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31-30 October 2019

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@IBCS7 IBCS7@shahroodut.ac.ir IBCS7. shahroodut.ac.ir

IN THE NAME OF GOD

Program book proceeding of the 7th Iranian Biennial Chemometrics Seminar

30-31 Oct. 2019, Shahrood University of Technology, Shahrood, Iran

WELCOME MESSAGE FROM THE SEMINAR'S CHAIR

In The Name of God

It is our honor to welcome you to the 7th Iranian Biennial Chemometrics Seminar (7IBCS) at Shahrood University of Technology on 30th and 31th October 2019. The 7IBCS provides the scientific meeting for the Chemometricians with invited speakers and make an opportunity for younger researchers to present their researches. The scientific program will feature to plenary talks, 11 invited speakers and 12 accepted oral presentations and 50 posters which are distributed in two days.

It is necessary to appreciate the Shahrood University of Technology authorities; the Iranian Chemical Society, Organizing Committee, Scientific and Referee Committees, Student Executive Committees, Novin Shimiar Chemical Company, Fanavari Pishrafteh Jahan, Petro Kimiagar Rad and all university staffs who helped us hold this Conference.

Sincerely Yours,

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N. Goudarzi

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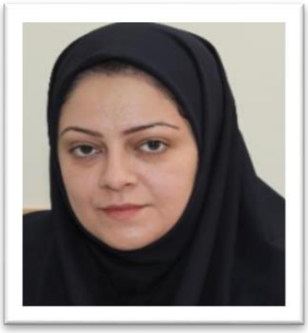

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Chemistry & Chemical Engineer Research Center of Iran

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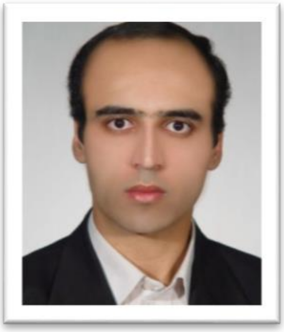

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Time Schedule of 7th Iranian Biannual Chemometrics Seminar

First Session	
Time	Program
8-8:45	Registration and Reception
8:45-9	Reading the Quran and playing the anthem
9-9:05	Presentation of the seminar's chairman report and greetings
9:05-9:10	Play a video clip and introducing the University
9:10-9:20	Speech and greeting of Shahrood University of Technology Chairman
9:20-9:30	Speech by Dr. Shamsipour, head of the Chemical Society of Iran
9:30-9:40	Speech by Dr. Khayamian
10:00-10:30 CoffeeBreak	

Second Session: Oral Presentations

Chairmen: Dr. Naseri & Dr. Khayamian

Time	Title	Presenter
10:30-11:00	Do Analytical Chemists Use the Theory of Analytical Chemistry?	Dr. Abdollahi
11:00-11:30	Class-wise LC-HRMS Data Mining for Environmental Pollution Monitoring	Dr. Vosoogh
11:30-11:50	Estimating confidence intervals in multivariate curve resolution by exploiting the principles of error propagation in least squares framework	Dr. Mani
11:50-12:10	How scaling can affect metabolite identification and estimated pathways in metabolomics studies	Dr. Khoshkam
12:10-12:25	A new strategy for calibrating IDA-based sensor systems	Somaiyeh Khodadadi Karimvand
12:25-12:40	Rapid determination of nitrate ions in drinking water based on image processing techniques using a smartphone platform	Ali Farahani

Third Session: Oral presentations

Chair men: Dr. Abdollahi & Dr. Fatemi

Time	Title	presenter
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14:30-15:00	About the error propagation and uncertainty estimation for the fitted parameters using Microsoft excel	Dr. Naseri
15:00-15:20	Some Misleading Issues in Drug Delivery Systems and their Associated Demands for Employing Multivariate Chemometric Approaches	Dr. Sajjadi
15:20-15:35	Geographical classification of olive oil using the PLS-DA technique and linking chemical content to classes	Mohaddeseh rezaei
15:35-15:50	Untargeted metabolomics changes of Gammarus Pulex in river water induced by designed exposure with selected pharmaceuticals: A chemometrics study	Mahsa Naghavi Sheikholeslami
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Forth Session: Oral Prentation		
Chairmen: Dr. Kompany-Zareh & Dr. Vosoogh		
Time	Title	Presenter
17:00-17:30	Where Pattern Recognition Meets Nanostructure-Based Optical Sensors	Dr. Hormozi-nezhad
17:30-17:45	Essential Spectral Pixel Selection in Hyperspectral Images	Dr. Mahdiyeh Ghaffari
17:45-18:00	Investigation of an interactive molecular autoburette for simultaneous determination of analytes by chemometric approaches of automatic spectrophotometric titration	Sanaz Sajedi Amin
City Tour 19:00-22:00		

Fifth Session: Oral presentation		
Chairmen: Dr. Goudarzi & Dr. Mani		
Time	**Title**	**Presenter**
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9:15-9:45	Application of near infrared spectroscopy and chemometrics for assessing food authenticity and adulteration	Dr. Yazdanpanah
9:45-10:05	Ensemble learning: a new concept in chemometrics?	Dr. Parastar
10:05-10:25	Bioinformatics in drug discovery	Dr. Gharaghani
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Chairmen: Dr. Gharaghani & Dr. Prarstar		
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11:35-11:50	Convolutional neural network as a new tool for classification of multisensor data: prostate cancer case	Kourosh Shariat
11:50-12:05	Application of a new hybrid of SCAD - artificial neural network in QSAR study of HIV inhibitors	Zeinab Mozafari
12:05-12:20	Simultaneous determination of cysteine enantiomers by chemometrics methods	Azam Safarnejad
12:20-12:35	External parameter orthogonalization combined with support vector machine as an efficient method for analyzing saffron NIR and ATR-FTIR spectra to assess saffron adulteration with plant-derived adulterants	Aryan Amirvaresi

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Do Analytical Chemists use "Theory of Analytical Chemistry"?

Somaiyeh Khodadadi[1]*, Robert Rajko*[2]*, john Kalivas*[3] *and Hamid Abdollahi*[1]
[1]*Department of chemistry, Institute for advanced studies in basic sciences, Zanjan, Iran*
[2]*Institute of Mathematics and Informatics, Faculty of Sciences, University of Pécs, Ifjúság útja 6., H-7624 Pécs, Hungary*
[3]*Department of chemistry, Idaho state university, Pacatello, ID, USA*
E-mail address: abd@iasbs.ac.ir

ABSTRACT

Twenty five years ago, a generalized theory of analytical chemistry (TAC) has been proposed by Booksh and Kowalski [1]. The main point of this guiding theory is to explain about the information and type of data which can be extracted from different analytical instrument and methods. Accordingly, the analytical chemist can select the appropriate instrument and its produced data based on their existing problem. Indeed, this theory can direct the analyst to solve their research problems intelligently. The essence of theory is that, for extracting maximum information from a determined chemical system, not only taking higher order data from developed instruments is important, but also type of applying method is effective. Analyzing higher order data with simple univariate methods is possible, but at the expense of losing information.

Hence, the nature of theory is to introduce a functional framework for guiding analytical chemist to solve their considered problems. By deep understanding of the analytical questions, analysts should use the theory to find the optimal, practical solution. Indeed, they should design their laboratory procedures based on the available instruments and required information to solve the problem of interest optimally. It should be noted that, the potential and capabilities of analytical devices and methods play a key role in choosing the optimal solutions. The figures of merit that completely relate to the order of data, reflect the performance of the chosen method. It can be concluded from the theory that, for optimum solving of many problems, the analytical chemist required to take the higher order data sets, and thus apply the multivariate methods. Also, the theory can lead analyst to design appropriate analytical devices and methods.

Keywords: ”univariate methods”, “optimum”, “information”

References:

[1] K.S. Booksh, B.R. Kowalski, “Theory of Analytical Chemistry”, Anal. Chem., 66 (15) **(1994)** 782-791.

Class-wise LC-HRMS Data Mining for Environmental Pollution Monitoring

Maryam Vosough

Department of Clean Technologies, Chemistry and Chemical Engineering Research Center of Iran, P.O. Box 14335-186, Tehran, Iran
E-mail address: vosough@ccerci.ac.ir

ABSTRACT

The use of chromatography coupled with high-resolution mass spectrometry (HRMS) becomes ever more important in many areas of science that rely on identification and quantification of a large variety of compounds. Over the past few years this trend has also started in environmental analysis, where suspect and non-target screening approaches are currently in the focus of intense research [1]. Proper use of HRMS requires processing of “Big Data” and in many cases insights obtained from the measured data are rather limited by inadequate data processing and evaluation. So, developing new methodological approaches and data mining strategies is increasingly demanding. By linking HRMS data and in-depth chemometric data evaluation a higher level of insight into the systems under scrutiny will be achieved.

Class-wise pollution pattern studies can be considered a suitable field where multivariate statistical and supervised classification methods can be utilized and developed. Implementation of methods such as classic/group-wise ANOVA-simultaneous component analysis, partial least squares-discriminant analysis and machine learning-based methods, especially in the challenging nontarget scenarios, would prioritize the investigation of class-relevant pollutants. Thereupon, the most meaningful pollutants that correlate with different classes of environmental samples can be further followed. Identification and characterization of transformation/degradation products of organic pollutants and unveiling the connections between parent-product compounds are amongst the main benefits of these methodologies [2].

Keywords: “LC-HRMS”, “Data Mining”, “Environmental Pollution”

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Estimating confidence intervals in multivariate curve resolution by exploiting the principles of error propagation in least squares framework

Ahmad Mani-Varnosfaderani [1,3*], *Eun Sug Park* [2], *Romà Tauler* [3*]

[1] *Department of Chemistry, Tarbiat Modares University, Tehran, Iran.*
[2] *Texas A&M Transportation Institute, 3135 TAMU, College Station, TX 77843-3135, USA*
[3] *Department of Environmental Chemistry, Institute of Environmental Assessment and Water Research (IDAEA), Consejo Superior de Investigaciones Científicas (CSIC), Jorsi Girona 18-25, Barcelona, 08034, Catalonia, Spain*
E-mail address: a.mani@modares.ac.ir

ABSTRACT

Calculation of the prediction intervals in Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS) is a challenging problem. Several algorithms including Bayesian methods, Monte-Carlo approach and jackknife resampling have been proposed previously to address this problem in MCR [1, 2]. In the present contribution, the confidence intervals (CIs) in MCR-ALS resolved profiles were estimated using the principles of error propagation in linear least squares (LS) parameter optimization. The proposed approach is named as Confidence Intervals based on Least Squares optimization (CILS). The weighted version of this approach has also been implemented and named as CIWLS. This method can be used for handling datasets with a known type of error structure. The performances of the CILS and CIWLS approaches have been evaluated in this work for the estimation of the CIs for simulated three component LC-MS and LC-DAD datasets, with different homo- and heterosedastic added noise levels. The patterns observed for the CIs calculated using CILS and CIWLS were compared with those of Monte-Carlo noise addition and multivariate curve resolution-alternating Bayesian least square (MCR-ABLS) approaches. The root mean squares of the differences (RMSD) between the $CI_{5\%}$ and $CI_{95\%}$ values and the coverage probabilities were used as measures of the level of uncertainty in recovered profiles. The results in this work revealed that the CILS method gives similar results compared to MCR-ABLS approach with non-informative prior for error variance. Moreover, the results of the CILS method were in agreement with those of the Monte-Carlo approach. The main advantage of the CILS method is that it requires less computation time and the calculations are faster. Finally, the performance of CIWLS algorithm was assessed in the analysis and source apportionment of particulate matter (PM) air samples from a real environmental dataset collected in Northern Spain. The results obtained by the CIWLS method were in agreement with those previously reported for this dataset.

Keywords: "error propagation", "matrix decomposition", "Bayesian methods", "multivariate curve" resolution", "alternating least squares", "Monte-Carlo"

References:

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How scaling can affect metabolite identification and estimated pathways in metabolomics study

Maryam Khoshkam

Chemistry Department, Faculty of science, University of Mohaghegh Ardabili, Ardabil, Iran

E-mail address: khoshkam@uma.ac.ir

ABSTRACT

Metabolomics has been successfully applied in many fields including clinical research, drug discovery, toxicology, and phytochemistry. [1]. However extracting relevant biological information from large data sets is a major challenge in this field [2]. From data acquisition to statistical analysis, metabolomics data need to undergo several processing steps, which all of them is critical in correct interpretation of data [3]. One of the most important preprocessing method which is critical is scaling method. There has been minimal investigation of pre-treatment methods and their influence on classification accuracy within the metabolomics literature [4].

In this study it was observed that the reported results in metabolomics data are strongly influenced by scaling methods. Among the methods, the effect of each method is different, and the metabolites obtained for the same data set and the different scaling methods are quite different. Here, a study has been conducted to investigate the influence of six pre-treatment methods including autoscaling, range, level, Pareto and vast scaling, as well as no scaling on three sets of 1HNMR based metabolomics data. One of the datasets was 1HNMR of mice plasma and the other one was 1HNMR spectra of kidney and liver tissues in rattus species. The CdTe quantum dots was injected in different doses to these animals to see the toxicity of CdTe QDs. The results showed that in plasma and tissue data, the choice of the best scaling method is dependent to type of datasets and in different datasets is not the same and should be checked for each data sets. In order to investigate the best method of scaling, classification performance parameters for each scaling method including Q^2x, Q^2y and R^2 were computed. The resulted metabolites and estimated biological pathways were obtained in each case. It was seen that quit different metabolites and pathways have been obtained in each case. Thus selection of a proper scaling methods play an important role in the metabolites identification and estimated pathway steps in metabolomics studies.

Keywords: “phytochemistry”, “quantum dots”, “autoscaling”

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Bayesian Methods in Chemometrics: A Simple Introduction

Mohsen Kompany-Zareh
Department of Chemistry, Institute for Advanced Studies in Basic Sciences (IASBS), Gava Zang, Zanjan 45137-66731, Iran. Trace Analysis Research Centre, Department of Chemistry, Dalhousie University, PO Box 15000, Halifax, NS B3H 4R2, Canada.
Email address: kompanym@iasbs.ac.ir

ABSTRACT

Chemometrics is increasingly being perceived as a maturing science. While this perception seems to be true with regards to the traditional methods and applications of chemometrics. Advances in instrumentation, computation, and statistical theory may combine to drive a resurgence in chemometrics research. Previous surges in chemometrics research activity were driven by the development of new ways of making better use of available information. Bayesian statistics can further enhance the ability to use domain specific information to obtain more accurate and useful models, and presents many research opportunities as well as challenges.

Recent Bayesian statistical methods are based on conditional probability and practical for a wide range of applications without making the common assumptions of Gaussian noise and uniform prior distributions. An overview of traditional chemometric methods from a Bayesian view and a tutorial of some recently developed techniques in Bayesian chemometrics, such as Bayesian PCA and Bayesian latent variable regression, will be discussed. Probabilistic analysis of non-trilinear fluorescence spectroscopic data and Naive Bayesian classification will be considered to show the flexibility and wide range of applicability of Bayesian statistics.

Keywords: “Bayesian”, “non-trilinear”, “fluorescence spectroscopic”

References:

[1] H. Chen, B.R. Bakshi, P.K. Goel, “Toward Bayesian chemometrics-a tutorial on some recent advances”, Anal Chim acta, 602, **(2007),** 1–16.

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About the error propagation and uncertainty estimation for the fitted parameters using Microsoft excel

Abdolhossein Naseri

Department of Analytical Chemistry, Faculty of Chemistry, University of Tabriz, Tabriz, Iran

E-mail: a_naseri@tabrizu.ac.ir

ABSTRACT

Uncertainty estimation and propagation of uncertainty of parameters are main topics in model fitting. Propagation of uncertainty (or propagation of error) is the effect of variable's uncertainties on the uncertainty of a function based on them. When the variables are the values of experimental measurements they have uncertainties which propagate due to the combination of variables in the function. The correlation between the variable is important thing in error propagation which can arise from different sources. In the error propagation, if the uncertainties are correlated then covariance must be taken into account. Unfortunately, the correlation between variables is ignored in most chemistry textbooks to get simplicity in calculation which leads to incorrect results [1, 2].

Microsoft Excel is the spreadsheet applications and commonly used for data analysis because of its simplicity and universal availability [2, 3]. It has a programming ability, Visual Basic for Applications (VBA).

The aim of this work is to show the ability of Microsoft excel in calculation of uncertainty of parameters in fitting and also getting of their correlation in different chemical systems. Then, propagation of uncertainty will be studied using this universal available software taking in to account covariance matrix.

Keywords: “error propagation”, “correlation”, “covariance matrix”, “fitting”, “Microsoft excel”

References:

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Some Misleading Issues in Drug Delivery Systems and their Associated Demands for Employing Multivariate Chemometrics Approaches

S. Maryam Sajjadi
Faculty of Chemistry, Semnan University, Semnan, Iran.
E-mail address: sajjadi@semnan.ac.ir

ABSTRACT

Drug delivery systems (DDSs) refer to the pharmaceutical technology employed for presenting the drug to the desired body site. In therapeutic goals, it is an urgent need to control the delivery of drugs in both desired dose and site, in order to decrease their adverse side effects. In the study of DDSs, pharmacokinetic investigations have gained much attention from researchers; however, in this regard, there are some misleading issues such as decomposition of some drugs during their release process [1]. Indeed, any changes in DDSs' formulations, either quantitatively or qualitatively, could influence drug release; therefore, it is crucial to have a deep insight into the mechanism of drug release and its side reactions.

There are a verity kind of multivariate chemometrics methods that can be utilized to find the kinetic mechanisms and estimate the profiles of all or some kinetic profiles of species involved in the reactions [2]. It should be noted that high-performance liquid chromatography (HPLC) is a common method used for most of DDSs assessments because it can produce selective responses for drug [3]. However, there is no limitation of using spectrophotometric methods for monitoring the kinetic processes in DDSs when they are coupled with chemometrics strategies which are able to resolve the data containing spectroscopically active species with severely overlapped signals.

In this study, it will be discussed how chemometrics approaches can be applied successfully to investigate different kinetic processes in drug delivery systems which are responsive to light, pH, or temperature. Moreover, it will be shown how the loading condition of drug can influence its release mechanism.

Keywords: “Drug Delivery”, “Pharmaco-kinetic”, “Multivariate Data; “Chemometric Methods”

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Where Pattern Recognition Meets Nanostructure-based Optical Sensors

M Reza Hormozi-Nezhad
Department of Chemistry, Sharif University of Technology, Tehran, Iran
E-mail address: hormozi@sharif.edu

ABSTRACT

Visual detection, as a universal sensing approach, holds great promise in various fields such as environmental monitoring, food safety, security issues, clinical and point-of-care diagnosis, and healthcare assays in especially resource-constrained areas, where sophisticated instrumentation may not be available. Many efforts have been made over the past few decades to develop optical probes which can be classified into two main groups: colorimetric and fluorometric approaches. In the former, changes in the absorption signal or wavelength is assigned to the concentration of an analyte whereas in the latter, changes in the emission characteristics is monitored for quantification. In either of these analytical signal modes, implementation of nanostructures can greatly enhance sensing. Owing to the high extinction coefficient of plasmonic nanoparticles together with their size, shape and environment dependent absorption profiles, they provide much better colorimetric probes compared to their conventional counterparts. Similarly, it has been shown that emitters in nanoscale such as quantum dots, nanoclusters and metal organic framework materials with incredible and tunable emission properties, have recently attracted great attention in the fields of sensing and bioimaging. Moving from single optical probes towards cross-reactive sensor arrays enables the recognition and discrimination of groups of target species. In array-based sensors, instead of relying on a specific lock and key interaction for sensing, an array of semi-selective sensor elements is used. These cross-reactive sensor elements provide differential responses and generate measurable fingerprint patterns which are analyzed by pattern recognition methods in order to classify the data and to detect unknown samples. Since the large amount of data provided in a sensor array usually has a high dimension and cannot be analyzed by basic calibration methods, a multivariate data reduction method is required to reduce the dimension of the data and to make it better visually interpretable [1-2].

