



8th Iranian Biennial
Chemometrics Seminar



هشتمین سمینار دوساله کمیوتریک ایران

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8th Iranian Biennial Chemometrics Seminar

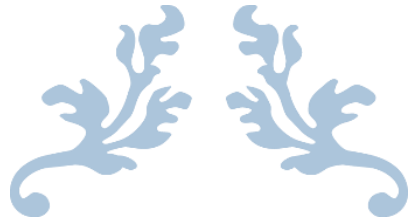


Program book proceeding of the 8th Iranian Biennial Chemometrics Seminar

Nov. 10, 11- 2021

Tarbiat Modares University





In the name of God



8th Iranian Biennial Chemometrics Seminar



WELCOME MESSAGE FROM THE SEMINAR SECRETARY



Dear Friends and Colleagues

It is a great pleasure and an honor to welcome you; honorable guests, lecturers, researchers and participants, to the 8th Iranian Biennial Chemometrics Seminar to be held 10-11 November 2021 at Tarbiat Modares University in Tehran.

We, organizing and executive committees, believe that this seminar is the largest meeting of chemometrics researchers and specialists which be held every two years in one of the Iranian universities. This seminar is a forum for presentation and discussion of the most recent advancements in all the fields of chemometrics.

Plenary and invited speakers, oral presentations, poster sessions, are arranged in program of present seminar. We look forward to that these specific topics could manifest the current central points and the trends of development in chemometrics research, thus direct us to work coordinately for the advancement of chemistry.

It is necessary to appreciate the Tarbiat Modares University of authorities; the Iranian Chemical Society, Chemometrics Committee, Organizing Committee, Scientific and Referee Committees, Student Executive Committees, and all university staffs who helped us hold this Conference.

Ahmad Mani-Varnosfaderani









Assistant Professor of Analytical Chemistry

Executive Scientific Secretary of 8IBCS

8th Iranian Biennial Chemometrics Seminar



The Brief History of Iranian Biennial Chemometrics Seminars

No.	City	Year	Chairman	Organizer	
1 st	Arak	2006	Dr. Ghulam Hassan Azimi	Arak University	
2 nd	Urmia	2009	Dr. Morteza Bahram	Urmia University	
3 rd	Tabriz	2011	Dr. Abdolhossein Naseri	Tabriz University	
4 th	Shiraz	2013	Dr. Bahram Hemmateenejad	Shiraz University	
5 th	Tehran	2015	Dr. Jahanbakhsh Ghasemi	Tehran University	
6 th	Mazandaran	2017	Dr. Mohammad Hossein Fatemi	University of Mazandaran	
7 th	Shahrood	2019	Dr. Nasser Goudarzi	Shahrood University of Technology	
8 th	Tehran	2021	Dr. Ahmad Mani-Varnosfaderani	Tarbiat Modares University	



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Invited Speakers



Prof. Mehdi Jalali-Heravi

Speech Topic:

Chemometrics in Iran: Past, Present and Future outlook



Prof. Roma Tauler

Speech Topic:

How we can measure the uncertainties associated to Multivariate Curve Resolution solutions due to the combined effect of rotation ambiguities and experimental errors?



Prof. Hamid Abdollahi

Speech Topic:

Multivariate Curve Resolution (MCR) Modeling for Pattern Recognition



Prof. Federico Marini

Speech Topic:

Classification/clustering/ and /class modeling/ with applications in Metabolomics studies

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Prof. Bahram Hemmateenejad

Speech Topic:

Data preprocessing in colorimetric sensor array: why and how?



Prof. Beata Walczak

Speech Topic:

Analysis of Variance of Multivariate Data



Dr. Hadi Parastar

Speech Topic:

Quantitative mass spectrometry imaging: a journey from multivariate resolution to deep learning



Dr. Maryam Khoshkam

Speech Topic:

Context dependency of pretreatment methods in metabolomics studies



Prof. Morteza Bahram

Speech Topic:

Classification of classification methods and some recent applications

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Prof. Mohammadreza Khanmohammadi

Speech Topic:

Spline regression for multivariate calibration



Prof. Hassan Yazdanpanah

Speech Topic:

The key role of chemometrics in rapid and innovative analysis for food authenticity using handheld visible and NIR spectroscopic techniques



Dr. Jamile Mohammad Jafari

Speech Topic:

Non-target ROIMCR LC-MS study of the disruptive effects over time of TBT on the lipidomics of Daphnia magna

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Conference Topics:

- *Curve Resolution*
- *Experimental Design*
- *Metabolomics*
- *Multivariate Calibration*
- *Structure-Activity Studies*
- *Clustering and Classification Methods*
- *Multivariate Regression*
- *Chemometrics applications in food and pharmaceutical industries, health domain, Criminalistics, etc.*

Sponsors :









