnegativity and selectivity constraint for the concentration profile. The present method was evaluated by the prediction performance for 27 spiked syrup samples. The samples were prepared by dilution with the buffers. As seen in Table 1, the present method well reproduced the concentration of BB, PBV, PBVF, FG and GS with $R^2 > 0.84$ while it considerably underestimated the concentration of IC.

Table 1. Coefficients of determination (R^2) and limit of detection (LOD) of the present method for the studied blue colorants.

	BB	PBV	PBVF	FG	GS	IC
R^2	0.901	0.845	0.863	0.877	0.949	0.158
LOD [mg/L]	0.38	0.46	0.22	0.21	0.29	1.01

1) a) D. W. Lachenmeier, W. Kessler, *J. Agric. Food. Chem.* **2008**, *56*, 5463. b) N. E. Llamas, M. Garrido, M. S. Di Nezio, B. S. Fernández Band, *Anal. Chim. Acta* **2009**, *655*, 38. c) A. Bordagaray, S. Dávila, R. Garcia-Arrona, M. Vidal, M. Ostra *J. Chemom.* **2019**, *33*, e3176.