In this presentation, basic principles in the design of nanostructure-based optical sensor arrays will be outlined. Focusing on our recent research in this field [3], we will present several examples of luminescent and plasmonic nanoparticles that have been used to produce the desired assembly of sensor elements for detection and discrimination of important analytes.

Keywords: “Bayesian”, “non-trilinear”, “fluorescence spectroscopic”

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Essential Spectral Pixel Selection in Hyperspectral Images

Mahdiyeh Ghaffari[1], *Nematollah Omidikia*[2], *Cyril Ruckebusch*[1]

[1]*Univ. Lille, CNRS, UMR 8516 LASIR, F-59000 Lille, France,*
[2]*Department of Chemistry, Faculty of Science, University of Sistan and Baluchestan,*
P .O. Box 98135-674, Zahedan, Iran.
E-mail address: m.ghaffari808@gmail.com

ABSTRACT

Spectral imaging techniques are now important tools in chemical analysis. These tools combine the spectroscopic attributes of chemical measurements with the ones of imaging. Challenging applications of spectral imaging can be found in chemistry, biology, medicine, food science or agriculture, at both the micro and macro scales [1,2]. However, while chemical images can now be acquired in routine, linear spectral unmixing with multivariate curve resolution (MCR), which assumes a low-rank approximation of the bilinear decomposition to extract spectra of the pure/est individual chemical components and distribution of their proportions in the image of a scene, remains a challenging problem. Despite recent advances both in the field of self-modeling curve resolution (SMCR) and on the practical side, (bio) chemical are difficult to analyze, because they are big and spatial-spectral information is highly mixed [3]. In this work we propose a methodology to select Essential Spectral Pixels (ESPs) (very important pixel instead) of chemical images. These pixels are on the outer envelope of the principal component scores of the data and can be identified by convex-hull computation. As they carry all the spectral information that is useful for linear unmixing, all other measured pixels can be removed resulting in simpler multivariate curve resolution (MCR) analysis of large hyperspectral images. The proposed procedure is used to analyze several chemical images of different spectroscopies, sizes and complexities and show that multivariate curve resolution analysis done on full data sets of hundreds of thousands of spectral pixels can be performed on reduced data sets composed of very sparse sets of ESPs.

Keywords: “Essential Spectral Pixels (very important pixels)”, “Multivariate Curve Resolution”, “convex-hull”, “SMCR”, “chemical images”

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Deep learning (past, present, future)

Hossein Khosravi

Faculty of Electrical and Robotic Engineering, Shahrood University of Technology,
Shahrood, P.O. Box 36199-95161, Iran.

E-mail address: Hosseinkhosravi@chmail.ir

ABSTRACT

Deep learning is making a big impact in many areas of human life for solving complex problems. Deep learning models share various properties and the learning dynamics of neurons in human brain. It covers many areas of artificial intelligence, including image classification, image captioning, machine translation, speech recognition, drug discovery and computational chemistry.

The main concept of deep learning is not new, it is about 30 years old. With the development of large data sets, huge computing power and new algorithms, the true power of the concepts are now revealed.

In this lecture we will review the historical perspective of deep learning including:

- Perceptron, the first model of neural network
- Backpropagation and MLP
- First Deep Network introduced by LeCun 1989
- Recurrent Neural Networks
- Restricted Boltzman Machine
- ImageNet and its Influence on development of Deep Learning
- GPUs and their Influence on Deep Learning

Furthermore, we will describe the present status of deep learning including:

- Convolutional Networks
- Regional Proposal Networks (R-CNN)
- Deep Recurrent Networks (RNN, LSTM)
- Deep Reinforcement Learning (Q-Learning)
- Applications of DNN

And finally, a few things about the future directions for deep learning:

- Quantum deep learning
- Automated Machine Learning
- Competing Learning Models
- Hybrid Learning Models

Keywords: “Deep learning”, “Convolutional Networks”, “Quantum deep learning”

Application of near infrared spectroscopy and chemometrics for assessing food authenticity and adulteration

Hassan Yazdanpanah
Food Safety Research Center, Shahid Beheshti University of Medical Sciences, Tehran, IR Iran
E-mail address: Hassan.yazdanpanah@gmail.com

ABSTRACT

Food authenticity and adulteration are major issues in the food industry and are attractive for consumers. The globalization of our food makes it more vulnerable to food adulteration with both unintentional and intentional fraud being perpetrated. The latter is very often used for economic gain, also called “economically motivated adulteration”. The risk for food adulteration increases proportionately with the complexity of the supply chain. Considering the fact that the prediction of possible adulterants is not always an easy or sometimes even a possible task, this in turn leads to opportunities to make huge financial gains with a very low risk of detection. This can make the task of deciding which analytical methods are more suitable to collect and analyse chemical data within complex food supply chains, at targeted points of vulnerability, that much more challenging. It is evident that those working within and associated with the food industry are seeking rapid, user-friendly methods to evaluate food authenticity and adulteration, and rapid/high-throughput screening methods for the analysis of food in general. In addition to being robust and reproducible, these methods should be portable and ideally handheld and/or remote sensor devices, that can be taken to or be positioned on/at-line at points of vulnerability along complex food supply networks and require a minimum amount of background training to acquire information rich data rapidly (ergo point and-shoot). There are several methods available to characterize authenticity of foods, but these methods are usually expensive and time consuming. In relation to the globally traded amount of foods, an adequate number of controls by several traditional analytical methods is not realistic. In contrast, near infrared (NIR) as a spectroscopic fingerprinting technique has been shown to be a low cost, rapid, convenient, precise, multi-analytical and non-destructive screening method for food authentication and adulteration. Along with chemometrics, a resolution of unique chemical information is provided, which allows rapid monitoring of subtle compositional changes. Therefore, the comparison of the fingerprints obtained from authentic samples to adulterated samples can reveal mis-description or adulterations. The use of NIR as an analytical tool for process control, food safety and quality has been well recognized and accompanied by the application of chemometrics for data pre-treatment and analysis and multivariate screening and modelling. The NIR as a rapid method could be networked and thus used to detect trends in the food market perhaps even before any food security threat/event is acknowledged by regulators and thus could very easily sit within the umbrella of the Internet of Things. A big advantage of spectrometric methods combined with chemometrics lies in the fact that once a database is established and a suitable data analysis protocol is determined, a new sample can be screened within a few minutes. With a suitable user interface, even non-specialist personnel (such as food inspectors and consumers) can undertake sample analysis on-site as well as in QC laboratories and factories.

Among foods, meat and fruit juices are among commodities that meet the criteria for a high risk of being affected by adulteration. In this regard, we evaluated the feasibility of a handheld NIR device (900 – 1700 nm) for speciation of mutton, beef, chicken, and pork. NIR

spectroscopy was coupled with two different chemometric methods including Partial Least Squares Discriminant Analysis (PLS-DA) and Support Vector Machine (SVM). After spectral acquisition, the 6 spectra of each sample was used for further analysis. Spectral datasets were divided into calibration (70%) and validation (30%) sets with duplex algorithm and pre-processed with Mean Center and 2nd derivative (Savitzky–Golay) for PLS-DA and SVM-C models. The best results were achieved with SVM model. For SVM model, sensitivity and specificity values in the validation set were 88% and 94% for mutton, 95% and 99% for beef, 84% and 96% for chicken, and 86% and 93% for pork, respectively. SVM model overall accuracy was 87%. The finding presents, for the first time, the potential of hand-held NIR spectroscopy with chemometrics models for rapid, inexpensive and non-destructive speciation of 4 different types of raw meat samples.

In another study, we investigated the novel application of a handheld NIR device (900 – 1700 nm) coupled with multivariate classification methodologies as a screening approach in detection of adulterated lime juices. Three diffuse reflectance spectra of 31 pure lime juices (collected from Jahrom, IR. Iran) and 25 adulterated ones were acquired. Principal component analysis was almost able to generate two clusters. PLS-DA and k-nearest neighbors algorithms with different spectral preprocessing techniques were applied as predictive models. In the PLS-DA, the most accurate prediction was obtained with SNV transforming. The generated model was able to classify juices with an accuracy of 88% and the Matthew’s correlation coefficient value of 0.75 in the external validation set. In the k-NN model, the highest accuracy and Matthew’s correlation coefficient in the external validation set (88% and 0.76, respectively) was obtained with multiplicative signal correction followed by 2nd-order derivative and 5th nearest neighbor.

The results showed that handheld NIR in combination with multivariate analysis can be a very promising rapid first-step screening method for evaluation of meat and lime juice authenticity. Handheld NIR is, therefore, an ideal tool for high throughput analysis of a high number of samples identifying suspects which require further examination by state-of-the-art confirmatory methods.

Keywords: “Chemometrics”, “Near Infrared”, “Food authenticity”, “Food adulteration”, “Lime juice”, “Meat species”

Ensemble learning: a new concept in chemometrics?

Hadi Parastar
Department of Chemistry, Sharif University of Technology, Tehran, Iran
E-mail address: h.parastar@sharif.edu

ABSTRACT

Ensemble learning is a machine learning paradigm where multiple learners are trained to solve the same problem. In contrast to ordinary machine learning approaches which try to learn *one* hypothesis from training data, ensemble methods try to construct a *set* of hypotheses and combine them to use [1]. An ensemble contains a number of learners which are usually called *base learners*. The generalization ability of an ensemble is usually much stronger than that of base learners. Actually, ensemble learning is appealing because that it is able to boost *weak learners* which are slightly better than random guess to *strong learners* which can make very accurate predictions. So, “base learners” are also referred as “weak learners” [2].

Ensemble learning is a new concept in computer science for analysis of “Big Data” especially for classification and regression purposes [3]. However, the potential use of this method is under question in chemometrics. Therefore, in this contribution, the concept of ensemble learning and different types of learners is discussed and then their potential for the analysis of chemical data is investigated. Furthermore, its performance will be compared with conventional chemometric methods. As an example, random subspace discriminant ensemble (RSDE) [4] as one of ensemble learning algorithms combined with handheld near-infrared (NIR) spectroscopy is used to show the potential of ensemble learning for analysis of chemical data. In this regard, we developed a powerful method to test chicken meat authenticity. The research presented in this work shows that it is both possible to discriminate fresh from thawed meat, based on NIR spectra, but even to correctly classify chicken fillets according to the growth conditions of the chickens with good accuracy. In all cases, the RSDE method outperformed other common classification methods such as partial least squares-discriminant analysis (PLS-DA), artificial neural network (ANN) and support vector machine (SVM) with classification accuracy of >95%. This study shows that handheld NIR coupled with machine learning algorithms is a useful, fast, non-destructive tool to identify the authenticity of chicken meat. By comparing and combining different protocols to measure the NIR spectra (i.e., through packaging and directly on meat), we show the possibilities for both consumers and food inspection authorities to check the authenticity of packaged chicken fillet.

Keywords: “Ensemble learning”, “Chemometrics”, “Classification; Machine learning”

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Bioinformatics in drug discovery

*Sajjad Gharaghani**
Laboratory of Bioinformatics and Drug Design, Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran
E-mail address: s.gharaghani@ut.ac.ir

ABSTRACT

The human community still faces the problem of finding an effective and potent drug. Until now, the discovery of new drugs has not been in line with the advancement of science and technology. The methods of drug design are divided into ligand-based and structure-based categories. Ligand-based methods include Quantitative Structure Activity Relationship (QSAR) and pharmacophore models. In the structure-based approach (molecular docking), the protein-drug interaction is usually used for modeling. While this method leads to the discovery of the active compounds, it fails in the clinical phase due to the side effect. Many of the side effects are due to drug interactions with off-target proteins. Therefore, the need for computational methods that take into account drug interactions with all proteins seems essential. Nowadays, using bioinformatics methods with machine learning and network-based approach considers drug and protein interaction networks to provide a solution to this problem.

Keywords: “Drug discovery”, “Bioinformatics”, “QSAR, “Docking”, “Pharmacophore”

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Set of Sparse Solutions in Bilinear Decomposition

*Nematollah Omidikia**
Department of Chemistry, Faculty of Science, University of Sistan and Baluchestan,
P .O. Box 98135-674, Zahedan, Iran
E-mail address: nematkia@gmail.com

ABSTRACT

Several constraints are designed to restrict bilinear decompositions further to get a unique solution [1]. Sparsity constraint was introduced to create solutions with zero elements [2]. As nor the number of zeros neither the place of zeros are not initially available, sparsity constraint should be incorporated with caution. Regarding sparsity constraint, two important issues can be addressed. The first issue is the effect of sparsity constraint on the possible solutions of bilinear decompositions, finding the set of sparse solutions. The second issue is the type of Lp-norm, {p=0,1,2}, for the sparsity implementation. Focusing on the geometry of bilinear data sets, outer-polygon as the non-negativity boundary in curve resolution contains all the possible sparse solutions [3]. In this contribution, we shed light on the all possible sparse solutions, and it was shown that outer-polygon is the set of sparse solutions. Not only sparse solution, but also sparset solutions are located on the outer boundaries. Finally, Lp-norms were calculated for the different feasible profiles, and it is revealed that L_0 minimization and L_2 maximization are correct strategies to reach the sparse/est solutions. However, L_1-norm is not appriate candidate for sparse non-negative decomposition.

Keywords: “unique solution”, “bilinear data sets”, “feasible profiles”

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A new strategy for calibrating IDA-based sensor systems

Somaiyeh Khodadadi Karimvand, Hamid Abdollahi *,
Department of Chemistry, Institute for Advanced Studies in Basic Sciences, Zanjan, Iran
E-mail address: abd@iasbs.ac.ir

ABSTRACT

Nowadays, the indicator displacement assay (IDA) has wide applications in chemistry due to its high potential to selective and sensitive determination of different analytes [1]. In order to calibrating IDA-based sensor arrays systems for simultaneous quantification of analytes, nonlinear calibration methods such as Artificial Neural Network (ANN) are mainly used. For minimizing the complication of the constructed models in different algorithms of ANN methods and hence for preventing the over fitting problem, removing of redundant input variables is unavoidable. For this reason, various variable selection methods have been introduced to performing this important task. So, as the results of calibration model in ANN are completely affected by the chosen variables, herein, we present a novel strategy for calibrating the IDA-based colorimetric sensors with ANN models using dramatically reduced number of input variables and without needing any variable selection method. The general unique feature of IDA-based sensor systems is that the species of signal generators, the indicator and probe (indicator-receptor complex), are known and their pure spectra can be easily available. As the target analyte(s) in IDA sensors is colorless, any obtained data from these systems are the result of changing in the equilibrium concentrations of these two species. Herein, we proposed that for calibrating IDA-based sensors, instead of using signals with a large number of variables, the equilibrium concentration of active species with smaller number of variables can be replaced. As a result, the number of input variables in the calibration and thus, the possibility of overfitting will be significantly reduced. Most equilibrium chemical systems including IDA sensors due to presence of matrix effect are intrinsically non-linear. So, the Beer-Lambert law is not valid in the non-linear systems, and the simple least square method (CLS) of data to pure spectrum does not result in correct free concentrations profiles. Thus, in this situations the generalized classical least square or Indirect Hard Modelling (IHM) approach can be applied as an alternative method for resolving the equilibrium concentrations of the spectroscopic active species [2]. The performance of the proposed strategy was evaluated in a designed sensor array for simultaneous quantification of Histidine and Cysteine.

Keywords: "Indicator Displacement Assay (IDA)", "Sensor array", "Simultaneous quantification", "Artificial Neural Network (ANN)", "Indirect Hard Modelling (IHM)", "Histidine and Cysteine"

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Rapid determination of nitrate ions in drinking water based on image processing techniques using a smartphone platform

Ali Farahani, Hassan Sereshti, Camelia Tashakori, Shamim Azimi*
School of Chemistry, College of Science, University of Tehran, Tehran, Iran.
E-mail address*:* sereshti@ut.ac.ir

ABSTRACT

Developing a simple operating, robust and affordable technique for monitoring the concentration of nitrate residues in drinking water has become a crucial issue which has led to the introduction of various nitrate determination methods [1]. The present study aims to introduce a rapid, low-cost and portable smartphone-platform sensing device based on image processing techniques for fast determination of nitrate ions in water samples. A sample holder and photography kit, as shown in Fig.1A, was designed using cost-effective components. A circle of 600 pixels in diameter with the best correlation and sensitivity to nitrate ion concentration, was chosen as the region of interest using Convolutional Neural Network (CNN) shown in Fig.1B. An application platform named nitrate hunter developed and lunched in smartphone by app inventor platform (Fig.1C). Application was conducted to measure the nitrate levels in drinking water samples collected from 42 different zones of Tehran and Alborz provinces (Iran). The nitrate level in each sample was determined using a smartphone and UV-vis spectrophotometry. Based on the statistical analysis, nitrate concentration read from UV-visible spectrometer and that of calculated from the smartphone provided high correlation of *R2*=0.982. Correspondingly, using image processing and deep learning techniques nitrate concentration were detected in the range of 5 to 100 µg mL-1 (Fig.1D) with a high determination coefficient (*R2* = 0.995). Besides, the smartphone device predicted an LOQ value (5.0 µg mL) lower than the maximum residual level set by WHO.

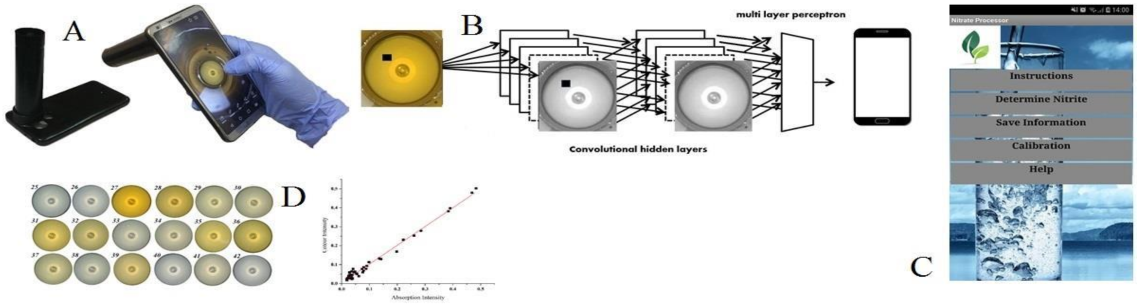

Figure 1: procedure of test and validation nitrate level in drinking water.