8th Iranian Biennial Chemometrics Seminar Timetable

Wednesday, November 10, 2021

First section

Title	Time
 Recite the holy Quran, National Anthem, schedule announcement	08:00 – 08:10
 Academic-executive head of the seminar presentation	08:10 – 08:20
 Tarbiat Modares University introduction clip	08:20 – 08:25
 Chemometrics pioneer speech (professor Jalali)	08:25 – 08:45

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Wednesday, November 10, 2021

Second section “scientific speeches”

Title	Presenter	Time
Data preprocessing in colorimetric sensor array: why and how?	Dr. Bahram Hemmateenejad	08:50 – 09:30
The key role of chemometrics in rapid and innovative analysis for food authenticity using handheld visible and NIR spectroscopic techniques	Dr. Hasan Yazdanpanah	09:30 – 10:00
Miniaturized Low-cost Paper-Based Electronic Noses for Discrimination of Volatile Organic Compounds by Chemometrics Method	Shiva Pesaran	10:00 – 10:15
Single-sensor voltammetry electronic tongue based on the pH variations and chemometrics preprocessing for the classification of the pharmaceutical samples by the neural networks	Mehdi Moghtader	10:15 – 10:30
P1-P10	1st Poster Session	10:30 – 11:00
Quantitative mass spectrometry imaging: a journey from multivariate resolution to deep learning	Dr. Hadi Parastar	11:00 – 11:40
Spline regression for multivariate calibration	Dr. Mohammad Reza Khanmohammadi	11:40 – 12:20
Ensemble learners combined with handheld near infrared spectrometer for detection of hydrogen peroxide adulteration in milk	Samaneh Ehsani	12:20 – 12:35
Gaussian apodization factor analysis for Rank analyzing of Ion mobility spectra	Amir Hossein Alinoori	12:35 – 12:50
Preparation and characterization of activated carbon from palm bio-waste by H ₃ PO ₄ for the simultaneous removal of Basic dyes in binary aqueous systems	Fatemeh Kiani Ghalesardi	12:50 – 13:05
☕ Lunch break ---2nd Poster Session	P11-P20	13:05 – 14:00

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Wednesday, November 10, 2021

Third section “scientific speeches”

Title	Presenter	Time
Non-target ROIMCR LC-MS study of the disruptive effects over time of TBT on the lipidomics of <i>Daphnia magna</i>	Dr. Jamileh Mohammad Jafari	14:00 – 14:30
In Silico study of a group of antibiotics affinity toward aptamers for biosensor development	Masoumeh Naseri	14:30 – 14:45
Signal Contribution Effects on Error Propagation in Self-Modeling Curve Resolution Methods	Samaneh Tavoosi	14:45 – 15:00
Exploring the independence of feasible solutions in two-component hyperspectral imaging data using mutual information map	Fatemeh-sadat Hasheminasab	15:00 – 15:15
How we can measure the uncertainties associated to Multivariate Curve Resolution solutions due to the combined effect of rotation ambiguities and experimental errors?	Prof. Roma Tauler	15:15 – 16:00
P21-P30	3rd Poster Session	16:00 – 16:30
Multivariate Curve Resolution (MCR) Modeling for Pattern Recognition	Dr. Hamid Abdollahi	16:30 – 17:10
The effects of selectivity on accuracy of multivariate curve resolution (MCR) results	Dr. Somayeh Khodadadi Karimvand	17:10 – 17:40
Descriptive Definition of Multivariate Calibration Model Vector	Dr. Somayeh Valizadeh	17:40 – 17:55
Outliers detection map in analytical chemistry calibrations	Fatemeh Ahmadiyeh	17:55 – 18:10
Comparison of perturbation and augmentation to solve rank deficiency problem	Yasaman Sefid-Sefideh khah	18:10 – 18:25
P31-P40	4th Poster Session	18:25 – 19:00

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Thursday, November 11, 2021

First section “scientific speeches”

Title	Presenter	Time
Classification of classification methods and some recent applications	Dr. Morteza Bahram	8:00 - 8:40
Network pharmacology in drug discovery	Dr. Sajjad Gharaghani	8:40 - 9:10
Theoretical cross-reactivity neutralizing study of some nanobodies for receptor binding domain (RBD) of SARS-CoV-2 using covid-19 molecular docking server	Zahra Pahlavan Yali	9:10 - 9:25
Ligand-based virtual screening for isoform-selective histone deacetylase inhibitors (class I)	Dr. Marzieh Sadat Neiband	9:25 - 9:40
QSAR study & Molecular docking of matrix metalloproteinase inhibitory activity of hydroxamate derivatives by MIA-QSAR & using OSC-GA-PLS	Delaram Salehpour Kahi	9:40 - 9:55
P41-P50	5th Poster Session	9:55 - 10:30
Context dependency of pretreatment methods in metabolomics studies	Dr. Maryam Khoshkam	10:30 - 11:10
Discriminating between patients with endometriosis and healthy women using gas chromatography-mass spectrometry and chemometrics techniques	Dr. Mohammad Javad Masroor	11:10 - 11:40
A Colorimetric Chemical Nose with Unmodified Gold Nanoparticles for Multiplexed Detection and Discrimination of Catecholamine Neurotransmitteres	Dr. Naeimeh Mohseni	11:40 - 11:55
Prediction of RT-PCR results using multivariate investigation of important blood biomarkers in patients with covid 19	Samaneh Sadat Momen Ghazvini	11:55 - 12:10
Comparison of prediction uncertainty in first order multivariate calibration methods	Taha Kafili	12:10 - 12:25
☕ Lunch break --- 6th Poster Session	P51-P60	12:25 - 13:30

