References


Determination of Sunset Yellow and Erythrosine in Binary Mixture Using of second-order calibration Methods
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Use of second-order calibration and second-order data allows to determination the interest analyte in the presence of uncalibrated sample constituents, a property known as the second-order advantage.

To determination synthetic food colors in the presence of other dyes compound with similar structures and overlay spectrums, the second order calibration algorithms based on the rank annihilation factor analysis (RAFA) were used[1].

In this method, pH in the range of 1-12 was changed gradually and the absorption spectra of standard dye and real samples were recorded in the range of 200-700 nanometer. Thus, the concentration of sunset yellow and erythrosine in black system[2][3] could be determined from the spectra matrices using second order calibration algorithms. This method is simple, convenient and dependable. The method has been used successfully to determine sunset yellow and erythrosine in simulated saffron sample with satisfactory results with 6% and 4% relative errors, respectively

Keywords: Sunset Yellow; Erythrosine; Saffron; Chemometric method; second-order calibration.

References


Support vector regression based QSAR for the prediction of retention times of various peptides in seven reversed-phase liquid chromatography systems
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In the present study, Quantitative Structure-Property Relationship (QSPR) models were developed to investigate the retention times (tR) of various peptides in seven reversed-phase liquid chromatography (RPLC) systems using Partial Least Squares (PLS), Artificial Neural Network (ANN) and Support Vector Machine (SVM) techniques. The data set of retention times of 93 peptides with known amino acid composition was extracted from the values reported by Put and Vander Heyden [1]. The retention times of the peptides were measured on seven RP chromatographic systems (C18-C77) [2]. Different types of molecular descriptors were calculated to represent the molecular structures of the various compounds studied using and Dragon packages [3]. Important descriptors were selected by a Genetic Algorithm-Partial Least Square (GA-PLS) method. The four descriptors selected using GA-PLS were used as inputs for PLS, ANN and SVM to build models to predict the retention times. These descriptors are: structural information content (neighborhood symmetric of 3rd-order) (SIC3), Geary autocorrelation lag 2/weighted by atomic polarizabilities (GATS2P), lowest Eigenvalue n.1 of Burden matrix/weighted by atomic masses (BELM1) and number of total primary carbons (NCP). Our study reveals that the relation between the chemical properties and retention time is a nonlinear phenomenon and that the PLS method is not capable to properly model it. The results obtained, demonstrate that, for all seven data sets, the tR values estimated by SVM were in good agreement with the experimental, and the performances of the SVM models were comparable or superior to those of PLS and ANN.

References


An integrated ANN-COA approach for modeling the microextraction of acidic and basic drugs
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In this paper, a Cuckoo Optimization Algorithm-based Artificial Neural Network (COANN) [1] was utilized for prediction of a mathematical model that describes the optimum criteria of a microextraction technique for acidic and basic drugs in biological samples, ion-pair based surfactant assisted liquid phase microextraction. A three-layer artificial neural network (ANN) model was applied to optimize and determine the variables affecting the extraction efficiency. A multilayer feed-forward neural network trained with an error back-propagation algorithm was employed for developing a predictive model. The chosen input parameters are the pH of sample, surfactant concentration and volume, extraction solvent volume and salt while the peak area of each analyte is the output. The results showed that a network with ten hidden neurons was highly accurate for predicting the peak area of analytes. The mean squared error (MSE) and the coefficient of determination (R) between the actual and predicted values were determined as 0.0024 and 0.9859 for training, 0.0199 and 0.8876 for validation and 0.0158 and 0.9375 for testing data sets. The highest peak area (215.096) was found after 20 times running COA at the following conditions: pH of sample, 12; surfactant concentration and volume, 1.1 mL of 0.5 mM cetyltrimethyl ammonium bromide (CTAB) in ultra pure water; extraction solvent volume, 60 μL n-octanol; and without salt addition.

References