Keywords: “Nitrate ions”, “Smartphone-based techniques”, “Water quality determination”, “Image processing”

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Geographical classification of olive oil using the PLS-DA technique and linking chemical content to classes

Mohaddeseh rezaei, Mohsen Kompany Zareh, Maryam Khoshkam*

Institute for Advanced Studies in Basic Sciences

E-mail address: mohirezaei@yahoo.com

ABSTRACT

One of the most important issues of the olive oil industry in Iran is the definition of the grade of olive oil. Internationally, most countries use the standards of the International Association of Olive Oils (IOOC) to define the quality of olive oil. Due to the high nutritional value of olive oil and its benefits to human health, there are many traditional methods for defining the grade of olive oil, but none of these methods are sufficient on their own and thus the definition of an economical, comprehensive and simple method for the definition of the quality of olive oil is important. In this study, the least squares split strain analyzer (PLS-DA) method and method (Multi-Block Data Analysis) has been used as a method for determining the relationship between the quality of olive oil. This study is important because in Iran, there is no way to classify olive oils according to their nutritional value and their geographical area, so most of the counterfeit olive oils are sold instead of virgin olive oil.

In addition to the study done in comparison with similar work in the world, it is advantageous to combine and compare the results of the PLS-DA and Multi-Block Data Analysis methods. The results of previous studies have shown that the issue of non-compliance of the quality label on glass of olive oil with its actual quality is a serious issue in Iran. In this research, it will be shown that these methods can be used as a comprehensive method for defining the degree of quality of olive oil successfully. This method can be an easy and economical way to define the grade of olive oil quality for the olive oil extraction industry [1-3].

Keywords: “olive oil”, “PLS-DA”, “Multi-Block Data Analysis”, “geographical”, “classification”, “chemical content”

Untargeted metabolomics changes of Gammarus Pulex in river water induced by designed exposure with selected pharmaceuticals: A chemometrics study

Mahsa Naghavi Sheikholeslami[1], *Maryam Vosough*[*,1] , *Roma Tauler*[*2] , *Cristian Gomez-Canela*[2]
[1]*Department of Clean Technologies, Chemistry and Chemical Engineering Research Center of Iran, Tehran, Iran, P.O. Box 14335-186 Tehran, Iran*
[2] *Department of Environmental Chemistry, Institute of Environmental Assessment and Water Research (IDAEA), Consejo Superior de Investigaciones Científicas (CSIC), Barcelona, 08034, Catalonia, Spain*
E-mail address: vosough@ccerci.ac.ir

ABSTRACT

Recently, the presence of pharmaceuticals and personal care products (PPCPs) in water due to incomplete removal in wastewater treatment plants (WWTPs) is a serious concern. In this work the effect of three pharmaceuticals (Propranolol, Triclosan, and Nimesulide) exposure on Gammarus pulex metabolic profiles in river water was assessed by liquid chromatography coupled to high resolution mass spectrometry (LC-HRMS), in an untargeted way [1]. The generated complex data sets in the different exposure experiments were processed by different chemometric tools based on the selection of regions of interest (ROIs) and on multivariate curve-resolution alternating least squares (MCR-ALS). Utilizing analysis of variance simultaneous component analysis (ASCA) on metabolite peak profile areas resolved by MCR-ALS showed significant changes between different contaminants, different pharmaceutical concentrations (exposed and non-exposed samples) and between different exposure times (2h, 6h and 24h). In addition, 34 metabolites were common between various contaminants, which they have been interpreted using ASCA [2,3].

Keywords: “PPCPs”, “WWTPs”,“Gammarus pulex”, “Metabolite”, “LCHRMS”, “ROI-MCR-ALS”, “ASCA”

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Investigation of an interactive molecular autoburette for simultaneous determination of analytes by chemometric approaches of automatic spectrophotometric titration

Sanaz Sajedi Amin[1], Abdolhossein Naseri[1], Hamid Abdollahi[,2]*
[1] Department of Analytical Chemistry, Faculty of Chemistry, University of Tabriz, Tabriz, Iran
[2] Department of Chemistry, Institute for Advanced Studies in Basic Sciences, Zanjan, Iran
E-mail address: abd@iasbs.ac.ir

ABSTRACT

The device is a tool that invented or constructed for a special goal. Chemical devices are molecular level devices, which can be used instead of physical ones and also expected to open the way to revolutionizing the science i.e. in drug delivery and solving the environmental pollution [1].A chemical system provides to change the value of an nenvironmental parameter (pH, temperature, etc.) inside a reaction vessel in a controlled way without any interfering with the progression of studied reaction. Here we studied the possibility of using any chemical devices that provide variable pH condition as a molecular burette in reaction vessel based on model based analysis. The chemical compounds such as cryptand, tert-buthylchloride or any chemical system that produce or entrap H+ in reaction vessel can act as a variable pH autoburette [2]. Proper simulation of this mechanism based on the kinetic or intertwined equilibrium-kinetic model; enable ones to design an experimental direction for its use as a molecular burette. The present study aims to investigate the optimum condition of molecular outoburette operating parameters to obtain better performance for various acid-base titration. In other words, a larger pH range of action or a balancing the rate of pH change, provide the almost ideal demand system for automatic titrations. So, the effect of different factors such as initial concentration of chemical device, starting pH and buffer capacity on tuning the pH-time profile of molecular burette were investigated. Finally, the proposed molecular device can be evaluated for simultaneous determination of binary mixtures of food colorants by chemometrics analysis of simulated pectrophotometric titration data, which was alternative to traditional extensive series of experiments. This kind of data structure, analyzed by multivariate curve resolution-alternating least squares (MCR-ALS) under the non-negativity, correspondence and trilinearity constraints [3] As a result, the concentration of each dye in the samples and their corresponding pure spectra were obtained.

Keywords: “molecular devices”, “automatic titration”, “food colorants”, “multivariate curve resolution-alternating least squares”

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Convolutional neural network as a new tool for classification of multisensor data: prostate cancer case

Kourosh Shariat[1], *Dimitry Kirsanov*[2], *Hadi Parastar**[,1]
[1]*Department of Chemistry, Sharif University of Technology, Tehran, Iran*
[2]*Departmetnt of Analytical Chemistry, Saint Petersburg State University, Saint Petersburg, Russia*
E-mail address: h.parastar@sharif.edu

ABSTRACT

Convolutional neural networks (CNNs) have shown excellent performance in the past few years on a variety of machine learning problems to process multidimensional data and to recognize local patterns which makes them useful for problems such as image analysis and sound recognition [1]. Additionally, a recent study showed that CNNs can be efficiently applied to classify vibrational spectroscopic data and it was claimed that CNN outperformed conventional classification methods such as partial least squares-discriminant analysis (PLS-DA), support vector machine (SVM) and logistic regression (LR) [2]. This implies the relevance of feasibility study of CNNs as a possible tool for data analysis in other applications. Prostate cancer (PCa) is the second most common cancer in males and it is one of the leading causes of cancer mortality. Early detection of prostate cancer is crucial for successful therapy and so far, the common methods of detection are either inaccurate or resource-consuming [3]. The potentiometric multisensor systems are the arrays of cross-sensitive electrodes which can be used for untargeted detection of biomarkers and therefore, a multivariate "fingerprint" can be obtained. The main objective of the present contribution was development of a chemometric classification method based on CNN for classification of multisensor data of prostate cancer towards early diagnosis of this cancer. The studied data set contained 89 samples (43 from biopsy confirmed PCa patients and 46 from control group) characterized with responses from 28 sensors [3]. The original data were splitted into calibration and test set using duplex algorithm. Then, different preprocessing methods including mean-centering, auto-scaling and smoothing were tested on the performance of CNN. In optimum CNN condition, CNN gave 95.6% sensitivity, 97.7% specificity and 95.0% accuracy which were really surprising. Also, CNN performance was superior of the conventional classification methods of PLS-DA and SVM. It is concluded that CNNs can be effectively used to classify multisensor data and more importantly, detect prostate cancer via potentiometric multisensor systems at early stage.

Keywords: **"**Convolutional neural networks", "Chemometrics", "Multisensor system", "Prostate cancer"

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Application of a new hybrid of SCAD - artificial neural network in QSAR study of HIV inhibitors

Zeinab Mozafari, [1], Mansour Arab Chamjangali[1], Mohammad Arashi[2], Nasser Goudarzi [1]*
[1]Department of Chemistry, Shahrood University of Technology, Shahrood, P.O. Box 36155-316, Iran.
[2]Department of Statistics, Faculty of Mathematical Sciences, Shahrood University of Technology,
Shahrood, P.O. Box: 316-3619995161, Iran.
E-mail address: Chemist.mozafari1991@gmail.com

ABSTRACT

A hybrid of smoothly clipped absolute deviation (SCAD) and Levenberg- Marquardt (LM) artificial neural network (ANN) was used as a new approach in the quantitative structure-activity relationship (QSAR) studies. Fan and Li presented the SCAD in 2001 to improve previous variable selection methods' [1] performance. The SCAD has advantages such as unbiased estimation, continuity, low prediction error, stability, good sparsity and high interpretation. Hence, SCAD as an oracle method has an efficient penalty function. Recently, SCAD has been used as modeling method in QSAR/QSPR studies [2,3].

57 new HIV inhibitors were used in the QSAR modeling and pEC_{50} of compounds were simulated. 3224 Dragon descriptors were computed for the thioacetamide/acetanilide derivatives [4]. Dataset were divided into the three categories of train set (35 compounds), validation set (11 compounds) and the test set (11 compounds). SCAD method [2] was applied on the train and validation set data (46 compounds) and 11 non-zero coefficients corresponded to the parameter with the lowest cross validation error (λ_{min}) were selected and used as inputs of modeling method. The predictability of the optimum LM-ANN model was evaluated using external test, leave one out (LOO) technique and statistical parameters. Statistical parameters such as determination coefficient (R^2) and mean square error (MSE) of the test set were 0.92 and 0.12 respectively, which prove the generalizability and predictability of the constructed model. According to the effects of descriptors on the biological activity, some active compounds were suggested and the interaction of ligand-enzyme were analyzed using Autodock4.2 and pyMOL softwares.

Keywords: "HIV", "QSAR", "SCAD", "Artificial neural network", "Molecular docking"

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Simultaneous determination of cysteine enantiomers by chemometrics methods

*Azam Safarnejad[1], M. Reza Hormozi-Nezhad[2,3], Hamid Abdollahi *[1]*
[1] Department of Chemistry, Institute for Advanced Studies in Basic Sciences, P.O. Box 45195-1159, Zanjan, Iran Zanjan, Iran
[2] Department of Chemistry, Sharif University of Technology, Tehran, 11155-9516, Iran.
[3] Institute for Nanoscience and Nanotechnology, Sharif University of Technology, Tehran, Iran
E-mail address: abd@iasbs.ac.ir

ABSTRACT

The determination and analysis of chiral compounds are of critical importance in chemical and pharmaceutical sciences. The Cysteine amino acid is one of the important chiral compounds that each enantiomer (L and D) has different effects on fundamental physiological Processes. The unique optical properties of nanoparticles make them a suitable probe for determination of different analytes. There are many reports in the chemistry literature which in applying nanoparticles for quantification and qualification of chiral compounds. For a chiral components containing varying composition of two enantiomers, both the concentration and enantiomeric composition should greatly influence the intensity of fluorescent sensor[1]. Water-soluble thioglycolic acid (TGA)-capped CdTe QDs as a nanoparticle exposing green emission[2]. In this work, under optimized conditions (pH, concentration of QD and Temperature) the CdTe QDs is used as an optical sensor for determination of Cysteine Enantiomers in the concentration range of 100-2000mM. The difference in the kinetics of the interactions between L- and D-cysteine with CdTe QDs led to chiral determination of these enantiomers. Compared to univariate methods that only applied for determination of enantiomeric excess at total enantiomer concentration or ratiometric methods that applied for determination of total concentration and composition of enantiomers, multivariate methods can determine the concentration of each enantiomers in the mixture. Herein, the Back Propagation-Artificial Neural Network (BP-ANN), and Partial Least Squares regression (PLS) was applied for the simultaneous determination of L and D Cysteine.

Keywords: “TGA-CdTe QDs”, “Artificial neural network”, “partial least squares regression”, “Enantiomers”, “Simultaneous determination”

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External parameter orthogonalization combined with support vector machine as an efficient method for analyzing saffron NIR and ATR-FTIR spectra to assess saffron adulteration with plant-derived adulterants

Aryan Amirvaresi [1], *Nastaran Nikounezhad* [2], *Maryam Amirahmadi* [2], *Bahram Daraei*[3], *Hadi Parastar**[1]
[1]*Department of Chemistry, Sharif University of Technology, Tehran, Iran*
[2]*Food and Drug Laboratory Research Center, Food and Drug Organization, Tehran, Iran*
[3]*Department of Toxicology and Pharmacology, School of Pharmacy, Shahid Beheshti University of Medical Science, Tehran, Iran*
E-mail address: h.parastar@sharif.edu

ABSTRACT

Data preprocessing is one of the most data mining tasks which include preparation and transformation of data into a suitable form to mining a procedure [1]. Data preprocessing especially important for spectroscopic data that is affected by systematic variation and multiple external parameters [2]. This study presents an application of near infrared (NIR) and attenuated total reflectance (ATR) spectroscopy with special preprocessing and pattern recognition techniques for evaluating saffron adulteration with four characteristic adulterants of plant origin (i.e. C. sativus style, calendula, safflower and rubia). The proposed method was test on two different classification techniques of partial least squares-discriminant analysis (PLS-DA) and support vector machine (SVM). External parameter orthogonalization (EPO) was applied in both model as an efficient preprocessing techniques. In this way, 100 saffron samples were provided. Then, NIR and ATR spectra of the samples were recorded. Samples were grounded and passed through a sieve according to ISO/TS 3632-2. The data matrix was analyzed using principal component analysis (PCA), PLS-DA and SVM with quadratic kernel function. PCA was performed for preliminary exploration of possible differentiation according to the purity of saffron and the type of adulterant used. Different preprocess and filter methods were applied, but differentiation of most samples was not possible, except for the case of EPO. Thus, pre-processed data with EPO filter was included as input to the models in the next step. Firstly, discrimination of pure saffron samples was performed and secondly, adulterated saffron samples were examined. In all cases, discrimination between saffron and adulterated samples was better in EPO-QSVM rather than EPO-PLS-DA and on average good classification figure of merit including sensitivity (91.5%), specificity (93.5%) and accuracy (92%) were achieved. The obtained results illustrated that the proposed strategy based on combining EPO-QSVM with rapid NIR and ATR analysis can be considered as a rapid test for food quality control.

Keywords: “Saffron adulteration”, “Spectroscopy”,” Chemometrics”,”Support vector machine”

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The extraction and measurement of nickel metal ion in crab,shellfish and rice samples using magnetic silk fibroin - EDTA ligand and chemometric method

*Manijeh yekrangi, Shahriar Jahanbani, Ali Benvidi**
Department of Chemistry, Faculty of Science, Yazd University, Yazd, I. R. Iran,
E-mail address: abenvidi@yazd.ac.ir

ABSTRACT

The main aim of the present study was the measurement of nickel metal ion in the real samples of crab and oyster by the designed magnetic nano adsorbent silk fibroin-EDTA ligand (SF-Fe3O4-EDTA). Due to the structure of silk fibroin (possessing lots of functional groups which are suitable for attachment of ligands and high surface area), it was used in the structure of fabricated nano adsorbent [1]. The optimization processes were performed with the chemometric method of response surface modeling with sufficient accuracy and precision [2]. Using this chemometric method, the optimum values of pH, absorption time, the concentration of nano-adsorbent and temperature were calculated to be 6, 21 min, 4 mg L-1 and 28 °C, respectively. Using the magnetic nano adsorbent of silk fibroin- EDTA ligand and furnace atomic absorption a detection limit of 0.0017 µg L-1 and a linear range of 0.0030-5.0 µg L-1 for determination of nickel metal ion was obtained.

Keywords: “SF-Fe3O4-EDTA”, “ nano adsorbent “

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Probing the binding mechanism of sorafenib to bovine α-lactalbumin using spectrometric methods, molecular docking

Fatemeh Bagheri *, *Mohammad Hossein Fatemi*
Laboratory of chemometrics, Faculty of chemistry, University of Mazandarn Babolsar, Iran
E-mail address: Bshimi999@email.com

ABSTRACT

Sorafenib, Multi-kinase inhibitor [1] and bovine α-lactalbumin (BLA) is an important Ca^{2+} binding protein of milk [2]. The affinity between sorafenib and (BLA) was investigated by molecular docking techniques and spectroscopic methods. The association behavior of Sorafenib was investigated at its various concentrations and using BLA concentration of 10µM in aqueous phosphate buffer (pH=7.4).in 297 K, 303K and 308 K. To estimate the character of the binding between studied quencher and BLA the Stern–Volmer method were used. The fluorescence spectroscopic results revealed that sorafenib could effectively quench the intrinsic fluorescence of BLA through a static quenching mechanism because the static quenching constant decreases with the increasing temperature. The binding affinity (KA) and the number of binding sites (n) between sorafenib and BLA at 297 K were estimated $9.12*10^4$ L_mol-1 and 1 respectively. However, the thermodynamic parameters(enthalpy change ($\Delta H0$) and entropy change (ΔS_0) in the binding process can be calculated by the van't Hoff equation. Evaluation of the thermodynamic parameters(both $\Delta H0$ and $\Delta S0$ 4 are negative), suggested that the binding process was spontaneous while hydrogen bonds and van der Waals forces played a major role in this interaction. The UV spectra of BSA in the presence of BLA sorafenib were done. The results revealed that the intensity of UV-absorption of BLA increased with the addition of sorafenib However, red shift of maximum peak of BLA at 280 nm were also noticed probably due to the formation of sorafenib–BLA complex. The results of docking studies indicated that sorafenib come closer to the Trp-104 than to other tryptophans also ΔG obtained from this method corresponds to the spectroscopic methods.

Keywords: "Sorafenib", "bovine α-lactalbumin", " α-lactalbumin", "fluorescence spectroscopy", "Molecular docking", "Multi-kinase inhibitor"

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Visualization of Component-wise Rotational Ambiguity Using Signal Contribution Function

Jamile Mohammad Jafari[1], *Robert Rajkó*[2], *Hamid Abdollahi*[1]*
[1] *Institute for Advanced Studies in Basic Sciences (IASBS)*
[2] *Department of Process Engineering, Faculty of Engineering, University of Szeged*
E-mail address: abd@iasbs.ac.ir

ABSTRACT

Soft modeling or multivariate curve resolution (MCR) are well-known methodologies for the analysis of multivariate data in many different application fields. Results obtained by soft modeling methods are very likely impaired by rotational and scaling ambiguities, i.e. a full range of feasible solutions can describe the data equally well while fulfilling the constraints of the system. There are a few methods that attempt either at determining a useful approximation the ranges of feasible solutions for the resolution problem. These methods have calculated and shown the rotational ambiguity for the profiles that exist in systems [1]. In other word, all profiles for each component have obtained in these methods. In fact, these were demonstrated the rotational ambiguity as profile-wise. In this work, a new way was proposed for visualizing and determining the rotational ambiguity. It is called component-wise rotational ambiguity. It means rotational ambiguity can be shown for any component instead of profile. An estimation of the extent of rotation ambiguity and of approximate ranges of feasible solutions has been proposed by Tauler [2], MCR-BANDS method. This method is based on the definition of an objective function that should be optimized, the $f_n(T)$ maximum, f_{max}, and minimum, f_{min}, values. The MCR-BANDS method was used for indicating the extent of rotational ambiguity for every resolved component in the system. In fact, two data were obtained for any component using f_{max} and f_{min}. The space between these two data is a displaying of rotational ambiguity. Several examples were simulated for examining this study. Rotational ambiguity has been shown for any component in different systems. This visualization has some advantages: the type of normalization is not affected by components-wise rotational ambiguity. In addition, the rotational ambiguity can be calculated by measuring a volume between two surface corresponding maximum and minimum data.