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Thursday, November 11, 2021

Second section “scientific speeches”

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Analysis of Variance of Multivariate Data	Prof. Beata Walczak	13:30 -14:20
Mixture QSAR/QSPR: a novel approach to define mixture descriptors	Dr. Vahid Zare Shahabadi	14:20 -15:00
Classification/ clustering/ and /class modeling/ with applications in Metabolomics studies	Prof. Federico Marini	15:00 -15:45
Application of Data Point Importance (DPI) Concept in Supervised and Unsupervised Pattern Recognition	Zahra Zare	15:45 -16:00
Comparison of embryo culture medium samples in IVF with infrared spectrometry using successive projections algorithm (SPA) - sum of ranking differences (SRD)	Dr. Shima Zandbaf	16:00 -16:15
Area of Feasible Figures of Merit (AF-FOMs) for second-order multivariate calibrations in MCR methods	Fariba Norooz Yeganeh	16:15 -16:30
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Miniaturized Low-cost Paper-Based Electronic Noses for Discrimination of Volatile Organic Compounds by Chemometrics Method

Shiva Pesaran, Zahra Shojaeifard, Bahram Hemmateenejad and Javad Tashkhourian*.*

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ABSTRACT

An integrated design of a paper-based colorimetric sensor array (including indicators and the sample injection zone) is described. To overcome previous limitation in volatile measurements by sensor array [1], a miniaturized chamber was designed to reduce the consumption volume, and made the work simple and affordable. In this regard, a 3D printer was used to design the 3×3 cm reaction chamber. Moreover, using the watercolor paper and placing the injection site on the surface of the paper are considered to reach these aims. The considered miniaturized chamber and analyte embedded location caused using the lowervolume of analyte (13μL) to create a vapor saturated environment. To show the applicability of the proposed sensor, a colorimetric sensor array was used for discrimination of volatile organic compounds (VOCs) related to different solvent families. The integrated colorimetric sensor (ICS) designed by spotting 12 sensing elements from three different groups (solvatochromic dyes, pH indicators and metallochromic dyes) with various properties and interactions. The color difference map (CDM) of the sensor array was obtained before and after exposure to VOCs, which was used as a fingerprint to discriminate VOC samples based on their functional group. The proposed device and sensor could discriminate 30 volatile organic compounds with linear discrimination analysis (LDA) method. They were classified in six chemical families including alcohols, amines, acids, ketones, aldehydes, nonpolar with 99% accuracy. In total, the designed device is portable, rapid, cost-effective and requires low volumes of sample that can be considered as a good candidate for various VOC analysis.

Keywords: Linear discriminant analysis, VOC sensor, Paper-based sensor array, Reaction chamber

References:

[1] H. Lin, W. C. Kang, H. J. Jin, Z. X. Man, and Q. S. Chen, (2020). "Discrimination of Chinese Baijiu grades based on colorimetric sensor arrays", *Food science and biotechnology*, 29, (2020), 1037-1043.



Single-sensor voltammetric electronic tongue based on the pH variations and chemometrics preprocessing for the classification of the pharmaceutical samples by the neural networks

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ABSTRACT

The imitation of the taste sensation process in human and animals can be used as an analytical tool for qualitative evaluation and classification of the food, drink and chemical samples. In this manner, the voltammetric Electronic Tongues (ETs) consisting of a set of solid-state electrodes with different electrochemical properties, have been extensively used in the analysis of the various real samples [1]. The IUPAC report defines an electronic tongue as “a multisensor system, which consists of a number of low-selective sensors and uses advanced mathematical procedures for signal processing based on the pattern recognition and/or multivariate data analysis”. Based on this definition, any parameter like pH or ionic strength of the solution, which induce a subtle difference in the voltammetric response of the electrode toward a specific analyte, can be used to fabricate an electronic tongue that uses the obtained responses to create a fingerprint for each of the analytes [2, 3]. As most of the analytes undergo the structural variations due to the change in the pH of the medium, which results in the different voltammetric behaviors, this parameter (pH) can be employed to design a voltammetric electronic tongue for the classification purposes without the need to the expensive and time-consuming electrode preparation and optimization procedures for each of the sensors. In this study a single glassy carbon electrode (GCE) modified with the MWCNTs was used for the classification of 14 different drugs at three concentrations in their pure form and binary mixtures using the Linear Sweep Voltammograms (LSV) recorded at three different pH values and three replications in the ranges 0.2 to 1.2 V. The obtained large data matrix (126×2985) was preprocessed by the first-order derivatization to reduce the overlapping and background interference and Discrete Wavelet Transform (DWT) with the Coiflet3 mother wavelet at five decomposition levels for the dimensionality reduction, which results in an about 96% compression ratio. The obtained approximation coefficients (126×109) together with the raw and first-derivative data matrices were analyzed by both PCA and XY-Fused neural networks as unsupervised and supervised pattern recognition techniques respectively. The results indicate that the XY-Fused neural networks due to their nonlinear characteristics can better classify the analyzed samples using their processed voltammetric responses compared to the PCA as a linear data processing chemometrics technique.

