

Simultaneous Spectrophotometric Determination of Food Colorants Employing Multivariate Calibration Methods

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ABSTRACT

This study investigated the simultaneous spectrophotometric determination of three food colorants – Tartrazine (T), Ponceau 4R (P) and Indigo carmine (I) – in mixtures employing multivariate calibration methods. Absorption spectra of 76 mixtures of the colorants were recorded. The 76 spectra were divided into three sets: calibration, validation and unknown. This study employed three multivariate calibration methods: principal component regression (PCR), partial least square 1 (PLS1) and partial least square 2 (PLS2). The study involved training set characteristics and signal characteristics. Concentration ranges and concentration ratios of the colorants were used as criteria in selection of training sets and found to be important parameters for predictive accuracy.

Keywords: Multivariate calibration method, Principal component regression, Partial least square 1, Partial least square 2, Food colorant, Simultaneous determination

INTRODUCTION

Existing approaches to simultaneous monitoring of food colorants in the food industry are based on spectrophotometry, thin layer chromatography and high performance liquid chromatography (HPLC) (Karaoglan et al., 2007; Nevado et al., 1999). UV-Vis spectrophotometry is used in many fields because it is quick, easy and low cost. Spectra due to some analytes in a mixture sample may be complicated due to overlapping of the signal, which would require separating, involving tedious experimental work. Investigation was made in derivatization of UV-VIS spectra of colorant mixtures for better sensitivity in the determination of colorants in a mixture (Bosch Ojeda and Sanchez Rojas, 2004; Capitán-Vallvey