Keywords: "Chemometrics", "self-modeling curve resolution (SMCR)", "signal contribution function (SCF)", "rotational ambiguity"

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Local Calibration Using Multivariate Curve Resolution Methods

Ali Pahlevan[1], Somaiyeh Khodadadi Karimvand[1], John Kalivas[2] , Hamid Abdollahi[1]*

[1]Department of Chemistry, Institute for Advanced Studies in Basic Sciences, Zanjan, Iran
[2]Department of Chemistry, Idaho State University, Pocatello, ID, 83209, USA
E-mail address: abd@iasbs.ac.ir

ABSTRACT

Multivariate Curve Resolution (MCR) strategies are powerful tools allowing the description, species identification and system understanding, of totally or partly unknown chemical processes and reactions where species cannot be easily isolated and where unknown intermediate species may be present. These methods are also powerful techniques for quantification of complex mixtures. Recently MCR-ALS was used for the analyte quantitation in first-order data sets and was compared with PLS regression [1, 2]. In most of compared cases, MCR-ALS quantitative analysis performed better than PLS. However, in some cases, MCR-ALS was also unable to build a robust regression model, especially when the sample to sample variability was low. The better quantitative results of MCR-ALS, when the minimum number of calibration samples we provided, can be attributed to the fact that both calibration and prediction samples are applied simultaneously in MCR-ALS algorithm. Thus, the prediction error decreases due to the signal averaging effect and the calibration space is better defined by MCR-ALS factors. In this study we have used MCR first-order calibration for evaluating its ability to local calibration in comparison with other calibration methods such as PLS. Matrix matching has been used as criteria for selecting most appropriate calibration sets. Several real experimental complex data have been used for evaluating the power of MCR methods for local calibration in the presence of matrix effects.

Keywords: "Multivariate Curve Resolution-Alternative Least Square (MCR-ALS)”,"Matrix effect", "Local calibration", "Matrix matching"

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Application of Box-Behnken design and response surface methodology in optimization of salting out assisted liquid-liquid microextraction of chromium species in environmental samples

Reza Tabaraki, Elham Heidarizadi, Mina Khodabakhsh*
Department of Chemistry, Faculty of Science, Ilam University, Ilam, Iran
E-mail address: rezatabaraki@yahoo.com

ABSTRACT

Chromium is a major pollutant for environment, usually as a result of some industrial pollutions. Chromium species exist mainly in two different oxidation states in the environment, Cr(III) and Cr(VI), which have contrasting physiological effects. In this work, salting out liquid-liquid microextraction (SALLME) combined with UV/Vis spectrophotometer was developed as an extraction method for Cr(VI) and Cr(III) in environmental water samples. Spectrophotometric determination of chromium using the diphenylcarbazide is an inexpensive and sensitive procedure and also permits the speciation of chromium. This colorimetric method is very selective for Cr(VI). Cr(VI) ions were converted into their cationic complex with 1,5-diphenylcarbazide (DPC) and then extracted into organic phase (ethanol) while Cr(III) remained in the aqueous layer. Total chromium was determined as Cr(VI) after oxidazing Cr(III) to Cr(VI) by the addition of $KMnO_4$ in acidic medium. Cr(III) concentration was calculated by difference between the concentration of total chromium and Cr(VI). Variables affecting the SALLME of chromium, such as type of extraction solvent, acidity, concentration of DPC (chelating agent) and salt type were optimized by one factor at a time approach. Afterwards, the main factors of SALLME including solvent extraction volume, salt amount and vortex time were optimized by response surface methodology (RSM) based on Box-Behnken experimental design. The Box–Behnken method was selected as the statistical prediction method with the aim of reducing the number of experimental runs which will directly save time and chemicals and thereby reducing the overall cost. In present study, ethanol volume [X1], salt amount (Na2CO3) [X2] and extraction time [X_3] were independent factors and extraction recovery was response variable. The levels of the variables were selected according to the preliminary studies. A quadratic polynomial equation was fitted to experimental data and terms significance were computed by analysis of variance (ANOVA). Under the optimum conditions, linear dynamic range (LDR) and limit of detection (LODs) were 5–40 (R^2= 0.995) and 2 µg L^{-1}, respectively. The extraction recoveries and enrichment factor ranged from 98% to 104% and 33, respectively. Repeatability of method based on five replicate measurements was 3.8%. The proposed method was also compared with the other method. Results showed that the proposed method is simple, rapid and environmentally friendly with high efficiency [1].

Keywords: "Response surface methodology", "Box-Behnken design", "salting out liquid-liquid extraction"

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Performance comparison of wavelet neural network and adaptive neuro -fuzzy inference system

Reza Tabaraki, Mina Khodabakhsh*
Department of Chemistry, Faculty of Science, Ilam University, Ilam, Iran
E-mail address: rezatabaraki@yahoo.com

ABSTRACT

Artificial intelligence has been applied to a wide variety of chemical problems such as nonlinear modeling for quantitative structure property relationships. Adaptive neuro Fuzzy Inference System (ANFIS) is an artificial neural network based on the Takagi-Sugeno fuzzy system. Since this system combines neural networks and fuzzy logic concepts, they can take advantage of both possibilities in a frame. Wavelet neural networks (WNN), which combine the wavelet theory and feed-forward neural networks, utilize wavelets as the basis function to construct a network. The wavelet neural network shows surprising effectiveness in solving the conventional problems of poor convergence or even divergence encountered in other kinds of neural networks. In this work, performance of WNN and ANFIS models were compared with multiple data sets by different criteria such as second order corrected Akaike information criterion (AIC), Schwartz Bayesian criterion (SBC), Nash–Sutcliffe efficiency (E_{NS}), mean relative error (MRE) and root mean squared error (RMSE). Another criterion was overfitting. To avoid overfitting, the ratio of training set observations to network adjustable parameters must be greater than two. Nine data sets were selected from literature and their data were divided to training, test and validation sets. Network parameters were optimized for WNN and ANFIS models and the best architectures with the lowest errors were selected for each data set. At first sight, results indicate that both WNN and ANFIS models are comparable based on mentioned criteria but ANFIS networks are faster in computation process (low epochs). Precise survey of networks showed that overfitting in the ANFIS networks is serious. Seven ANFIS models (from total 9 models) had overfitting and even five models had higher total number of adjustable parameters than number of observations in training sets. When the number of inputs is more than five and the number of membership functions is greater than two, overfitting is serious in ANFIS models [1].

Keywords: “wavelet neural network”, “adaptive neuro-fuzzy inference system”, ” overfitting”

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Experimental and theoretical studies on interaction of some drugs with human serum albumin

Fatemeh Mohammadnia[*,1], *Mohammad Hossein Fatemi*[1], *Seyed Mojtaba Taghizadeh*[2]
[1] *Laboratory of chemometrics, Faculty of chemistry, University of Mazandarn Babolsar, Iran*
[2]*Novel Drug Delivery systems, Faculty of Science, Iran Polymer and Petrochemical Institute, Tehran, Islamic Republic of Iran*
E-mail address: f.mohammadnia@ippi.ac.ir

ABSTRACT

The interaction of 14 anti-inflammatory drugs with human serum albumin (HSA) was studied by fluorescence quenching technique, molecular docking studies, and "quantitative structure activity relationship" (QSAR) method. Binding constants of the drugs obtained by fluorescence quenching method. Molecular docking was used for estimation of binding sites and binding constants of these anti-inflammatory drugs. The results of molecular docking indicated the role of hydrogen binding of the selected drugs in interaction with HSA. Finally, the QSAR model constructed between experimental binding constants of the drugs and theoretical descriptors. Theoretical descriptors were classes of constitutional, geometrical, functional group counts, atom-centered fragments, 2D frequency fingerprints, and molecular properties of DRAGON software [1]. A stepwise multiple linear regression (MLR) was used in the selection of the most relevant descriptors. Finally, a two-parameter model was developed. Descriptors revealed in model were sum of conventional bond orders (SCBO) and presence/absence of N and O at topological distance of 03 (B03 [N-O]). In order to assess the robustness of model, the leave-one out cross validation test was applied. The correlation coefficient of model was 0.95. The value of cross-validation correlation coefficient (Q^2) was found as 0.62, which showed robustness of the model.

Keywords: “Anti-inflammatory drugs”, “Human serum albumin”, “Fluorescence quenching”, “Quantitative structure activity relationship”, “Molecular docking”

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The experimental and theoretical studies of Biopartitioning Micellar Chromatography to mimic the drug-protein binding of some drugs

Fatemeh Mohammadnia[*,1], *Mohammad Hossein Fatemi*[1], *Seyed Mojtaba Taghizadeh*[2]
[1] *Laboratory of chemometrics, Faculty of chemistry, University of Mazandarn Babolsar, Iran*
[2]*Novel Drug Delivery systems, Faculty of Science, Iran Polymer and Petrochemical Institute, Tehran, Islamic Republic of Iran*
E-mail address: f.mohammadnia@ippi.ac.ir

ABSTRACT

In this work, biopartitioning micellar chromatography (BMC) was used to the assessment of affinity binding of 13 pain-relief drugs to HSA molecule. BMC retention factors (k_{BMC}) of tested compounds were calculated as $k_{BMC} = (t_R - t_0)/t_0$, where t_R is the retention time of the test compound and, t_0 corresponds to dead time. Values of k_{BMC} are determined based on averaging of at least triplicate measurements and are used in a logarithmic scale (log k_{BMC}). The values of BMC retention factors were determined by aqueous CTAB solution as mobile phase. Then, these values were correlated to some molecular structural descriptors by using quantitative structure retention relationship (QSRR) methodology. Four QSRR Models are developed by using the stepwise-MLR procedure and considering log k_{BMC} as dependent variable and descriptors calculated by DRAGON [1], CODESSA [2], and LFER parameters as independent variables. Correlation coefficients (R) values of these four models were 0.892-0.947. Results indicated that selected descriptors can address the most important structural features influencing the binding affinity of studied drugs to HSA.

Keywords: quantitative structure retention relationship, biopartitioning micellar chromatography, CTAB, HSA

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Partial least squares- residual bilinearization for simultaneous determination of ten pesticides in milk using QuEChERS-dispersive liquid-liquid microextraction followed by gas chromatography

*Farnoosh Koleini, Parvaneh Balsini, Hadi Parastar**
Department of Chemistry, Sharif University of Technology, Tehran, Iran
E-mail: h.parastar@sharif.edu

ABSTRACT

Milk is one of the best sources of proteins, lactose, and minerals which virtually all ages among people consume it at least one time in a week. Unfortunately, sometimes due to an inferior feeding of cows, it could be possible to detect some kinds of pesticides in their product. As a result, the quality control of milk to achieve the healthiest production is incredibly considerable for users. Plenty of efforts have been developed to determinate the amount of pesticides in complex matrices such as water, fruits, vegetables and milk [1]. In the present study, ten pesticides including dichlorvos, carbofuran, carbaryl, atrazine, ametryne, diazinon, pirimiphos methyl, chlorpyrifos, prothioconazole, and tebuconazole were extracted from milk by utilizing quick, easy, cheap, effective, rugged, and safe (QuEChERS) combined with dispersive liquid-liquid microextraction (DLLME) [1]. It should be noted that central composite design (CCD), multiple linear regression (MLR), and Nelder-Mead simplex optimization method were used in order to design, model, and optimize all of the effective factors of QuEChERS-DLLME for simultaneous determination of these mentioned pesticides with gas chromatography-flame ionization detector (GC-FID). Accordingly, global optimum conditions were gained which were 0.25 mL of acetonitrile, 42.1 μL of chloroform, 25 min of sonication time and 3.8 % (w/v) NaCl in pH 6.1. In the next section, partial least squares-residual bilinearization (PLS-RBL) [2] was utilized to build a multivariate calibration model in concentration range of 0.5-100 ngmL^{-1}. R^2 for calibration and cross validation were 0.997 and 0.973 respectively. Moreover, RMSEC and RMSECV were 1.758 and 7.332, and analytical figures of merit (AFOM) including sensitivity (the first and most important analytical parameter), analytical sensitivity, selectivity, limit of detection (LOD), and limit of quantitation (LOQ) were evaluated [3]. The validity of this proposed method was confirmed based on the comparison between calculated LOD and MRL guideline of European Union (EU). the value of recovery and RSD were 77.69-147.69% and 1.57-9.67%. This validated method was successfully applied for quantitative determination of 10 pesticides in milk samples and would be powerful to exploit in quality control laboratories as a reliable method.

Keywords: “Pesticides”, “QuEChERS”, “Dispersive Liquid-Liquid micro extraction”, “Gas chromatography”, “Multi-response optimization”, “partial least squares- residual bilinearization”

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Random Augmented Classical Least Squares: A Modified Calibration with CLS and ILS Advantages

Saeed Khalili Ali Abad[1], *Nematollah Omidikia*[2*], *Hamid Abdollahi**[,1]
[1]*Department of Chemistry, Institute for Advanced Studies in Basic Sciences, Zanjan, Iran.*
[2]*Department of Chemistry, University of Sistan and Baluchestan, Zahedan, Iran.*
E-mail address: abd@iasbs.ac.ir

ABSTRACT

Calibration is finding a relationship between instrument response and physical or chemical property of an analyte(s) [1]. Multivariate calibrations are divided into two directions, Classical Least-Squares (CLS) and Inverse Least-Squares (ILS) [2]. ILS methods such as Principle Component Regression (PCR), Partial Least Squares (PLS) are more popular than CLS because inverse methods allow one to study multicomponent samples where only one or few analytes are of interest, but the concentration, spectra, and chemical identities of other components in the calibration samples are unknown while the complete knowledge of chemical and physical components such as concentration, baseline, offset and etc. is necessary for CLS [3]. On the other hand, CLS method allows one to do qualitative and quantitative analysis, simultaneously due to estimated regression coefficients since they are pure spectra of components. The important issues have been highlighted and handled concern with CLS, which partial knowledge of concentration profiles in the calibration set is available while doing CLS is of interest. In this contribution a new procedure is proposed with a purpose of modifying classical calibration to the inverse models. To this goal, a series of random concentration vectors were augmented to compensate unknown components contributions. Finally, an algorithm was developed to optimize the required number of random augmented vectors and was tested on simulated and several real data sets.

Keywords: “Multivariate Calibration”, “Modified-CLS”, “Duality”, “Net Analyte Signal”, “Inverse Advantages”

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Combination of Multivariate Curve Resolution Alternating Least Squares Method and Experimental Design to Optimize the Simultaneous Photocatalytic Degradation of some Nitro phenols

Seyedeh Maryam Sajjadi, Javad Yousefi*
Faculty of Chemistry, Semnan University, Semnan, Iran.
E-mail address: sajjadi@semnan.ac.ir

ABSTRACT

In this study, photo-catalytic degradation processes of 2-nitrophenol (2-NP) and 4-nitrophenol (4-NP) were optimized simultaneously at acidic and basic media using the combination of central composite design (CCD)[1] and second-order data. ZnO nanoparticles were used as the photo-catalyst in this research. Spectrophotometric method as a cheap, simple and an available technique was employed to monitor experimental condition. Since the degradation processes have kinetic nature, the time dimension was used to create second-order time-spectral data at each experiment. During the degradation at both acidic and basic media, nitrophenols were converted to some spectrophotometrically active products. Both nitrophenols and their products show overlapping spectra; however, thanks to the second-order advantages of the data, the concentration profiles of 2-NP and 4-NP were resolved by matrix augmentation multivariate curve resolution method (MA-MCR-ALS) [1, 2].

At each experimental condition, the standard deviation of the concentration profiles of the analytes was introduced as a new criteria to quantify the degradation progress of nitrophenols and employed as response in the CCD design. Given that, the more standard deviations of the profiles are, the more progress in the degradations of analytes are, the optimal conditions were obtained based on maximizing the standard deviations of both analytes.

The results showed both analytes were more degradable in acidic media at the following condition: the amount of the catalyst , the volume of H2O2, 2-Np concentration, 4-NP concentration, tempreture were 3mg , 0.2 mL, 7.6 ppm, 25.1 ppm and 36.5 0C, respectively.

Keywords: “Standard deviation”, “MA-MCR-ALS”, “Nitrophenol”, “Photo-catalytic Degradation”

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Comparison of molecular based modelling for predicting gas heat capacity of organic compounds

*Aboozar Khajeh**
Department of Chemical Engineering, Birjand University of Technology, Birjand, Iran.
E-mail address: akhajeh@birjandut.ac.ir

ABSTRACT

The gas heat capacity is one of important property of organic compounds in design and application of chemical processes. With regard to the experimental measurement of physical-chemical property of organic compounds is expensive, laborious and time-consuming, having accurate models for predicting especially based on molecular structure is necessary. Group contribution (GC) and quantitative structure-property relationship (QSPR) are two methods that is commonly used for estimating various properties of organic compounds. In our previous study [1], a new QSPR model with three descriptors was developed for the prediction of heat capacity of 1174 common organic compounds in gas phase at 298.15 K. In the present study, a new linear group contribution model was produced using multiple linear regression (MLR) method. The gas heat capacity data were collected from the Yaws' Handbook [2] which to proper comparison between QSPR and GC model, same training and test sets were used. In GC modelling, by using MLR the best relationship between the chemical functional groups and the heat capacity values of chemical compounds were developed. The obtained results by GC method based on 71 functional groups (group contributions) show the squared correlation coefficient (R^2) of 0.9812 and root mean square error (*RMSE*) of 14.3419 for training set, 0.9935 and 10.3931 for test set. The high R^2 and low *RMSE* values obtained from the proposed GC model suggest that the presented model provides a simple and straightforward way to predict gas heat capacity of organic compounds from their structures alone with high accuracy. The comparison between GC and QSPR model indicates, the QSPR model (R^2= 0.9958 and *RMSE*=7.1358 for total data) showed slightly better statistical quality, however the application of GC, due to simplicity of calculation the number of groups for a compound, is easier compared with the QSPR. However QSPR is more accurate than GC model, the GC model has enough accuracy for engineering purposes and can be used as simpler alternative in many applications. The interpretability of QSPR models is one of their advantage because the selected descriptors in QSPR modelling have definite meanings.

Keywords: "QSPR", "Heat capacity", "Group contribution", "Multiple linear regression", "Modelling"

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The feasibility of applying hand-held NIR for speciation of beef, chicken, mutton and pork with chemometrics

Abolfazl Dashti[1], Hassan Yazdanpanah [1,2], Hadi Parastar[4], Farzad Kobarfard[2,3], Bahram Daraei[1]*

[1] Department of Toxicology and Pharmacology, School of Pharmacy, Shahid Beheshti University of Medical Sciences, Tehran, IR Iran.

[2] Food Safety Research Center, Shahid Beheshti University of Medical Sciences, Tehran, IR Iran.