Keywords: Electronic tongue, Voltammetry, Wavelet transform, Neural networks, Pattern recognition

References:

- [1] F. Winquist, Voltammetric electronic tongues-basic principles and applications, *Microchim. Acta*, 163 (2008) 3–10.
- [2] P. Ciosek and W. Wróblewski, Sensor arrays for liquid sensing-electronic tongue systems, *Analyst*, 132 (2007) 963–978.
- [3] Y. Zou, H. Wan, X. Zhang, D. Ha and P. Wang, *Bioinspired Smell Tast. Sensors*, Springer, 2015.



Ensemble learners combined with handheld near infrared spectrometer for detection of hydrogen peroxide adulteration in milk

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Abstract:

Milk is wholesome nutritious dairy product, which has been confronted with various adulterations. Hydrogen peroxide (H_2O_2) is widely used for disinfection purposes by food industry enterprises, and it is one of the major adulterants in milk and dairy industry. Even though due to chemical processes inside raw milk, it can contain small quantities of H_2O_2 ($1-2 \text{ mgL}^{-1}$), the concentration must be 10 times higher in order to destroy pathogens. At the same time, high concentrations of H_2O_2 in milk can lead to changes in its chemical composition which, in turn, can lead to negative effect for the consumers [1]. Therefore, the main objective of this work is to use a handheld near infrared spectrometer (NIRS) as a rapid and non-destructive technique in combination with ensemble learners to detect H_2O_2 adulterant in milk. For this purpose, authentic raw bovine milk samples were collected from two dairy farms located in Iran. After pooling the samples, appropriate amount of a standard solution of H_2O_2 were added at 10 concentration levels ranged 0.05% to 18% (v/v). A handheld NIRS device (Tellspec Inc., Toronto, Canada) was used to acquire NIR spectra in the reflectance mode in the spectral range of 900-1700 nm. First of all, the pattern of the milk samples (pure and adulterated) and of the 256 NIR variables was explored by principal component analysis (PCA). The first two principal components explained 98% of the total variance. Then, the dataset was split into training (70%) and test (30%) sets using duplex algorithm. Additionally, a five-fold randomized cross-validation was used for internal model validation. Random subspace discriminant ensemble (RSDE) [2, 3] was used for classification. The performance of the RSDE method was evaluated in terms of sensitivity (Sen), specificity (Spe), and accuracy (Acc). All the values for Sen, Spe and Acc were above 95% in each case, which showed the reliability and robustness of the developed model. Furthermore, the RSDE method outperformed partial least squares-discriminant analysis (PLS-DA) and support vector machine (SVM) as common classification techniques used in food authenticity.

Keywords: Milk adulteration; Handheld near infrared; Ensemble learner; Random subspace discriminant ensemble; Hydrogen peroxide.

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Gaussian apodization factor analysis for Rank analyzing of Ion mobility spectra

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ABSTRACT

Evaluation of raw data on ion mobility spectrometry is very important in detection of the trace chemical of interest. It is truly ideal to reach a new technical methods that can extract ions mobility signals from all acquired raw data without manipulation of it. In many cases, weak signals are manipulated during the data collection process and some weak signals are eliminated. Quickly and clearly finding of a rank map is the main problem in resolving the elution profiles of all the chemical components in such data. In the past decade, a variety of non-iterative methods for the correct determination of the number and range of each factor based on singular value decomposition (SVD) have had widespread applications in analytical chemistry and other fields. Gaussian apodization factor analysis (GAFA) has been developed as an enhanced algorithm to assess the peak purity of the two-dimensional data, by weighting the fixed-size moving window via Gaussian formula. In GAFA method, submatrices are extracted by Gaussian apodization moving window. Therefore, each submatrix mainly characterizes the spectrum and by performing factor analysis on this Gaussian weighted submatrix, the number of principal components for each evaluated spectrum, is determined [1]. This precise and quick determination of a rank map is successfully used for extract pure components from Ion mobility spectra.

Keywords: Ion mobility spectrometry, Gaussian apodization factor analysis, Local rank map, Curve resolution.

