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Application Of Multivariate Calibration And

Therefore, multivariate calibration tools may be used to develop models that aim for the determination of total methylxanthines, resorting to the spectral signal found in the NIR region. Similar procedures have been adopted by several authors, for instance for the characterization of coffee and green tea (Paradkar and Irudayaraj, 2002 , Chen et al., 2006 , Shinija and Mishra, 2009).

Application of multivariate calibration and NIR ...

Application of multivariate calibration and artificial neural networks to simultaneous kinetic-spectrophotometric determination of carbamate pesticides

Application of multivariate calibration and artificial ...

Application of multivariate calibration and NIR spectroscopy for the quantification of methylxanthines in yerba mate (Ilex paraguariensis)

Application of multivariate calibration and NIR ...

Article History: Two simple, precise and accurate multivariate calibration methods, partial least square (PLS) and principal component regression (PCR) have been applied for the simultaneous determination and dissolution profile evaluation of atorvastatin (ATV) and ezetimibe (EZT) in their binary mixtures and commercial tablets.

Application of Multivariate Calibration Methods, in ...

The combination of multivariate calibration and spectroscopic analysis technology can achieve the rapid analysis of substance. However, when the exter...

Progress and Applications of Multivariate Calibration ...

Application of multivariate calibration to the simultaneous routine determination of ethanol, glycerol, fructose, glucose and total residual sugars in botrytized-grape sweet wines by means of near-infrared reflectance spectroscopy

Application of multivariate calibration to the ...

Abstract The combination of multivariate calibration and spectroscopic analysis technology can achieve the rapid analysis of substance. However, when the external environmental conditions such as instruments or accessories are replaced or temperature changed, the current master calibration may be “invalid”.

Progress and Applications of Multivariate Calibration ...

Application of multivariate calibration to the simultaneous routine determination of ethanol, glycerol, fructose, glucose and total residual sugars in botrytized-grape sweet wines by means of near-infrared reflectance spectroscopy.

Application Of Multivariate Calibration And Nir

Univariate Linear Regression: This will be familiar to most people as finding the line of best fit through a cloud of points. We assume that the relationship between a single X variable and one Y variable is linear. i.e. $Y = bX + a$, where b is the slope of the line, while a is the intercept at the Y axis. Univariate linear regression estimates the values of b and a by minimising the sum of ...

An Introduction to Multivariate Calibration

The Kalman filter is a recursive, digital filtering algorithm which can be used for a variety of applications in analytical chemistry, including multivariate calibration 1, 2and the determination of instrumental response drift 3, 4, 5, 6. The latter application provides both a method of correcting for drift in a series of calibration spectra, and a means of determining when the precision of a calibration parameter (e.g. baseline or sensitivity) falls below a desired level, which can be used ...

Application of Kalman filtering to multivariate ...

Multivariate calibration involves a series of mathematical models for processing partially selective instrumental signals, particularly near-infrared (NIR) spectra, to determine analyte concentrations or sample properties in complex samples. These models are trained by establishing a relationship between a sample set with known property values (calibration phase), which is then applied to unknown specimens to estimate their properties (prediction phase).

Developing and Implementing an R Shiny Application to ...

Multivariate calibration. Many chemical problems and applications of chemometrics involve calibration. The objective is to develop models which can be used to predict properties of interest based on measured properties of the chemical system, such as pressure, flow, temperature, infrared, Raman, NMR spectra and mass spectra. Examples include the development of multivariate models relating 1) multi-wavelength spectral response to analyte concentration, 2) molecular descriptors to biological ...

Chemometrics - Wikipedia

Application of multivariate calibration and artificial neural networks to simultaneous kinetic-spectrophotometric determination of carbamate pesticides . HOME ; Application of multivariate calibration and artificial neural networks to simultaneous kinetic-spectrophotometric determination of carbamate pesticides

Application of multivariate calibration and artificial ...

Multivariate data analysis is capable of not only large dataset management but also interpret them surely and rapidly. Application of chemometrics and cheminformatics methods may be useful for design and discovery of new drug compounds.

Application of Multivariate Linear and Nonlinear ...

Use of the Cross-Section Technique Linked with Multivariate Calibration Methods To Resolve Complex Pesticide Mixtures. Analytical Chemistry 1999, 71 (21), 4844-4850. DOI: 10.1021/ac990024s. Judith Pink,, Marian Naczka, and, David Pink.

An Introduction to Multivariate Calibration and Analysis ...

Application of FTIR Spectroscopy and HPLC Combined with Multivariate Calibration for Analysis of Xanthones in Mangosteen Extracts by Endjang Prebawa Tejamukti 1, Widiastuti Setyaningsih 2, Irnawati 3, Budiman Yasir 4, Gemini Alam 4 and Abdul Rohman 1,5,* 1

Sci. Pharm. | Free Full-Text | Application of FTIR ...

NIR and Raman spectra are considered a source of multivariate data, as they contain information related to physical and chemical properties of the analyzed sample. Thus, the application of chemometric methods for extracting predictive spectral variability and reducing orthogonal sources of variation is indispensable [11].

Multivariate Calibration for the Development of ...

The statistical parameters of multivariate calibrations of Principle Component Regression (PCR) and Partial Least Square (PLS) for quantitative analysis of gartanin (GT).

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