[3] Department of Medicinal Chemistry, School of Pharmacy, Shahid Beheshti University of Medical Sciences, Tehran, IR Iran.

[4] Department of Chemistry, Sharif University of Technology, Tehran, Iran

E-mail address: yazdanpanah@sbmu.ac.ir

ABSTRACT

Meat species identification is a significant authenticity issue [1]. This study evaluates the feasibility of a handheld NIR device (900 – 1700 nm) for speciation of mutton, beef, chicken, and pork. NIR is used as a prescreening technology to increase the cost effectiveness of more expensive laboratory methods (like DNA, histology or microscopy). Raw meat samples of mutton (15 frontshank and rear shank samples), beef (19 foreshank and hind shank samples) and chicken (30 breast and drumstick samples) were collected from local butchers in Tehran and Yazd cities, IR Iran in 2019. Thirteen pork samples (from different parts of the animal body) were collected from different countries in 2019. Each sample was placed in a plastic plate in order to collect the spectral information. For each individual sample, 6 reflectance spectra were acquired (5 at the edges of the sample and 1 at the center) by contacting the probe of the instrument with the sample. NIR spectroscopy was coupled with two different chemometric methods: Partial Least Squares Discriminant Analysis (PLS-DA) and Support Vector Machine (SVM). After spectral acquisition, the 6 spectra of each sample was used for further analysis. Spectral datasets were divided into calibration (70%) and validation (30%) sets with duplex algorithm and pre-processed with Mean Center and 2nd derivative (Savitzky–Golay) for PLS-DA and SVM-C models. In these two models, mutton and pork classes were difficult to separate. But other classes were very much different and well separated. For PLS-DA model, sensitivity and specificity values in the validation set were 91% and 93% for mutton, 95% and 99% for beef, 81% and 95% for chicken, and 72% and 90% for pork, respectively. The overall accuracy of the method was 83%. For SVM model, sensitivity and specificity values in the validation set were 88% and 94% for mutton, 95% and 99% for beef, 84% and 96% for chicken, and 86% and 93% for pork, respectively. SVM model overall accuracy was 87%. The finding presents, for the first time, the potential of portable NIR spectroscopy with chemometric models for rapid, inexpensive and non-destructive speciation of 4 different types of raw meat samples including mutton, beef, chicken, and pork which could be used as a basis for meat adulteration determination.

Keywords: “Hand-held NIR”, “Meat”, “Chemometrics”

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QSPR study of linear retention indices of some organic compounds extracted from Lupinus Pilosus Murr plants

*Razieh Hamidi *, Mansour Arab Chamjangali, Nasser Goudarzi*

Faculty of chemistry, Shahrood University of Technology, Shahrood, Iran

E-mail address: razieh.hamidi58@gmail.com

ABSTRACT

In this paper, a predictive quantitative structure-property relationship (QSPR) model was created for the prediction of linear retention indices for 47 organic compounds extracted from Lupinus Pilosus Murr[1]. First, the structures of the compounds were drawn in Hyperchem software[2] and optimized using the semi-empirical AM1 method. After that, molecular descriptors for all compounds in data set were calculated using Dragon 5 software[3]. The calculated descriptors as the independent variables and experimental linear retention indices as the dependent variable were used for variable selection via stepwise regression method in SPSS software. Six descriptors (Dz, Mor26e, Mor30e, O060, G3s and C025) were selected as the most significant descriptors and used as inputs in artificial neural network (ANN) as a nonlinear modeling method. Data set was divided into two categories of training (37 molecules) and test (10 molecules) sets. Training set was used for the training of ANN through the cross validation method and test set was used for the external evaluation of method. ANN model was constructed between these six descriptors and the linear retention index and all affecting parameters on the performance of the model were optimized. During the optimizing of ANN model, minimizing of the mean squared error (MSE) was selected as the criterion. Finally, the optimized model was applied for the prediction of linear retention indices for the compounds in external test set. The obtained results ($R2_{test}$=0.9937, $R2_{traning}$=0.9971 and MSE=745.2977) indicate that proposed QSPR model is accurate and suitable.

Keywords: “QSPR”, “ANN”, “Linear Retention Index”, “Lupinus Pilosus Murr”, “Molecular Descriptors”

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Geochemometrics Analysis of Cr, As, Hg, Cd, Pb in Tarom soil samples by spectroscopic methods

Somayeh Veyseh[1] *Ali Niazi*[2], *Shabnam Najafi Aslipashaki*[1]
[1]*Geological research center of geological survey and mineral explorations Country Alborz*
[2] *Arak Branch, Islamic Azad University, Arak, Iran*
E-mail address: somayeh.veyseh@gmail.com

ABSTRACT

In this study distribution of Cr, As, Hg, Cd, Pb in soil samples of Tarom in Zanjan province was investigated. 217 soil samples were taken in Taron (T) according to standard sampling methods. Sample digestion was done according to ASTM D4698 by fusion methods [1]. Analysis was done by ICP-MS, ICP-OES and AF and resulted data were processed by Geochemometrics methods. Geochemoemtrics is a new method for receiving the most profitable data from a huge mass of complicated data [2]. PCA is the most useful mathematical method in chemometrics. KNN method is used for classification and determination of the coherence between data [3].

The analysis of principle components was done according to heavy metals and three main components are PC1=26.94%, PC2=21.18% and PC3=19.11% which contain more that 67% of the change. Distribution of samples was studied according to the Score plots of the first and second principle components and T211, T87, T172 in has got a significant variance. The effect of elements on samples was investigated by Biplot diagram and results show that Cr and Cd have got an effect on distribution of Tarom.

According to the studies about T^2-Hotelling the significant difference in T103, T173, T203 and T211 was obvious. KNN was used to study the correlation and clustering of elements and results show that Cr and Pb have got relative correlation in this region. In this plot As and Cr were placed in a different classification in compare with other elements also Pb and Cd are in this classification and have got closer correlation with As and Pb in comparison with Cr and Hg.

Results show that ICP-MS and ICP-OES analyses have got good accuracy and precision and the method is applicable in determination of trace elements in Geology.

Keywords: “Geochemometrics”, ”ICP-MS”, “ICP-OES”, “K_Nearrest Neighbor (KNN)”, “Heavy elements”

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The effect of random noise and spectral overlapping on the accuracy of the extracted profiles from spectroscopic data by soft modeling method

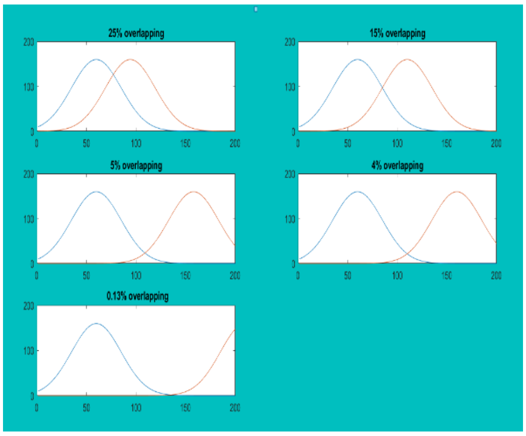
*Mahsa Zarei**
Department of Chemistry, Faculty of Science, University of Tehran, Tehran, Iran
E-mail address: Mahsa.zarei@ut.ac.ir

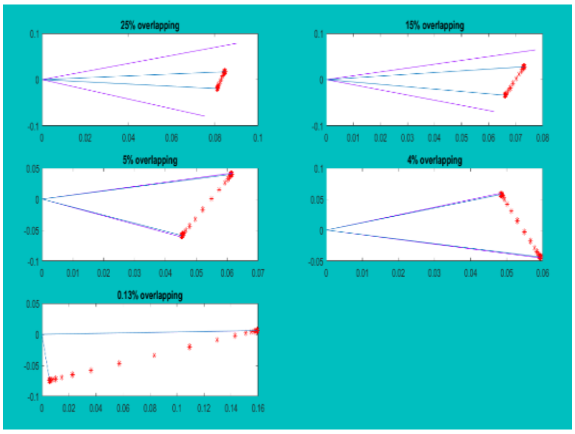
ABSTRACT

After the presentation of milestone paper by Lawton and Sylvester [1] in 1971 about rotation ambiguity, many important and novel modifications for extraction of pure concentrations and response profiles were reported.

In this report we studied the effect of the added noise level and degree of spectral overlapping of binary absorbing system. All calculations and simulations were performed in MATLAB. The obtained results were compared to the previous reported soft modeling methods. The effect each influenced parameter was thoroughly discussed.

Double Sigma value	Sigma value	Overlapping Percentage
1.3686	0.6843	**25%**
2	1	**15%**
3.92	1.96	**5%**
4	2	**4%**
6	3	**0.13%**





Keywords: “rotation ambiguity”, “response profiles”, “MATLAB”

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Discovery of New Inhibitors of AChE by Virtual Screening, Molecular Docking and Molecular Dynamics Simulations

Fatemeh Ansari[*1], *Pedram Bakhshi*[2], *Jahan B Ghasemi*[2], *Ali Niazi*[3]
[1] *Department of Chemistry, Arak Branch, Islamic Azad University, Arak, Iran*
[2] *Drug Design in Silico Lab, School of Sciences, Chemistry Faculty, University of Tehran, Teheran, Iran*
[3]*Department of Chemistry, Central Tehran Branch, Islamic Azad University, Tehran, Iran*
E-mail address: fansari94@iau-arak.ac.ir

ABSTRACT

In the present report we carried out a combination of molecular modelling method to discover a new class of AChE inhibitors. To do this, NCI database was screened by using a docking model which was built by AChE-Rivastigmine (1GQR) complex. Molecules were filtered by Lipinski, TOPKAT and ADMET limitations. Afterward, the similar molecules chosen by Tanimoto method and the retrieved molecules based on the dock score were fed to pharmacophore modeling. A Molecular dynamics simulation was applied to recognize and have a better insight to type and importance of molecular interactions including H-bonding and other molecular nonbonding and bonding counterparts [1]. The identified key residues in the active site of AChE were TYR121, GLY123, SER 124, ASP 72, PHE 330, TRP 84 and HIS 440. The results of this work improve our understanding of the mechanisms of AChE inhibitors and give valuable information that should assist in the design of novel potential AChE inhibitors [2,3].

Keywords: "AChE inhibitor", "Molecular Dynamics (MD)", "pharmacophore modelling", "Docking"

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Multi-Stimuli Responsive Molecularly Imprinted Polymer Based on Chain Transfer Agent Modified Chitosan Nanoparticles for Microextraction of Capecitabine: An Experimental Design Study

Saeedeh Ansari, *Saeed Masoum* *
Department of Analytical Chemistry, Faculty of Chemistry, University of Kashan, Kashan, Iran
E-mail address: masoum@kashanu.ac.ir

ABSTRACT

Capecitabine (CAP) is an anticancer pro-drug which is widely used as monotherapy or a combination chemotherapy agent in breast, colorectal, gastric, and esophageal cancers. Amongst the promising alternatives for solid sorbents, molecularly imprinted polymers (MIPs) that offer high selectivity and high binding affinity, widely utilized to generate synthetic receptors in solid-phase microextraction (SPME) [1]. This work provides an ultrasonic-assisted dispersive solid-phase microextraction by a multi-stimuli responsive MIPs based on chain transfer agent modified chitosan nanoparticles for highly selective enrichment and separation of trace CAP in real samples. The synthetic particles were carefully characterized and the results indicated that a uniform pH-sensitive imprinted layer was coated on the Fe_3O_4@CS core successfully, and enough saturation magnetization (29.45 emu/g) was obtained for magnetic separation. The reversible addition-fragmentation chain transfer (RAFT) polymerization, as one of the CLRP strategies, due to the unique advantages in MIPs preparation involving mildly polymerization conditions, living/controlled nature, fast mass transfer, uniform imprinted shell layer and almost no chain termination reaction has received impressive attention [2]. The desirable adsorption capacity (90.90 mg/g) and high imprinting factor (IF=3.61) toward CAP were exhibited by Langmuir isotherm model. Under optimized conditions, which achieved by Box-Behnken design (BBD) under response surface methodology (RSM), good linearity was obtained with correlation coefficients (R^2) over 0.999 and the detection limit (S/N=3) was 1.87 ng/mL. The average recoveries of CAP were calculated from 93.41% to 102.50% in human plasma samples with RSD less than 5.45%. This work provides the ultrasonic-assisted dispersive solid-phase microextraction (UA-DSPME) based on pH-sensitive MMIP@CS NPs for highly selective enrichment and separation of trace CAP in real samples.

Keywords: “Dispersive solid-phase microextraction”, “Magnetic molecularly imprinted nanoparticles”, “pH-sensitive polymer”, “Ultrasound assisted extraction”, “Pro-drug capecitabine”

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QSAR Study of Diarylpyrimidine Derivatives as HIV-1 Nonnucleoside Reverse Transcriptase Inhibitors by Particle Swarm Optimization Feature Selection- Multiple Linear Regression and Artificial Neural Networks

Seyed Mohammadreza Motalebi Tabaei[1] , *Mehdi Nekoei*[2*], *Safa Aliasgari*[2]
[1]*Department of Biochemistry,Shahrood Branch, Islamic Azad University, Shahrood, Iran*
[2]*Department of Chemistry,Shahrood Branch, Islamic Azad University, Shahrood, Iran*
E-mail address: m_nekoei1356@yahoo.com

ABSTRACT

Diarylpyrimidines (DAPYs), acting as HIV-1 nonnucleoside reverse transcriptase inhibitors (NNRTIs), have been considered to be one of the most potent drug families in the fight against acquired immunodeficiency syndrome (AIDS) [1]. QSAR models were developed for predicting activity of a series of diarylpyrimidine derivatives as HIV-1 nonnucleoside reverse transcriptase inhibitors. Particle swarm optimization (PSO) is a population-based stochastic optimization algorithm motivated by intelligent collective behavior of some animals such as flocks of birds or schools of fish. PSO algorithm simulates animal's social behavior, including insects, herds, birds and fishes. These swarms conform a cooperative way to find food, and each member in the swarms keeps changing the search pattern according to the learning experiences of its own and other members [2]. The suitable set of the molecular descriptors was calculated and the important descriptors by using the particle swarm optimization (PSO) were selected. The predictive quality of the QSAR models were tested for an external set of compounds by MLR and ANN. Statistical parameters for PSO-MLR and PSO-ANN were: R^2_{test}=0.627, 0.719, RMSEP= 0.665, 0.552 and REP=8.234, 7.312 respectively. The results of this research can be used to design new diarylpyrimidine compounds as HIV-1 nonnucleoside reverse transcriptase inhibitors.

Keywords: "QSAR", "Diarylpyrimidines (DAPYs)", "AIDS, particle swarm optimization", "Multiple linear regression", "Artificial neural networks"

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Combining chemometrics and the TOPSIS: a new approach to optimizing HPLC parameters using multiple-responses

Leila Mousavi[1], *Zahra Tamijia*, [2], *Mohammad Reza Khoshayand*[1,2,*]
[1]*Department of Drug and Food Control, Faculty of Pharmacy, Tehran University of Medical Sciences, Tehran, Iran*
[2]*Department of Chemometrics, The Institute of Pharmaceutical Sciences, Tehran University of Medical Sciences, Tehran, Iran*
E-mail address: khoshayand@tums.ac.ir

ABSTRACT

Some devices are used in the pharmaceutical industry to produce and control the quality of a variety of pharmaceutical products; therefore, it would be helpful to identify the factors affecting the performance of those devices and optimize them in terms of time and cost. In this regard, the use of experimental design approaches to optimization is important as it can help a device achieve its highest efficiency. One of the most popular devices in the pharmaceutical industry is high-performance liquid chromatography (HPLC). In view of its wide use in the industry and the number of factors affecting it, it is necessary to design and validate a new method that can simultaneously optimize its different parameters [1]. In this study, the method of the simultaneous optimization of the parameters was implemented using the Box-Behnken design and multiple-criteria decision-making (MCDM) by Derringer's desirability function and technique for the Order of Preference by Similarity to Ideal Solution (TOPSIS) method 2,3]. In doing so, mobile phase ratio, flow velocity, and pH were simultaneously changed, and capacity factor, total analysis time, and resolution were considered as responses [4]. To validate the method, the key parameters of the method were determined and used for all the validation steps. Therefore, this approach to optimizing HPLC factors is new and very cost-effective with diverse applications in the pharmaceutical industry.

Keywords: "multiple-criteria decision-making", "Derringer's desirability function", "experimental design", "multiple responses"

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A QSAR Study of GC-MS Retention Indecies of Essential Oils Extracted From Polygonum Minus Huds

Shokoufe Khani[1], *J.B. Ghasemi*[1]*,*, Fatemeh Ansari*[2]
[1]*Department of Chemistry, Faculty of Science, Tehran University, Tehran, Iran*
[2] *Department of Chemistry, Arak Branch, Islamic Azad University, Arak, Iran*
E-mail address: jahan.ghasemi@ut.ac.ir

ABSTRACT

A quantitative structure activity relationship (QSAR) modeling was carried out on the GC-MS retention indices of essential oils extracted from Polygonum minus Huds [1]. The usual pipeline flow chart was followed for the drawing, optimization and descriptor generation by hyperchem and dragon. Kennard-Stone algorithm was performed on the data set to diversely split the data into training and test set. Variable selection was carried out by genetic algorithm (GA) followed by model building using by partial least squares technique. Using this technique, a well-correlated model was achieved both for the training set (R2cal=0.932, RMSEC= 0.056, and R2cv= 0.824, RMSECV= 0.092) and for the test set (R2pred= 0.873, RMSEP= 0.091) the relation of the final descriptors to the endpoint values, relation indices were described and discussed.

Keywords: "QSAR", "partial least squares", "Polygonum minus Huds", "retention indecies"

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Multivariate Methods Enhanced Nontarget LC-HRMS Assessment of the River Upstream and Downstream Water Pollution Impressed by Wastewater Treatment Effluents

Reza Lotfi Khatoonabadi, *Maryam Vosough**
Department of Clean Technologies, Chemistry and Chemical Engineering Research Center
of Iran, P.O. Box 14335-186, Tehran, Iran
E-mail address: vosough@ccerci.ac.ir

ABSTRACT

Nontarget analysis is considered one of the most comprehensive tools for the identification of unknown compounds in a complex sample analyzed via liquid chromatography coupled to high-resolution mass spectrometry (LC-HRMS). Different LC-HRMS data analysis packages have been developed in the last few years to facilitate this work. However, most of these strategies involve challenging tasks of "feature" (each chromatographic peak associated with a unique m/z fragment) alignment, componentization and feature grouping to reduce data dimension effectively [1]. As an alternative to the vendor and open source software, multivariate chemometric methods have brought about great progress in processing of big data obtained from high dimensional chromatographic systems [2]. The goal of the current study is a nontarget assessment and comparison of pollution patterns of upstream river water samples with the downstream ones impressed by effluent of wastewater treatment plant (WWTP) as a case study. Here, the regions of interest (ROI) strategy was evaluated and applied to compress LC–HRMS data, then multivariate curve resolution alternating least-squares (MCR-ALS) was applied for simultaneous resolution of 18 up/downstream river water samples together with a set of blank samples, extracted using SPE method and measured by LC-Q-Orbitrap mass spectrometry in full scan data dependent acquisition mode. Then, the resolved and cleaned matrix of peak areas were subjected to ANOVAsimultaneous component analysis (ASCA) and partial least-squares-discriminant analysis (PLS-DA) for multivariate statistical investigation of significant features and differentiation and tentative identification of emerged organic contaminants in downstream water, respectively. The present work showed high potential for comprehensive evaluation of the environmental impacts of poor pollution removal during wastewater treatment in WWTPs.