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Preparation and characterization of activated carbon from palm bio-waste by H_3PO_4 for the simultaneous removal of Basic dyes in binary aqueous systems: optimization by central composite design, equilibrium, kinetic and thermodynamic studies

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ABSTRACT

In recent decades, extensive attempts have been made to use biomass-based materials for wastewater treatment¹⁻². The first aim of this study was to prepare activated carbon (AC), a practical biosorbent from palm bio-waste. It was characterized via Fourier transform infrared spectroscopy (FTIR), high-resolution transmission electron microscopy (HRTEM), Field Emission-Scanning Electron microscopy (FE-SEM), Energy-dispersive X-ray spectroscopy (EDS), X-ray diffraction (XRD), Brunauer–Emmett–Teller (BET) specific surface area and zeta potential measurement. As the second purpose, use of the prepared activated carbon was assessed and optimized for the simultaneous removal of Basic Blue 41 (BB41) and Basic Red 46 (BR46) dyes in binary aqueous systems, by Central Composite Design (CCD) under Response Surface Methodology (RSM). The optimum values for removing BB41 and BR46 systems were found to be 8.27 mg of adsorbent dosage, 48 min of contact time, 15 mg L⁻¹ for the concentration of BB41, and 5 mg L⁻¹ for the concentration of BR46 and the removal percentage equal to 99.81% and 95.76% for BB41 and BR46, respectively. In individual solutions, the adsorption process fitted well with Langmuir isotherm and pseudo-second-order kinetic models with the maximum adsorption capacities (q_m) of 344.83 and 263.16 mg g⁻¹ for BB41 and BR46, respectively. Extended Langmuir isotherm was used in binary systems to calculate q_m for BB41 and BR46 as 271.81 and 127.23 mg g⁻¹, respectively. Finally, it could be concluded that the mechanism of the adsorption procedure is monolayer, physical, spontaneous, endothermic, and more desirable at higher temperatures.

Keywords: Palm bio-waste; Activated carbon; Basic Blue 41; Basic Red 46; Central Composite Design; Response surface methodology.

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Non-target ROIMCR LC-MS study of the disruptive effects over time of TBT on the lipidomics of *Daphnia magna*

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ABSTRACT

Metabolomic studies of biological samples using statistically designed experiments produce large multivariate datasets which can be arranged in three-way data structures and modelled using bilinear and trilinear factor decomposition methods¹. The goal of these studies is the discovery of the hidden sources of data variability to facilitate their biochemical interpretation. In this presentation, the application of the new ROIMCR method² is shown as a means to recover the maximum number of lipids in non-target LC-MS studies of the disruptive effects over time of TBT on *Daphnia magna*³. Results of the ROIMCR method allowed the resolution of a large number of distinct lipid profiles (elution and spectra profiles) whose concentration changes are associated with the different time phases of *D. magna* intermolt development and with TBT dose. Results of the comparison of the results obtained in the non-target analysis with those previously obtained in the target analysis of the same samples are given³. Whereas most of the lipids were found in both studies, the non-target analysis provided a larger number of lipids showing statistically significant changes in their concentration due to TBT exposure and time, some of them could be de novo identified, and others were not identified using current databases. The relationship between the effects of the experimental design factors, the interaction between these factors, the structure of the generated three-way datasets and their more appropriate modelling (bilinear or trilinear) are investigated.

Keywords : Lipidomics, two-factor interaction, three-way data analysis, ASCA, MCR-ALS

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In Silico study of a group of antibiotics affinity toward aptamers for biosensor development: Molecular Dynamics Simulations and Molecular Docking Studies

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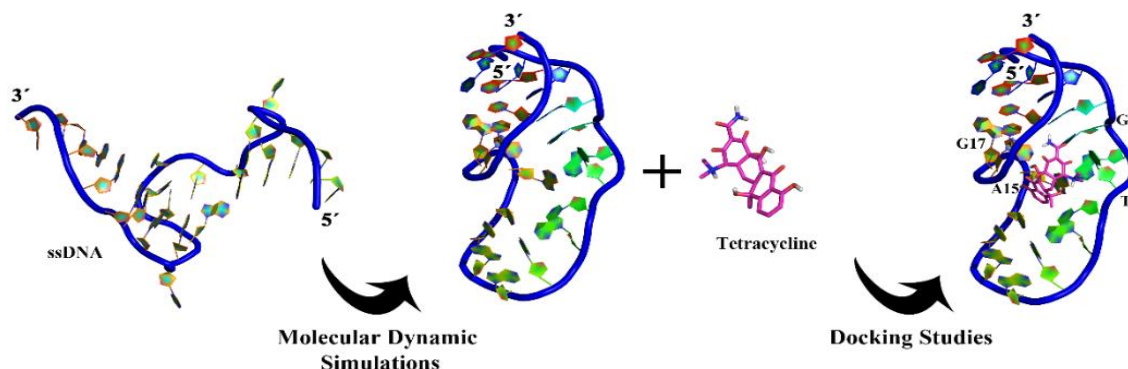
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ABSTRACT

Aptamers are short single-stranded DNA (ssDNA) or nucleotide sequences prepared by a random library through an iterative in vitro process called SELEX (systematic evolution of ligands via exponential enrichment), which that can bind with high affinity and specificity to various targets, such as drugs, proteins or other organic or inorganic compounds. These single chains have many advantages such as cost effectiveness, flexibility, easy modification and high stability [1]. In this study, the affinity of sequences of specific aptamers for various antibiotics was studied using molecular dynamics simulations (MDs) method and molecular docking studies [2]. The desired sequences structures were generated and went through molecular dynamics simulations, using GROMACS 5.1.5, to investigate the molecules conformational and obtain a stable structure at the desired conditions. The target antibiotics affinity and tendency to interact with the aptamers was computed with the aid of molecular docking methodology, employing Schrodinger maestro software (version 12.5).



The stability of the antibiotic-aptamer complexes interactions was further investigated using molecular dynamics simulations. The aptamers that the target antibiotics predicted to have more tendency to interact with were selected to design aptasensors to detect the antibiotics in different samples.

Keywords: Aptamer, Molecular Dynamics Simulation, Molecular Docking, ssDNA

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Signal Contribution Effects on Error Propagation in Self-Modeling Curve Resolution Methods

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ABSTRACT

Multivariate curve resolution (MCR) methods are powerful tools to investigate complex chemical systems whenever there is little or no knowledge about the system [1]. Despite of its high resolution power in the analysis of overlapping chromatographic and spectroscopic signals, MCR-ALS solutions usually suffer from noise propagation uncertainties and rotational ambiguities. It is important to know the extent of uncertainties in the resolved solutions. Without quantifying these uncertainties, one might mistakenly consider that the obtained solution is the true one [2]. When ambiguity is present, every resolved profile can be represented by a band of feasible solutions instead of by a unique profile. In the presence of experimental noise, the estimation of this band of feasible solutions is even more difficult and uncertain [3]. If the intensity of a component in a data set changes, it does not change the overlap of the profiles, but the rotational ambiguity will change. The aim of this work is to investigate how signal contribution and reduction of the data set dimensions affect the reliability of feasible solutions. To study the effect of the signal contribution, several identical two-component systems with different intensities of concentration profiles were simulated and the uncertainties of feasible solutions were investigated. To study the effect of the reduction of the data set dimensions, several simulated data sets and their reduced sizes have been systematically investigated. The obtained results by simulated data sets showed that increasing the intensities of concentration profiles decrease the uncertainties of the feasible solutions, and reduction the data sets dimensions increase the uncertainties of the feasible solutions.

Keywords: Signal Contribution Effects, Data Reduction, Error Propagation, Uncertainty

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Exploring the independence of feasible solutions in two-component hyperspectral imaging data using mutual information map

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ABSTRACT

In recent years, independent component analysis (ICA) has gained attention in chemistry as a blind-source separation technique (BSS) to find underlying components in multi- and hyper-spectral imaging (MSI/HSI) data [1]. Independence is the main constraint of ICA and it is believed that this constraint is a mathematical constraint which make ICA inappropriate for multivariate resolution purposes [2]. On the other side, multivariate curve resolution (MCR) methods are confronted with rotational ambiguities which means instead of a unique solution, a set of feasible solutions fulfilling the constraints can be obtained. The application of the strong constraint of independence, like in ICA, eliminate rotation ambiguities, but then the solution obtained is usually outside the range of MCR feasible solutions. In some implementations of ICA (like in mean-field ICA, MFICA), the independence constraint is relaxed by the application of non-negativity constraints and the solution can be then feasible. In these cases, ICA finds the more independent solution within the range of feasible solutions [3]. Consequently, there is a major concern about ICA application for multivariate resolution purposes. On this matter, there are two main questions which need clear answers by chemometricians; (i) is there any change of independence among solutions in the feasible bands? and (ii) which ICA algorithm can give solutions inside the feasible band? Therefore, the main objective of the present contribution is answering to these two important questions for HSI data. In this regard, mutual information (MI) was used to calculate independence between different solutions [4]. Additionally, three different two-component HSI datasets were simulated with different degrees of overlap in spatial profiles. Feasible solutions were obtained by two common approaches of grid search and Lawton-Sylvester plot and error maps were calculated. Then, MI values were calculated for all solutions especially for solutions in feasible bands and MI maps were obtained for the different datasets. Inspection of the results showed that different solutions in the feasible bands have different MI values and therefore different independence. Additionally, the MI values were lower for spectral profiles (more independent) and bigger for elution profiles (more dependent) based on duality. In general, the know solution in MI maps was near to more dependent solutions for concentration profiles and near to less dependent solutions for spectral profiles which is due to applying “independence” constraints to the spectral profiles. The performance of three well-known ICA algorithms of MFICA, mutual information based least dependent component analysis (MILCA) and joint approximate diagonalization of eigenmatrices (JADE) as well as multivariate curve resolution-alternating least squares (MCR-ALS) were investigated using MI maps for simulated datasets. MI maps showed that the solutions of MFICA and MCR-ALS are in the feasible bands but the MILCA and JADE solutions which are just based on the independence maximization are outside the MI maps. Finally, a real two-component hyperspectral imaging dataset was used to confirm the applicability of the proposed method.