Keywords: "LC-HRMS", "River Water, MCR-ALS", "ASCA, PLS-DA"

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Quantitative structure activity relationship study of azine derivatives as NNRTIs using artificial neural network

*Mozhgan Beglari *[1], Nasser Goudarzi [1], Davood Shahsavani [2], Zeinab Mozafari [1]*
[1]Department of Chemistry, Shahrood University of Technology, Shahrood, Iran
[2]Department of statistic, Shahrood University of Technology, Shahrood,, Iran
E-mail address: Biglari55@Yahoo.com

ABSTRACT

AIDS that is caused by HIV-1, threatens human life and spreads rapidly worldwide because of no effective vaccine. Non-nucleoside reverse transcriptase inhibitors (NNRTIs), that directly inhibit HIV-1 reverse transcriptase (RT) enzyme by binding to the allosteric site near the polymerase active site are highly specific, and play an important role in drug therapy [1].

In this study, QSAR model based on Bayesian Regularized artificial neural network (BR-ANN) was developed for the modeling and accurate prediction of biological activities of 73 azine (pyridone, pyrimidine, pyridine, pyridazine and triazine) derivatives as potent NNRTIs [2-4]. for this, The chemical structure of each compound was optimized using hyperchem 8.0.5 and all structures were converted to 16 drug like indexes (DLIs) using DRAGON 5.5 software and 10 molecular docking descriptors were extracted by docking the understudied compounds into the active site of the protein with the PDB codes of 3M8Q (for compounds 1 to 43) and 3MEC (for compounds 44 to 73) using the AutoDock4.2 software. Stepwise regression was applied on 26 descriptors and only 4 significant descriptors were selected and then they were used as inputs of artificial neural network. The parameters of neural network were optimized. The prediction ability of the best model was evaluated using the test set. The mean square error (MSE) and the coefficient of determination (R^2) for the test set data were 0.09 and 0.96, respectively. According to the results, the QSAR model showed superior prediction ability in the prediction of biological activities of these 73 anti HIV inhibitors.

Keywords: “Drug-like index”,” Molecular Docking”, “azine derivatives”, “Anti-HIV”,” QSAR”

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Optimization of process parameters for Paraquat and Diquat removal from binary solution by Angelica adsorbent using Box-Behnken experimental design

*Nasrin Mehmandost**, *Nasser Goudarzi, Mansour Arab Chamjangali, Ghadamali Bagherian*
Department of Analytical Chemistry, Faculty of Chemistry, Shahrood University of Technology, Shahrood, Iran
E-mail address: Nasrin0100@gmail.com

ABSTRACT

Some quaternary ammonium herbicides are known as quats, have been widely used in agricultural applications [1]. Paraquat and Diquat are toxic to humans and have been classified as moderately hazardous by the World Health Organization[2]. For drinking water, the US Environmental Protection Agency has determined a maximum contaminant level (MCL) of 20 and 3 ppm for Diquat and Paraquat respectively[3]. Natural adsorbent containing cellulose have good absorption potential for various pollutants. So plant adsorbents are affordable, accessible and environmentally friendly[4].

The present work focuses on investigating and optimizing paraquat and Diquat removal from binary aqueous solution by Angelica as low-cost adsorbent using Box–Behnken experimental design combining with response surface methodology (RSM). This adsorbent was characterized by several techniques such as Fourier transform infrared (FT-IR) spectroscopy, scanning electron microscope (SEM) and Brunauer–Emmett–Teller (BET).The design was carried out at Five independent variables, (the effect of pH ranging from 3 to 9, amount of the adsorbent ranging from 20 to70 mg, time ranging from 1 to 15, the concentration of Paraquat and Diquat ranging from 14.6 to 64.8ppm) and three-level. Then the number of experiment generated 44 experiments. Analysis of variance (ANOVA) was performed to evaluate the significant effect of independent variables on the response variable. The Statistical analysis shows that contact time was not significant. The optimal conditions for Paraquat and Diquat removal were ph=7.6, contact time t = 5 min, sorbent dose=58 mg, the concentration of Paraquat and concentration of Diquat=21ppm. R^2 = 0.97, Adjusted R^2 = 0.94 and Predicted R^2=0.86 for Paraquat and R^2 =0.98, R^2 Adjusted=0.96 and Predicted R^2 = 0.91 for Diquat were obtained. Furthermore, the isotherms and kinetics of adsorption were also explore.

Keywords: “Paraquat, Diquat”, “Optimization, Experimental design”, “Box–Behnken design”

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Adsorptive Removal of Phthalocyanine Using Nano-$CoFe_2O_4$ as a Sorbent from Aqueous Solution; Optimization and Adsorption Characterization

*Javad Zolgharnein, Mostafa Kazemi**
Department of Chemistry, Faculty of Science, Arak University, Arak 38156-8-8394, Iran
E-mail address: kazemichem1@gmail.com

ABSTRACT

Phthalocyanine dyes (PCs) are colors that are resistant to bacterial decomposition. Phthalocyanine reactive dyes are metal complexes used to produce shades of blue and blue-green and are highly water-soluble and its inefficient removal by biomass in wastewater treatment systems, leads to the formation of colored effluents [1, 2]. These high-risk colored wastewaters need to be purified before being released in nature. In the present study, magnetic cobalt ferrite nanoparticles are synthesized in an alkaline media through a co-precipitation method of cobalt chloride and ferric chloride. The acquired Cobalt Ferrite nanocomposite was characterized by FT-IR, FE-SEM, EDX, and XRD analyses. The ability of cobalt ferrite nanoparticles (CFNs) for the adsorption of PC has been investigated. The effects of pH, adsorbent dosage, contact time and initial dye concentration on the PC removal percentage were investigated. Implementing a response surface methodology (RSM) leads to an empirical mathematical model related to the percentage of removal (% R) absorbed with its effective variables and their interactions. In order to achieve maximum removal efficiency, using the box-Behnken design (BBD), the effects of the initial concentrations of PC, dosage of sorbent, pH, and contact time, modeling and optimization were performed. Significances of various parameters and the model obtained has been evaluated by analysis of variance (ANOVA). Absorption isotherms can be used to calculate the absorption capacity at equilibrium state for each adsorbent; therefore, the Langmuir, and Freundlich models were applied to describe the adsorption of PC on to $CoFe_2O_4$. The adsorption isotherm experiments were conducted at the optimum adsorbent mass, optimum pH. Langmuir isotherm successfully describe the equilibrium behavior of Cobalt Phthalocyanine by nano-$CoFe_2O_4$ adsorbent. To investigate the adsorption of Cobalt Phthalocyanine on the $CoFe_2O_4$ surface various kinetic models have been proposed to examine the controlling mechanism of adsorption process. In this study, the adsorption kinetics of dye onto $CoFe_2O_4$ was examined by two models of pseudo-first-order, and pseudo-second-order, at the optimum condition .The data did not fit well to the first-order equation in the entire region of Cobalt Phthalocyanine concentration used in this work, but it did fit very well with the pseudo-second-order model and the computed q_e values also consistent well with the experimental data. These results indicate that the overall rate of the Cobalt Phthalocyanine adsorption process appears to be controlled by the chemical adsorption or chemisorption process.

Keywords: "$CoFe_2O_4$ nanoparticles", "Adsorption", "Dye removal", "Box-Behnken design"

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On MCR-BANDS and FACPACK under unimodality constraints

Somaye Vali Zade[1], *Klaus Neymeyr*[2], *Hamid Abdollahi*[*1,] *Mathias Sawall*[3]

[1] *Institute for Advanced Studies in Basic Sciences (IASBS)*
[2] *Universität Rostock, Institut für Mathematik, Ulmenstrasse 69, 18057 Rostock, Germany*
[3] *Leibniz-Institut für Katalyse, Albert-Einstein-Strasse 29a, 18059 Rostock, Germany*
E-mail address: abd@iasbs.ac.ir

ABSTRACT

Multivariate curve resolution methods suffer from non-unique solutions. Due to the rotational ambiguity there is often a range of feasible solutions for the decomposition of the data set. This ambiguity is covered in a low-dimensional way by the so-called area feasible solutions (AFS-sets). Several methods have been proposed for the estimation of the AFS-sets. One of them is the polygon inflation algorithms, implemented in FACPACK [1]. Another method in order to analyze the rotational ambiguity of spectral data is the MCR-BANDS method [2] that provides an easy and flexible estimation of the extension of the ambiguity for any number of components and different types of constraints. In this work, results obtained by MCR-BANDS are compared with the AFS-sets obtained by FACPACK. In particular we apply both approaches only with nonnegativity constraints as well as with nonnegativity and unimodality constraints. For a three-component model problem we demonstrate how the MCR-BANDS solutions shift from the boundary of the AFS-sets by nonnegativity constraints to the boundary of the AFS-sets by nonnegativity and unimodality constraints.

Keywords: “Multivariate curve resolution”, “self-modeling curve resolution”, “area of feasible solutions”, “FACPACK”,” MCR-BANDS”, “unimodality constraint”

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Designing an IDA-based sensor array including a single indicator and receptor with multiple concentrations for quantitation of mixtures

Vahideh Mahram, Somaiyeh Khodadadi Karimvand, Hamid Abdollahi *
Faculty of Chemistry, Institute for Advanced Studies in Basic Sciences, Zanjan, Iran
E-mail address: abd@iasbs.ac.ir

ABSTRACT

A chemical sensor is a device that converts an input signal into a readable output signal. Nowadays, chemosensors have found a wide variety of applications in the fields of chemical detection. One of the important categories of chemical sensors includes sensors working based on the competitive displacement between species. The basis of numerous competition-based sensors is the Indicator Displacement Assays (IDA) approach being principally well explored by the Anslyn groups [1]. In a competitive IDA approach, an indicator is first reversibly bound to a receptor. In the presence of a competitive analyte with higher-affinity binding to the receptor, a displacement reaction takes place, leading to the release of the indicator in the system. As a result, the optical signal of the system changes. Based on the IDA principles, the binding affinity between the analyte and the receptor must be higher than that between the indicator and the receptor. In our research group, it was shown that, for simultaneous analysis it is possible to obtain two or more different compositions of two analytes with identical signals. Utilizing sensor arrays with at least two IDA sensor elements and different competitive equilibrium behavior can be a logic solution. There are several ways to modify the equilibrium behavior of sensor elements. One of them is to change the total concentration of involved components. In this way, the spectroscopic response of each sensor element would be different for a given mixture composition. Finally, the results reveal unique responses of sensor arrays for the mixture compositions. The efficiency of the proposed strategy for designing a simple sensor array is evaluated for simultaneous quantification of Sulfate and Phosphate [2]. In this work, the 1-(2-Pyridylazo)-2-naphthol (PAN) is used for indicator and Pb^{2+} metal ion as receptor. Also, Radial Basis Function Neural Network (RBFNN) and Partial Least Squares (PLS) methods were applied for quantitative analysis.

Keywords: "Simultaneous determination", "Indicator-Displacement Assay (IDA) " , "Sensor array," "Radial Basis Function Neural Network (RBFNN) ", "Partial Least Squares (PLS) " ,"Quantitation of mixtures" ,"Phosphate and Sulfate"

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Probing the binding mechanism of Nilotinib to bovine α-lactalbumin using spectrometric method, molecular docking

Fatemeh Bagheri *, *Mohammad Hossein Fatemi*
Laboratory of chemometrics, Faculty of chemistry, University of Mazandarn Babolsar, Iran
E-mail address: Bshimi999@email.com

ABSTRACT

Drug interaction with α-lactalbumin significantly affects in vivo drug transport Breast milk. Nilotinib (NIL), is a new, orally bioavailable, amino-pyrimidine-derived tyrosine-kinase inhibitor[1]. a-Lactalbumin (a-LA) is a protein present in the milk of all mammals. Its molecular weight is 14.2 kDa and its isoelectric point is between 4.2 and 4.5[2]. Under native conditions, the tertiary structure of a-LA is composed of a large domain (α) and a small domain (β) divided by a cleft. It comprises eight cysteines which form four disulfide bridges[3] and showed that the a-LA molecule contains one strong binding site for Ca2+ and a weaker binding site for Zn2+. To gain insight into the binding mechanisms of tyrosine-kinase inhibitor nilotinib (NIL) to (BLA), an approach combining an approach, steady-state fluorescence quenching, and molecular modeling was adopted. The association behavior of nilotinib was investigated at its various concentrations and using BLA concentration of 10μM in aqueous phosphate buffer (pH=7.4).in 297 K. To estimate the character of the binding between studied quencher and BLA the Stern–Volmer method were used. The fluorescence spectroscopic results revealed that nilotinib could effectively quench the intrinsic fluorescence of BLA. The binding affinity (KA) and the number of binding sites (n) between nilotinib and BLA at 297 K were estimated 5.01*105 L_mol-1 and 1 respectively. Modeling Molecular modeling was performed using a Lamarckian genetic algorithm implemented in Auto Dock 4.2 program package.The structure of NIL was illustrated using Hyper chem optimized using the AM1 semi-empirical method . The BLA crystal structure was obtained from the Brookhaven Protein Data Bank. The protein–ligand complex was visualized and analyzed using Auto Dock Tools also ΔG obtained from this method corresponds to the spectroscopic methods.

Keywords: “Nilotinib”, “bovine α-lactalbumin”, “fluorescence spectroscopy”, “Molecular docking”,”tyrosine-kinase inhibitor”, “Stern–Volmer”

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Analysis of residual moisture in a freeze-dried sample drug by multivariate fitting regression method

<u>Mahsa Akbari Lakeh</u>[1, 3]*, Somayeh Khodadadi Karimvand*[1]*, M. Khoshayand*[2, 3]*, Hamid Abdollahi*[*1,3]*,*

1. Faculty of Chemistry, Institute for Advanced Studies in Basic Sciences, P.O. Box 45195-1159, Zanjan, Iran

2. Department of Drug and Food Control, Faculty of Pharmacy, Tehran University of Medical Sciences,

3.Department of Chemometrics, The Institute of Pharmaceutical Sciences(TIPS), Tehran University of Medical Sciences,

E-mail address: abd@iasbs.ac.ir

ABSTRACT

The moisture content of many pharmaceutical products, like some type of vaccines and lyophilized drugs, is one the most important quality control parameters in the product qualification and drug attributes. Freeze-drying is a widely applied technique for the preservation and storage of such products. Karl Fischer titration is the standard method for the determination of residual moisture in freeze-dried samples, though this is a time-consuming and destructive method that requires the handling of organic solvents. Instead, Near-infrared (NIR) spectroscopy is a fast and non-invasive method that is well suited to the measurement of water due to the strong adsorption band of water in NIR. The determination of moisture content by NIR spectroscopy in both transmittance and reflectance modes have been described in literatures [1]. In this study multivariate fitting regression with Gaussian function (MFRG) [2] is used to predict the water content of a freeze-dried sample drug from NIR spectra. Also, the prediction performance of the MFRG was compared to the results of the well-known PLS method. Several simulated datasets and an experimental data were used to evaluate the performance of the MFRG method. In the case of experimental data, a number of mathematical pre-treatments were applied to check whether they lead to better models or not. It is found that, in nearly all the examined cases, the MFRG model performance was comparable or better than the PLS regression method. This is due to fact that MFRG models nonlinearity better than the PLS method. It is further found that the untreated data lead to a more robust model while the pre-treatment methods did not improve the model significantly.

Keywords: “Water determination”, “freeze-dried pharmaceuticals” ,,“near-infrared spectroscopy” “Karl Fischer titration” ,“multivariate fitting regression with Gaussian function”

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Metabolomic study of the effects of parabens and pharmaceuticals in recycled water on metabolic pathways of lettuce using NMR and GC-MS followed by chemometric techniques

*Neda Feizi, Mahsa Seraj, Reyhane Shavandi, Nastaran Nikzad, Hadi Parastar**
Department of Chemistry, Sharif University of Technology, Tehran, Iran
E-mail address: h.parastar@sharif.edu

ABSTRACT

A great number of integrated water resource management schemes are being implemented with focus on utilization of non-conventional water resources, such as treated wastewater (TWW) [1]. TWW may contain undesirable chemicals such as contaminants of emerging concern (CECs). Plant metabolomics aims to study the plant system at the molecular level to provide a non-biased characterization of the metabolome of a plant's tissue in response to its environment [2]. In this study, a non-targeted metabolomic analysis was performed on lettuce exposed to nine CECs by irrigation and the subsequent changes have been traced comprehensively by nuclear magnetic resonance (NMR) and gas chromatography-mass spectrometry (GC-MS) and the huge amount of acquired data was analyzed by chemometric techniques. Lettuce seedling was planted in pots and watered with Hoagland solution. The plants were watered with mixture of CECs 30 days after the transplantation of seedlings for 33 days under controlled conditions. This dataset contains three doses groups consist of: low dose (10 µg L^{-1}), medium dose (50 µg L^{-1}) and high dose (100 µg L^{-1}) and a control sample. Each dose group consists of three replicates. Samples were collected three, four and five weeks after exposure to CECs. After sampling, the leaves were comminuted with liquid nitrogen and stored at -20°C until analysis. The extraction of metabolites was performed as reported elsewhere [2]. For NMR analysis, 550 µL of D_2O was added to the dry residue and the analysis was performed. For GC-MS analysis, 100 µL of 30 µL of N-methyl-N-(trimethylsilyl) trifluoroacetamide (MSTFA) with 1% trimethylchlorosilane (TMCS) was added to the dry residue and the mixture was injected. The NMR and GC-MS data of control and exposed samples were arranged in a data matrix and then analyzed using principal component analysis (PCA), partial least squares-discriminant analysis (PLS-DA) using variable importance in projection (VIP) and ANOVA-simultaneous component analysis (ASCA). The metabolic response indicates that exposure to CECs at environmentally relevant concentrations causes large metabolic alterations in plants (carbohydrate metabolism, TCA cycle, pentose phosphate pathway and glutathione pathway) linked to changes in morphological parameters.