Keywords: Independent component analysis, Area of feasible solutions, Mutual information, Hyperspectral imaging.

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The effects of selectivity on accuracy of multivariate curve resolution (MCR) results

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ABSTRACT

The use of multivariate methods in order to analyze chemical data sets and extract useful information is inevitable. Multivariate curve resolution is the popular resolution methods. But, the results are always associated with the rotational-ambiguity (RA) problem. By using chemical information in the form of constraints, the amount of rotation can be reduced. Since applying different physical/chemical constraints can effect on the extent of RA and the accuracy of the SMCR results, herein, the effects of presence and utilizing selectivity constraint on the accuracy of the results is investigated. The selectivity constraint was defined as regions with presence of one component in the concentration or spectral profiles [1]. It is assumed that in the local rank-based methods the number of components in each region is equal to its rank. Thus, implementing local rank information as a constraint in can significantly diminish rotational ambiguity. It has been showed that the implementing of local-rank as a mathematical constraint for restricting the rotational ambiguity can lead to incorrect solutions due to the local-rank-deficiency problem [2]. Thus, obtaining information about selective windows by local rank information is not reliable. In order to investigate the effect of presence, detection and applying the information of selective regions, different simulated data and real experimental was checked out (hyperspectral image and HPLC-DAD). The effects of presence of selective window(s) of profiles on accuracy of the MCR methods was investigated. For this, the range of feasible solutions by using only non-negativity constraint was calculated. Then, the selectivity of resolved profiles for rank-one windows, for different solutions were checked out. Presence of one, two, or three components can be observed in sub-windows with rank one. Thus, due to the rotational ambiguity, there is an ambiguity in the presence pattern of concentration profiles. Thus, the local-rank-one sub-windows is not necessarily selective. This is the local-rank deficiency problem which is unavoidable in local rank-one sub-windows. It is notable that, although different sets of MCR solutions have variety of presence pattern, all are consistent with the scheme of rank windows obtained by EFA. The selective window size also varies in different feasible solutions. When the data conditions are such that the profile of at least one of the involved components is unique, then, because there is no rotational ambiguity for that profile, the observed selectivity status is true. Thus, it is possible to detect real selective profiles in data only with non-negativity constraint.

Keywords: Selectivity, Multivariate curve resolution, Rotational ambiguity, Local rank, EFA, Hyperspectral Image data, HPLC-DAD data, Data based uniqueness.

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Descriptive Definition of Multivariate Calibration Model Vector

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ABSTRACT

Multivariate calibration relates a dependent variable such as a chemical or physical property to independent variables such as spectroscopic measurements via the model vector. The model vector is commonly estimated by the methods of partial least squares (PLS), the Tikhonov regularization (TR) variant of ridge regression (RR), or principal component regression (PCR). However, multivariate calibration models often fail to extrapolate beyond the calibration samples because of changes associated with the instrumental response, environmental condition, or sample matrix. Most of the current methods used to adapt a source calibration model to a target domain exclusively apply to calibration transfer between similar analytical devices, while generic methods for calibration model adaptation are largely missing. Considering that the calibration model vector carries on all information of the calibration model. In fact, the calculation of model vector **b** is the core of all different first-order multivariate calibration methods. So we have focused on basic properties of model vector **b** for proposing a clear descriptive definition of this magic vector in first-order multivariate calibrations. This magic vector carries on the most information of calibration samples related to analyte and non-analyte constituents behaviors. This vector is sensitive and selective to its related analyte and can exploits the analyte concentration from the measured spectrum of unknown samples in almost same conditions of calibration samples. Clear imagine and understanding of model vector **b** can help analytical chemist to improve the multivariate calibration methods for more accurate and precise prediction of analyte concentrations in unknown samples. Descriptive definition of model vector **b** can create a new calibration transfer method via adopting the proposed procedure to inconsistency problem for two different measurement instruments. We have simulated a three-component data set for investigating regression coefficients of different methods (PCR, PLS and the proposed descriptive method). This data (64×221) is divided to calibration/prediction sets (38/26). The results are shown in figure 1 and table 1. Also, a real data set (corn data) is used for comparing our descriptive method and calibration transfer method [1].