Keywords: "Metabolomics", "Chemometrics", "NMR", "GC-MS", "CEC", "ASCA"

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Response surface modelling by using principal component analysis followed by partial least squares for optimizing efficient factors in micro-solid phase extraction of polycyclic aromatic hydrocarbons in oil spills

Nazanin Saburouh[1,2], *Ali Jabbari*[2], *Hadi Parastar**[,1]

[1] *Department of Chemistry Sharif University of Technology, Tehran, Iran,*

[2] *Department of Chemistry, K. N. Toosi University of Technology, Tehran, Iran*

E-mail address: h.parastar@sharif.edu

ABSTRACT

Nowadays oil pollution is an important problem for human and environment[1]. In this respect, the purpose of this study was removal and measurement of remaining pollutants using reduced grapheme oxide (rGO) synthesized using two different methods [2]. rGO was characterized using SEM, TEM and Raman spectroscopy. After separating the oil from the water using rGO, the amount of residual oil pollution dissolved in water was determined using rGO. For this purpose, mixture of seven polycyclic aromatic hydrocarbons (PAHs) was used as model compounds for optimizing absorption and desorption processes. Consequently, a monitoring method based on the micro solid phase extraction (µ-SPE) was developed and was analyzed using gas chromatography (GC). The six extraction factors of sorbent amount, sorbent volume, sample volume, desorption volume, extraction time and salt concentration were designed using central composite design (CCD) and were optimized by scores of principal component analysis (PCA) as a novel response factor for multi-response optimization. On this matter, 54 runs of experimental design resulted in a matrix of responses having 7 columns (the areas of the 7 peaks of analyte). The scores of the first PC on which all the variables had positive loadings and which was explaining a very high percentage of the total variance (i.e., 92.2%), was used as a response vector for optimizing the extraction factors. All the statistical parameter were improved for model obtained by the principal components with no preprocessing. For instance, R^2 increased from 0.53 to 0.75 for calibration and validation set. Also, mean-centering, auto-scaling, pareto-scaling and normalization was tested to develop a desirability function to include the response of seven analyte peak areas, but none of them had better result than PCA. Then, PLSR was used for quantitation of seven target PAHs in the presence of uncalibrated interferences. In this regard, calibration set for external calibration strategy was randomly designed in concentration range 0.1-100 ngmL^{-1}. Then, multivariate analytical figures of merit (AFOM) including sensitivity (SEN), selectivity (SEL) and limit of detection (LOD) were calculated. In all cases, the AFOMs were in acceptable ranges. It is concluded that the present multi-stage analytical strategy using rGO as an effective absorbent in combination with chromatography and chemometrics in order to remove oil spills from water and investigate the residual oil pollution in water.

Keywords: “Oil spill”, “rGO”, “µ-SPE”, “GC-FID”, “PCA”, “Experimental Design”, “Chemometrics”.

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PLS-DA vs. Q/LDA for classification of isotope ratio mass spectrometry data: a new way for food authentication

Ali Ghiasi[1]*, Arash Rabiee*[2]*, Hadi Parastar**[1]
[1]*Department of Chemistry, Sharif University of Technology, Tehran, Iran*
[2]*Department of Chemistry, Arak University, Arak, Iran*
E- mail: h.parastar@sharif.edu

ABSTRACT

Isotope ratio mass spectrometry (IRMS) of five bio-elements (H, C, N, S and O) has been reported as an alternative tool for food quality control. Isotopic profile has been used as a descriptor to establish differences between products for classification and authentication purposes [1]. The choice of the most appropriate classification technique depends on many factors including class criteria definition, homogeneous sample distribution, number of input variables and number of samples. Therefore, it is a common practice to apply more than one classification technique and evaluate their fitness for the problem under study [2]. The objective of this work was to propose elemental analysis (EA)-IRMS and gas chromatography (GC)-IRMS fingerprinting combined with chemometrics for authentication of saffron provided from main regions of Iran. In this regard, performance of frequently used classification models including partial least squares-discriminant analysis (PLS-DA) vs. linear discriminant analysis (LDA) and quadratic discriminant analysis (QDA) were studied in details. For this reason, three main classification model parameters including accuracy (acc), specificity (spe) and sensitivity (sen) were taken into account. Sixty-two saffron samples were provided from Khorasan province. For EAIRMS, the samples were powdered and then analyzed for measuring bulk carbon and nitrogen isotope ratios. Saffron metabolites were also extracted using ultrasonic-assisted extraction-dispersive liquid-liquid micro extraction (UAE-DLLME) before GC-IRMS. To gain GC-IRMS data, first, baseline was corrected using asymmetric least squares (AsLS) and elution time shifts were corrected using interval correlation optimized shifting (iCOShift). After that, eleven major peaks were chosen to obtain the components delta for GC-IRMS. As the class labels were not in accordance with the chemical composition of samples, then, the data matrix of EA-IRMS and GC-IRMS was clustered by principal component analysis (PCA) and hierarchical cluster analysis (HCA) and the number of classes by these two methods were considered for supervised classification. As a consequence, the best classification performance was observed for QDA with four classes (sen, spe and acc values were higher than 95.0%). In other words, it was seen that the best PLS-DA and LDA performance was observed for two classes but for more than two classes, the accuracy drops suddenly from ~92.0% to ~85.0%. In summary, QDA showed better performance for classification of EA-IRMS and GC-IRMS of saffron samples.

Keywords:“LDA”, “QDA”, “PLS-DA”, “IRMS”, “Adulteration”, “Saffron”

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Multiple response optimization of simultaneous biosorption of methylene blue and fuchsin acid by green alga Ulva fasciata

Reza Tabaraki, Mohsen Azadbakht, Mina Khodabakhshi*
Department of Chemistry, Faculty of Science, Ilam University, Ilam, Iran
E-mail address: rezatabaraki@yahoo.com

ABSTRACT

In response surface methodology (RSM), data is obtained from experimental design; different mathematical models are fitted to the experimental results, statistical techniques used to model verification and interactions between variables and responses studied. Finding the optimal conditions for a single response is relatively simple. However, in many situations, several responses must be simultaneously optimized. In multicriteria methodology, RSM is combined with the Derringer's desirability function. This function transforms a several response variables into a single response case (desirability value), which can be optimized by univariate techniques [1]. Algae as renewable natural biomass exhibit different affinities toward different metals and dyes. Uptake capacities of certain marine and river algae are reported to be much higher than agriculture wastes, natural zeolite and synthetic ion-exchange resin [2]. In this work, simultaneous biosorption of methylene blue and fuchsin acid by a green alga Ulva fasciata was optimized using multiple response optimizations and Box-Behnken experimental design. Biosorbent dose [X_1], pH [X_2] and contact time [X_3] were independent factors and biosorption capacities of dyes in mixture were response variables. The levels of the variables were selected according to the preliminary studies. Initial concentration of methylene blue and fuchsin acid in mixture was 5.0×10^{-5}M. The concentration of methylene blue and fuchsin acid were analyzed using an UV/Vis spectrophotometer at 664 nm and 554 nm, respectively. A quadratic polynomial equation was fitted to experimental data and terms significance were computed by analysis of variance (ANOVA). The optimum condition for simultaneous biosorption of these dyes was: biosorbent dosage 0.1 g L^{-1}, pH 10 and contact time 90 min with maximum overall desirability of 0.977. The maximum uptake capacities of Ulva fasciata for methylene blue and fuchsin acid were 0.340 and 0.354 mmol/g at optimum conditions, respectively. The Langmuir and Freundlich isotherm models were fitted to biosorption equilibrium data and the Freundlich isotherm was the most suitable model. Kinetic results indicated that in the optimum conditions, dyes biosorption better described with the second-order kinetic model. FT-IR analysis showed that biosorption of dyes is related to COOH, OH, SO_3 and NH_2 functional groups on the cell wall of biomass. Biosorption capacity of Ulva fasciata and other biosorbents were also compared.

Keywords: “Multiple Response optimization”, “Box-Behnken design”, “Biosorption”

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Principal component-adaptive neuro-fuzzy inference systems for the QSPR modeling of CMC of anionic gemini surfactants

Reza Tabaraki, Mina Khodabakhshi*
Department of Chemistry, Faculty of Science, Ilam University, Ilam, Iran
E-mail address: rezatabaraki@yahoo.com

ABSTRACT

Quantitative structure property relationships (QSPR) were developed for prediction of critical micelle concentration of anionic gemini surfactants. Data set consisted of 85 experimental critical micelle concentrations of anionic Gemini surfactants. The -log [CMC] was used as dependent variable. The data set was randomly divided into training (60 molecules) test (15 molecules) and validation sets (10 molecules). All molecules were drawn in the HyperChem 6 software and their molecular structures were optimized by semi-empirical AM1 method using the Fletcher–Reeves algorithm until the root mean square gradient was 0.01. The resulted geometry was loaded into Dragon software to calculate 1497 descriptor in 18 different classes. Then, all descriptors with zero or same values for all the molecules in the training set were eliminated. Co-linearity of the descriptors were calculated and one of the two descriptors which had the pairwise correlation coefficient above 0.9 ($R > 0.9$) and a large correlation coefficient with the other descriptors was eliminated. Finally, 386 descriptors were remained for next section. Modeling of the relationship between selected descriptors and cmc was achieved by genetic algorithm–partial least squares (GA–PLS) as linear model and principal component-adaptive neuro-fuzzy inference systems (PC-ANFIS) as nonlinear model. 21 molecular descriptors were selected as the most feasible descriptors for prediction of cmc in GA–PLS. The optimum PLS model had three latent variables. The predicted residual error sum of squares was 2.182. The principal component analysis (PCA) was applied to twenty one PLS descriptors for dimensional reduction and the scores of the PCs were selected as inputs. The ranked PCs were then entered into the ANFIS model successively. The best ANFIS model was obtained with four inputs. The root mean squares error (RMSE) for training, test and validation sets was 0.386, 0.668 and 0.617, respectively [1].

Keywords: "Adaptive neuro-fuzzy inference system", "GA–PLS", "anionic gemini surfactants"

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QSPR model for adsorption of organic compounds by multi-walled carbon nanotube (MWCNT): Comparison between MLR and ANFIS

*Aboozar Khajeh**
Department of Chemical Engineering, Birjand University of Technology, Birjand, Iran.
E-mail address: akhajeh@birjandut.ac.ir

ABSTRACT

Carbon nanotubes (CNTs) have attracted great attention in various area due to their special chemical and physical properties. Due to the large surface area, the CNTs can be considered as promising adsorbents. However, many experimental studies have been done for CNT adsorption of many common organic compounds, theoretical models to prediction the CNT adsorption of new compounds, instead of expensive and complicated experiments, is necessary. Quantitative structure-property relationship (QSPR) is a proper approach to understand the relationships between adsorption coefficients and molecular properties of compounds. In the present study, in order to developing QSPR model for prediction the MWCNT adsorption of organic compounds, a data set of diverse molecules were collected from [1]. After optimization the molecular structure of each compound, the descriptors were calculated by using Dragon software. The modified particle swarm optimization-multiple linear regression (MPSO-MLR) [2, 3] as a proper computational method was used for descriptor selection and linear model developing. By using MPSO-MLR following novel and efficient model was developed:

$$LogK = 0.1845 \times MLOGP2 + 0.8388 \times H\text{-}048 + 0.3020 \times C\text{-}001 + 0.1624 \times Mor02m - 3.0423 \times Depressant\text{-}80 - 2.6013$$

$N=68$; $R^2 = 0.7970$; $R^2_{adj} = 0.7806$; $Q^2_{LOO} = 0.7536$.

The standardization of the regression coefficients, indicates *MLOGP2* is the most important descriptor in the developed model. Therefore, it is suggested that the hydrophobic character of a compound, is the most important factor affecting its adsorption on MWCNT. For considering the nonlinear behaviour of selected molecular descriptors by MPSO-MLR, a nonlinear model developed by adaptive neuro-fuzzy inference system (ANFIS) to get the best fit of response data. The ANFIS model produced good results according to the squared correlation coefficient (R^2) and the root mean squares error (*RMSE*) values, which were 0.8727 and 0.4264, while the R^2 and *RMSE* for the linear model were 0.797 and 0.5386. Therefore the accuracy of developed model by ANFIS is higher, however the MPSO-MLR linear model is simpler and more interpretable.

Keywords: “QSPR”, “Adsorption”, “Multi-walled carbon nanotube”,” MLR”, “ANFIS”

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Particle swarm optimization with various mutations for descriptor selection in QSPR studies

*Aboozar Khajeh**
Department of Chemical Engineering, Birjand University of Technology, Birjand, Iran.
E-mail address: akhajeh@birjandut.ac.ir

ABSTRACT

Quantitative structure-property relationship (QSPR) is a promising approach for correlating the physical and chemical properties of materials to their molecular structures. One of the main important steps in the QSPR modelling process is the selection of the most relevant of descriptors from a pool of descriptors calculated from optimized structure of molecules. Several stochastic search algorithms such as ant colony optimization, simulated annealing and genetic algorithm were used for descriptor selection in QSPR studies. The particle swarm optimization (PSO) is another stochastic algorithm that can be applied to variable selection. Due to some drawback of original PSO such as premature convergence and plunge into a local optimum, various modifications have been suggested to improving its performance. In our previous works [1, 2] a mutation operator were proposed to modification of PSO and were successfully used for prediction Gibbs energy and entropy of formation of organic compounds. In this work two other mutation operators were used to modification of PSO as follows:

$X_{mut} = G_{best} + rand(\cdot) \times (X_{m1} - X_{m2})$ $\qquad$ $X_{mut} = X_{m1} + rand(\cdot)$

The new modified particle swarm optimization methods, incorporated with multiple linear regression (MLR) were employed to descriptor selection in QSPR modelling of the liquid heat capacity of alcohols as a case study. The heat capacity is one of the most important thermo-physical properties of compounds used in various area of studies. The obtained results indicated that the previous mutation operator $X_{mut} = X_{m1} + rand(\cdot) \times (X_{m2} - X_{m3})$ is the most efficient mutation operator, however the new mutation operators improved the original PSO. Moreover based on data collected from [3] the best following equation for prediction the liquid heat capacity of alcohols was derived:

$Cp = 8.3224 * TIC0 + 108.6048 * E2s + 22.9557 * Lop + 14.3471$
$N=106;\ R^2= 0.9241;\ R^2_{adj} = 0.9219;\ Q^2_{LOO}= 0.9166.$

The squared correlation coefficient of 0.92 for 26 test data, show that the proposed model can be used for prediction the liquid heat capacity of new alcohols with high accuracy. Analysis of selected descriptors suggest that the molecular branching and size of alcohols is the most important factor affecting their liquid heat capacity.

Keywords: “QSPR”, “Particle swarm optimization”, “Heat capacity”, “Mutation”, “Descriptor selection”

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Classification of three ground meat species using FTIR and chemometrics method

Abolfazl Dashti[1], Hassan Yazdanpanah [1, 2], Farzad Kobarfard [2, 3], Hadi Parastar[4], Bahram Daraei[1]*
[1]Department of Toxicology and Pharmacology, School of Pharmacy, Shahid Beheshti University of Medical Sciences, Tehran, IR Iran.

[2] Food Safety Research Center, Shahid Beheshti University of Medical Sciences, Tehran, IR Iran.
[3] Department of Medicinal Chemistry, School of Pharmacy, Shahid Beheshti University of Medical Sciences, Tehran, IR Iran.

[4] Department of Chemistry, Sharif University of Technology, Tehran, Iran
E-mail address: farzadkf@yahoo.com

ABSTRACT

The analysis of food authenticity and the detection of adulteration are major issues in the food industry and are attractive for consumers. Concerns about meat authenticity are increasing recently, due to great fraud scandals [1]. In the present research, the feasibility of diffuse reflectance infrared Fourier transform Spectroscopy (DRIFTS) (MIR; 4000 – 650 cm-1; 2500-15384 nm) in combination with chemometrics was used for meat speciation of beef, chicken and pork. Spectral data were pre-processed using different techniques and explored by a Principal Component Analysis (PCA) to find out differences among pure samples. Partial Least Squares Discriminant Analysis (PLS-DA) with Median Center and 2nd derivative (21) (Savitzky–Golay) was used for meats classification. Meat samples of beef (19 foreshank and hind shank samples) and chicken (30 breast and drumstick samples) were collected from local butchers in Tehran and Yazd cities, IR Iran in 2019. Thirteen pork samples (from different parts of body) were collected from different countries in 2019. Samples were first cleaned, removing the remaining skin and fat that could interfere in the analysis, and they were minced by a Moulinex (1000 W) mincer to homogenize them. Due to the high percentage of moisture in meat and the high intensity absorbance of the bands that appeared with the vibration of the water bonds, samples were dried in order to be able to observe the specific bands from protein and lipids in more detail. The samples were dried with freeze-dryer for 24 h. The spectra were recorded as transmittance values at each data point from 650 to 4000 cm−1 at a resolution of 8 cm−1. The spectra of each sample were taken as an average of 60 successive scans. Measurements are calibrated against the background gold. Spectral datasets were divided into calibration (70%) and validation (30%) sets with duplex algorithm. For PLS-DA model, sensitivity and specificity values in the validation set were 89% and 100% for beef, 100% and 100% for chicken, and 100% and 94% for pork, respectively. The overall accuracy of the method was 95%. In summary, a combination of infrared spectroscopy technology with PLS-DA can be used as an effective method to identify beef, chicken and pork meat samples.

Keywords: “FTIR”, “Meat”, “chemometrics”

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Analysis of U and Th in Mahneshan soil samples by ICP-MS and Geochemometrics

Somayeh Veyseh[1*] *Ali Niazi*[2], *Shabnam Najafi Aslipashaki*[1]
[1] *Geological research center of geological survey and mineral explorations Country Alborz*
[2] *Arak Branch, Islamic Azad University, Arak, Iran*
E-mail address: somayeh.veyseh@gmail.com

ABSTRACT

In this study inductively coupled plasma mass spectrometry was used to determine the uranium and thorium composition of 180 soil samples of Mahneshan in Zanjan province. Cluster analysis (CA) and principal component analysis (PCA) were used for multivariate statistical modeling of the input data. CA displays the object similarity [1]. Sample digestion was done according to ASTM D4698 by fusion methods [2]. Analyzes revealed an excellent separation between soil samples according to their type with the efficiency of LDA model as 100%. Analysis was done by ICP-MS and resulted data were processed by Geochemometrics methods. In conclusion, this study achieved satisfactory discrimination among soil samples from Mahneshan region of Iran by uranium and thorium analysis using ICP-MS. Distribution of samples was studied according to the Score plots of the first and second principle components. The data obtained and related to concentrations of elements in different soil samples was used for their classification by means of the pattern recognition.

Keywords: “Geochemometrics”, “ICP-MS”, “U, Th, K_Nearrest Neighbor (KNN)”, “Mahneshan”

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Analytical Figures of Merit for Feasible Solutions of Second-Order Calibration methods

Fariba Norouz Yeganeh[1], *Hamid Abdollahi*[2], *Morteza Bahram*[1].
[1] *Department of Analytical Chemistry, Faculty of Chemistry, Urmia University, Urmia*
[2] *Institute for Advanced Studies in Basic Sciences (IASBS)*
Email address: abd@iasbs.ac.ir

ABSTRACT

Figures of merit are numerical parameters that help to characterize the performance of a device or a system relative to alternative ones. The search for new ways to improve analytical figures of merit is an important driving force in modern analytical chemistry research, with the sensitivity and selectivity occupying one of the prominent places among these figures. analytical sensitivity, which is important for the comparison of methodologies based on widely different signals, because it is independent of the instrument and technique applied; selectivity, which helps to assess the possibility of analyte quantitation in the presence of interferences [1]. Different approaches have been proposed during recent years to improve the results obtained by soft methods, particular multivariate calibrations. However, univariate model predictions for unknown samples are only reliable if the signal is sufficiently selective for the analyte of interest. By contrast, multivariate calibration methods may produce valid predictions also from highly unselective data. But among them studies on circumstances that result in unique answers are of particular importance. As we know, results obtained by model-free methods often are complicated by rotational ambiguity, meaning that a range of feasible solutions describing and fitting experimental data equally well and fulfilling the constraints of the system are possible. Thus, when a soft-modeling method is used as a tool in analyzing a system, checking the range of the feasible solution and evaluating the error prediction range is highly recommended [2]. In order to analysis of the effect of rotational ambiguity in the accuracy of the analytical sensitivity, the systematic grid search minimization algorithm in two component chromatography system with high profile overlapping in the instrumental data modes was employed. Sensitivity was calculated for all points in feasible solution. It was demonstrated that sensitivity is different for every feasible solutions.

Keywords: “Analytical Figures of Merit”, “Feasible Solutions”, “Rotational ambiguity”, “Second-Order Calibration”

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Preparation of Magnetic Molecularly Imprinted Polymer coated Multi-Walled Carbon Nanotubes for Ultra-Detection of Sotalol: An Experimental Design Study

*Saeedeh Ansari, Saeed Masoum **
Department of Analytical Chemistry, Faculty of Chemistry, University of Kashan, Kashan, Iran
E-mail address: masoum@kashanu.ac.ir

ABSTRACT

Sotalol (SOT) is a chiral β-adrenoceptor antagonist marketed in a racemic form, which is used in individuals with rhythm disturbances (cardiac arrhythmias) of the heart, and is employed to treat hypertension in some individuals [1]. The measurement of SOT in plasma offers useful information in the study of possible pharmacokinetic interactions with other drugs and also for clinical drug-based studies in cases of intoxication in controlling the therapy compliance of the patients [2]. In this work, a magnetic molecularly imprinted polymer-coated multiwalled carbon nanotube (MWCNT-MMIP) was pre-designed using a computational approach and synthesized for selective extraction and preconcentration of SOT in biological fluid samples. The MWCNT-MMIP and non-imprinted polymer were characterized by Fourier transform infrared spectroscopy (FTIR), transmission electron microscopy (TEM), and vibrating sample magnetometry (VSM). The screening of ultrasonic-assisted dispersive solid-phase microextraction (UA-DSPME) was preliminary performed by Plackett-Burman design (PBD) and subsequently, central composite design (CCD) under response surface methodology (RSM) was used individually for evaluation of the significant factors and their possible interaction effects on the adsorption process. Under optimized conditions, the SOT was selectively and effectively extracted in real biological samples and good linearity was obtained with correlation coefficients (R^2) over 0.996 and the detection limit (S/N=3) was 0.31 ng/mL. The maximum adsorption capacity of SOT using MWCNT-MMIPs was calculated as 79.36 mg/g. The average recoveries of the spiked human plasma samples at four concentration levels of SOT ranged from 97.40-101.60 percent, and the relative standard deviation was found to be lower than 4.50%. Combined with high performance liquid chromatography analysis, the MWCNT-MMIPs were used to UA-DSPME of SOT in biological fluid samples.

Keywords: "Central composite design", "High performance liquid chromatography", "Human plasma, Molecularly imprinted polymer", "Multi-walled carbon nanotube", "Sotalol"

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Application Constant center and Ratio difference Methods for Simultaneous Determination of m-nitroaniline and p-nitroaniline whit high overlapping spectra

Fatemeh Mosayebi, *Ghadamali Bagherian*[*], *Mansour Arab Chamjangali, Motahare S. Ashrafi*

College of Chemistry, Shahrood University of Technology, Shahrood, Iran
E-mail address: fmosayebi2017@yahoo.com

ABSTRACT

Nitroanilines are important intermediates or precursors in the synthesis of azo dyes, antioxidants, fuel additives, pharmaceuticals, and pesticides [1]. They are strongly toxic and are now widely considered as potential carcinogens, and most of them have been included in the list of priority pollutants in many countries [2]. They can be released into the environment directly as industry waste or indirectly as breakdown products of herbicides and pesticides. Due to their solubility in water, anilines can readily permeate through soil and contaminate ground water. They can be taken up by humans via the skin, respiratory tract, and gastrointestinal tract [3]. Since isomers usually possess similar physical and chemical properties, their separation is one of the most challenging areas of separation science. Two simple and accurate spectrophotometric methods manipulating ratio spectra were developed and validated for the simultaneous determination of m-nitroaniline and p-nitroaniline in their binary mixture without prior separation. Method A is a constant center (CC) spectrophotometric method and method B is a ratio difference (RD) spectrophotometric one [4]. Linear correlations were obtained in the range of 5.00-60.0 mg/L for m-nitroaniline and 1.00-10.0 mg/L for p-nitroaniline. Both the RD and CC methods were successfully applied to determine the concentration of both nitroaniline isomers in water samples.

Keywords: **“**m-nitroaniline”, “p-nitroaniline”, “Constant center”, “Ratio difference”

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QSAR Study of New 1H-Pyrrolo [3, 2-c] Pyridine Derivatives against Melanoma Cell Lines by Firefly Algorithm-Support Vector Machine (FF-SVM)

*Mehdi Nekoei**,1, *Seyed Mohammadreza Motalebi Tabaei*[2]
[1]*Department of Chemistry, Shahrood Branch, Islamic Azad University, Shahrood, Iran*
[2]*Department of Biochemistry,Shahrood Branch, Islamic Azad University, Shahrood, Iran*
E-mail address: m_nekoei1356@yahoo.com

ABSTRACT

Melanoma is the most aggressive form of skin cancer. It is a malignant tumor that arises from melanocytic cells. The major risk factors for development of melanoma include exposure to solar ultraviolet irradiation, fair skin, dysplastic nevus syndrome, and a family history of melanoma. Melanomas can metastasize either by the lymphatic or by the hematogenous route [1]. Metastatic melanoma is a particularly aggressive form of cancer that is resistant to standard anticancer therapies. Quantitative structure–activity relationship (QSAR) models were developed for predicting activity of a series of pyridine derivatives against A375P human melanoma cell line. The suitable set of the molecular descriptors was calculated and the important descriptors using the firefly algorithm (FFA) as a new method of variable selection were chosen. Firefly algorithm is classified as swarm intelligent, metaheuristic and nature-inspired, and it is developed by Yang in 2008 by animating the characteristic behaviors of fireflies [2]. In fact, the population of fireflies show characteristic luminary flashing activities to function as attracting the partners, communication, and risk warning for predators. As inspiring from those activities, Yang formulated this method under the assumptions of all fireflies are unisexual such that all fireflies has attracting potential for each other and the attractiveness is directly proportionate to the brightness level of individuals [3]. Hence, the brighter fireflies attract to the less bright ones to move toward to them, besides that in the case of no fireflies brighter than a certain firefly then it moves randomly. The predictive quality of the QSAR model was tested for an external set of compounds by support vector machine. Statistical parameters for FF-SVM model were: R^2_{test}=0.894, RMSEP= 0.686, Q^2_{LGO}=0.847. Attained results indicated the superiority of the firefly algorithm in the feature selection. The predicted results of this study can be used to design new inhibitors of melanoma to treatment of cancer.

Keywords: “QSAR”, “Melanoma”,”Firefly algorithm”, “Support vector machine”

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Hybrid QSPR models for the prediction of the linear retention index of volatile compounds in flour

*Zeinab Mozafari**, [1], *Mansour Arab Chamjangali*[1], *Mohammad Arashi*[2], *Nasser Goudarzi* [1]
[1]*Department of Chemistry, Shahrood University of Technology, Shahrood, Iran.*
[2]*Department of Statistics, Faculty of Mathematical Sciences, Shahrood University of Technology, Shahrood, Iran.*
E-mail address: Chemist.mozafari1991@gmail.com

ABSTRACT

The data reduction methods are divided into two general categories. The classical methods as the first group, are including forward, backward and stepwise regression methods, which have disadvantages such as high bias in the estimation of regression coefficients, low performance in the presence of collinearity, and so forth [1]. The second group is penalized methods, which include variable selection methods such as least absolute shrinkage and selection operator (LASSO), smoothly clipped absolute deviation (SCAD) and adaptive LASSO (ALASSO). In these methods, coefficients of variables that do not have a significant relationship with the response shrinkaged to zero, and hence, the sparse models are obtained, so, the interpretation of the model increases. In this study 52 volatile compounds in flours from normal and waxy wheats were used in the QSPR modeling and linear retention index (LRI) of compounds were simulated. 3224 Dragon descriptors were computed for all volatile compounds [2]. Dataset were divided into the three sets of training set (30 compounds), validation set(11 compounds) and the test set (11 compounds). SCAD method [3] was applied on the train and validation set data (41 compounds) and 8 coefficients corresponded to the parameter with the lowest cross validation error (λ_{min}) were selected and used as inputs of Bayesian-Regularization artificial neural network model (BR-ANN). The predictability of the optimum BR-ANN model was evaluated using external test, validation set. Determination coefficient (R^2) of the test set and valid set were 0.89 and 0.99 respectively, which prove the generalizability and predictability of the constructed model.

Keywords: "volatile compounds", "QSPR", "SCAD", "Artificial neural network"

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Chemometrics Study Of Dye-Surfactant Interaction By Spectroscopic And Conductometric Methods

*Anita Parsaei, Jahanbakhsh Ghasemi**
Analytical Chemistry Department, School of Chemistry, Faculty of Sciences, University of Tehran, Tehran, Iran
E-mail address: jahan.ghasemi@ut.ac.ir

ABSTRACT

Dye molecules play basic and fundamental roles in a variety of fields including textile industries, dye-sensitized solar cells, medicine, separation science and understanding the biochemical reactions in living cells. In this study, the interaction of two cationic dyes, Methylene Blue and Nile Blue A with CTAB and SDS as cationic and anionic surfactants were evaluated. The spectrophotometric titration profile made a special type of evolving data, therefore different chemometrics techniques as deconvolution tools were used to extract the concentration and spectral profiles of formed species. Conductometric data verified the CMC points and the presence of free anions, cations, and ion-pair compounds in the pre-micellar and post-micellar phase of the reaction. The results to the following data reveal that the spectrophotometric method is a much better probe than conductometry. As we may see from its data there is a subtle change in conductometry in both the pre-micellar and post-micellar phase of the reaction even though data from spectrophotometry reveals considerable changes in absorption resulting from four kinds of species including dye monomer and dimer, ion-pairs and eventually extracted dye.

Keywords : “Dye”, “dye-sensitized solar cells”, “surfactants”, “conductometry”, “spectrophotometry”, “CMC”

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Quantitative structure activity relationship study of DAPY-like derivatives as NNRTIs using artificial neural network

Mozhgan Beglari[1], Nasser Goudarzi [1], Davood Shahsavani [2], Rahele Doosti[1]*
[1]Department of Chemistry, Shahrood University of Technology, Shahrood, Iran
[2] Department of statistic, Shahrood University of Technology, Shahrood,, Iran
E-mail address: Biglari55@yahoo.com

ABSTRACT

Acquired Immunodeficiency Syndrome (AIDS) is an infectious disease, first identified in 1983. AIDS is caused by the human immunodeficiency virus (HIV) that affects the immune cells in the blood (lymphocytes) and in the tissues and is still a significant pandemic worldwide. Highly active antiretroviral therapy (HAART) has become the most standard and efficient treatment regimen for HIV infection. Among currently available reverse transcriptase (RT) inhibitors, non-nucleoside RT inhibitors (NNRTIs), are an important component of the HAART regimen, owing to their unique antiviral activity, high specificity and low cytotoxicity. [1]. In this research, a nonlinear quantitative structure activity relationship (QSAR) study was performed for modeling and predicting inhibitory activity of 73 diarylpyrimidine like (DAPY-like) derivatives [2,3] as potent NNRTIs. Dataset (ligands) were drawn and optimized in hyperchem software. Chemical structures were digitized using DRAGON software and 154 functional group descriptors were obtained. 10 molecular docking descriptors were extracted from the enzyme-ligands interactions (PDB code of 3MEC for compounds 1 to 48 and PDB code of 3M8Q for compounds 49 to 73) using AutoDock4.2 software. All 163 descriptors were combined with each other and 7 descriptors as the most significant descriptors were selected by Stepwise regression (SR). The selected descriptors were used as inputs of artificial neural network (ANN). The neural network was trained and optimized using Bayesian Regularized (BR) and the best BR-ANN model was obtained according to the minimum MSE value of the valid set data. The prediction ability of the model was evaluated using the test set data. The MSE and the coefficient of determination values for the test set data were 0.10 and 0.86, respectively. The results obtained, showed the superior prediction ability of the proposed model in the prediction of inhibitory activities.

Keywords: “DAPY-like derivatives”,” Anti-HIV-1”, “Functional group descriptors”, “Molecular Docking”, “Stepwise regression”, “QSAR”

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Discrimination of Iranian vegetable oils by coupling of colorimetric sensor arrays and chemometrics techniques

*Bahram Hemmateenejad *, Javad Tashkhourian *, Mahsa Chaharlangi*
Chemistry Department, Shiraz University, Shiraz, 71454, Iran
E-mail address: hemmatb@shirazu.ac.ir , tashkhourian@susc.ac.ir

ABSTRACT

Oil is one of the essential ingredients in food and cosmetics industries. Due to the importance of oil in various industries, the study of its fraud is very important. There is an increasing need for developing appropriate methodologies for quality control of vegetable oils, as well as for identifying geographical or cultivar origin [1,2]. Colorimetric sensor arrays (CSA) are examples of simple and cost-effective analytical devices that have been developed by Suslick et al. in 2000 [3], these methods have been used in very different quality control assessments. For extraction of useful information from colorimetric sensor array patterns used multivariate statistical techniques, Among this chemometrics techniques, pattern recognition methods have found widespread applications in sensor arrays[4].

In this work, we developed a cross-responsive colorimetric sensor array (CSA) for discrimination of different oil samples. The sensor array was constructed from a (4 × 5) array of pH and redox indicators. The pH and redox indicators were spotted on a reverse phase silica gel plates using automatic micropipette. These sensors were placed on the cap of vessel containing oil samples vapor and let it to be exposed to the VOCs of the oils. A visual color change was observed after a certain time (e.g., around 3 hours). The color map of the pH and redox indicators after exposing to the vapor of oil sample was recorded by a scanner. Red, green and blue (RGB) color Intensity values of each element of the array calculate by using ImageJ software then difference in the color intensity of each spot of the array before and after exposure to the oil samples was considered as the corresponding signal. Then, Principal component analysis (PCA) , partial least squares discriminant analysis (PLS-DA) and linear discriminant analysis (LDA), as supervised pattern recognition techniques were used to analyze the data matrix for discrimination of different Iranian vegetable oils based on geographical or cultivar origin.

Keywords: “Colorimetric sensor array”, “Anions discrimination”, “Gold nanoparticles”, “Silver nanoparticles”, “Principal component analysis”, “Hierarchical clustering analysis”

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A nanozyme-based colorimetric sensor array for discrimination of anions in water samples

*Hoda Sharifi, Bahram Hemmateenejad *, Javad Tashkhourian*
Chemistry Department, Shiraz University, Shiraz, 71454, Iran
E-mail address: hemmatb@shirazu.ac.ir

ABSTRACT

Anions, such as halide ions (fluoride, chloride, bromide, and iodide), sulphide, chromate, phosphate, oxalate, nitrate and nitrite, play important roles in a wide range of environmental, chemical, and biological processes. Hence, the evaluation and discrimination of anions have attracted a lot of attention in chemical analysis, especially in water [1-3]. Here, a sensor array consisted of silver and gold nanoparticles stabilized with different organic capping agents for detection and identification of anions based on nanozymes-catalyzed 3,3',5,5' tetramethylbenzidine (TMB)-hydrogen peroxide (H_2O_2) reaction system is reported. In this sensor array, the anions depending on their type were showed different influence on the reaction between TMB and H_2O_2, resulting in different colorimetric response patterns. The obtained patterns for twenty eight anions, including fluoride, chloride, bromide, iodide, sulphate, chromate, bicarbonate, carbonate, acetate, nitrate, nitrite, phosphate, cyanide, sulphide, thiocyanate, oxalate, azide, hydroxide, dichromate, hydrogen phosphate, dihydrogen phosphate, periodate, benzoate, bromate, borate, arsenate, citrate and perchlorate at concentration of 12.5 mg/L, were successfully discriminated using principal component analysis (PCA) and hierarchical clustering analysis (HCA). Best discrimination performance of the sensor array was found in optimized condition including volume of nanoparticle of 40 μL, TMB concentration of 7.5×10^{-4} mol/L, H_2O_2 concentration of 3%(V/V), time of 2 min and temperatureof55ºC.

Keywords: "Colorimetric sensor array", "Anions discrimination", "Gold nanoparticles", "Silver nanoparticles", "Principal component analysis", "Hierarchical clustering analysis"

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Multiple implementation of MARS as a new descriptor selection method in the QSAR study of a new NNRTIs using artificial neural network

Mozhgan. Beglari *, [1,2], *Nasser Goudarzi* [2], *Davood Shahsavani* [3], *Zeinab Mozafari* [2]
[1]*Department of Chemical Industry, Faculty of Girls Shahrood, Technical and Vocational University (TVU), Shahrood Branch, Semnan, Iran*
[2]*Department of Chemistry, Shahrood University of Technology, Shahrood, Iran*
[3]*Department of statistic, Shahrood University of Technology, Shahrood, Iran*
E-mail address: Biglari55@yahoo.com

ABSTRACT

Acquired Immune Deficiency Syndrome (AIDS) is created by the Human Immunodeficiency Virus (HIV) via infecting a group of immune system cells called CD4 + T-lymphocytes [1]. HIV is a retrovirus whose genome is made up of RNA and consequently, HIV needs to reverse transcriptase (RT) enzyme to replicate its genome as DNA. Most anti-HIV drugs inhibit RT enzyme action. Non-nucleoside reverse transcriptase inhibitors (NNRTIs) inhibit the RT enzyme activity through the binding to an allosteric site of RT called NNRTI-binding pocket (NNIBP). NNRTIs are an important component of the HAART regimen, owing to their unique antiviral activity, high specificity and low cytotoxicity. [2]. The aim of this study was to develop a nonlinear quantitative structure-activity relationship (QSAR) to predict the pharmacological activity of a group of azine compounds [2,3] as potent NNRTIs using the molecular docking descriptors (MDDs). The 3D structures of azine derivatives were drawn and optimized in Hyperchem 8.0.5 software. For the extraction of MDDs from ligand-receptor (LR) interaction the optimized structures were individually docked at the active site of the respective proteins (PDB code of 3M8Q for compounds 1 to 43 and PDB code of 3MEC for compounds 44 to 73) using AutoDock4.2 software. Multiple implementation of MARS was used for the selection of the most important descriptors. The most relevant descriptors (3 descriptors) were used as the inputs in the artificial neural network (ANN) modeling. The prediction ability of the proposed ANN model was evaluated by the prediction of the pEC$_{50}$ of the test set data. The results showed R^2_{test} and MSE_{test} values equal to 0.78 and 0.18, respectively. The results obtained showed the superior prediction ability of the proposed model in the prediction of inhibiton activities.

Keywords: “Azine derivatives”,” Anti-HIV-1”, “Molecular Docking”, “Multivariate adaptive regression spline”, “QSAR” “Artificial neural network”,

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دبیرخانه : شاهرود، دانشگاه صنعتی شاهرود، دانشکده شیمی

@IBCS7 IBCS7@shahroodut.ac.ir IBCS7. shahroodut.ac.ir