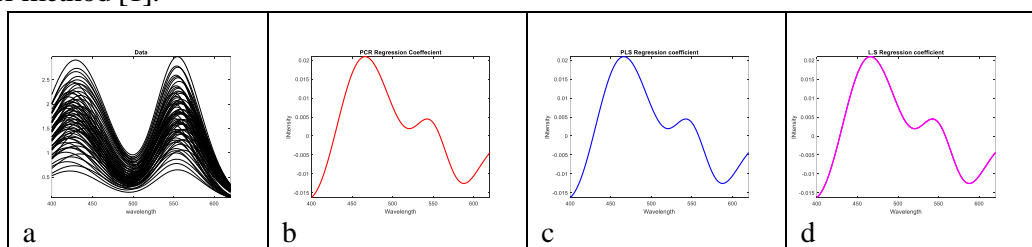


Fig. 1. Data (a), the regression coefficients of PCR (b), PLS (c) and descriptive method (d).

Table 1. Root mean square errors of calibration and prediction sets for PCR, PLS and descriptive b.

	PCR	PLS	Desc. b
RMSEC	1.44×10^{-16}	2.22	1.02×10^{-14}
RMSEP	3.27×10^{-17}	7.18×10^{-16}	6.73×10^{-15}

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Outliers detection map in analytical chemistry calibrations

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ABSTRACT

Recognizing outlier data and discarding them is one of the steps in data processing that has been considered in various sciences. The existence of outliers in chemistry data is not unexpected [1]. Regression for calibration and prediction of analyte concentration can be affected by outlier data. In performing the calibration, if the outliers are not identified and discarded, the constructed model will not have much validity and we will also make mistakes in estimating the concentration of unknown samples. [2]. In this work, the data will be divided into two categories, univariate and multivariate, and in the case of univariate data, which we will encounter in most analytical techniques, we will extract a map that recognizes the following: a) large error in the experimental process: the recorded signal does not match the desired concentration. B) The existence of data with high regression coverage that is far from the rest and will strongly affect the accuracy of the calibration equation, high leverage data. C) Detection of data with a signal less than the standard deviation of regression, the concentration of which cannot be predicted by the extracted equation. The proposed roadmap on various analytical techniques will be reviewed and its efficiency studied, and this will give a new look at the calibration equation, how to distinguish the upper and lower limits of the equation, and a solution to avoid common mistakes in chemistry. In the case of multivariate data [3], we will extract an outlier map similar to the univariate data outliers map, also has another special ability; detection of the presence of a non-calibrated interference in unknown samples, first-order data advantage. These methods will be implemented for different types of multivariate calibration data and models.

Keywords: Outlier, Regression, Univariate and multivariate data, High leverage.

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Comparison of perturbation and augmentation to solve rank deficiency problem

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ABSTRACT

Hard modeling (HM) and soft modeling (SM) approaches have been developed to resolve concentration profiles and pure absorption spectra from two-way kinetic-spectral data during a chemical reaction. HM techniques are based on fitting of experimental data to mathematical models. To estimate the reaction order and rate constants at the same time, different approaches are used (1). When the number of major contributions to data variance, as estimated by singular value decomposition or other related factor analysis approaches, is less than the real number of chemical components present in the system, the data matrix is rank-deficient. In the case of rank deficient system, analysis of single data matrix leads to correct estimation of rate constants and thus concentration profiles but the spectral profiles can not be estimated correctly. Thus in presence of rank deficient system full resolving the system is impossible and it should be solved. The problem of rank deficiency can be solved by two strategies (i) matrix perturbation by adding a single component or combinations of components during the process; (ii) matrix augmentation by simultaneous analysis of two or more data matrices (2). In this study, both of these strategies was used for resolving two types of kinetic data. 1) a simple full rank first-order kinetic system which is not rank deficient and used to test the performance of perturbation and 2) a simulated rank deficient second order consecutive reaction in which the problem of rank deficiency is serious and should be solved for full resolving the kinetic data. Then the method was applied for experimental data. In the experimental system, o-ABA reacts with diazonium salt in a second order consecutive reaction.



Our results show that in the case of non bilinearity in data, augmentation leads to incorrect results and thus systematic errors whereas perturbation works properly and its results are correct. In the next step the relation between the extent of reaction and perturbation was investigated. It was shown that the uncertainty of results in the case of perturbation strongly depends on the time of perturbation. It was shown that in the early stage of reaction the effect of perturbation is significant.

Keywords: perturbation, augmentation, rank deficiency, first order, second order consecutive, fitting, extent of reaction.

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Theoretical cross-reactivity neutralizing study of some nanobodies for receptor binding domain (RBD) of SARS-CoV-2 using covid-19 molecular docking server

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ABSTRACT

Severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2) is an infectious cause with exceptional character of its swift outbreak which led to epidemic far away from where it was first observed in Wuhan, China [1]. SARS-CoV-2 neutralizing antibodies primarily target trimeric spike glycoproteins on viral surface and mediate entry into host cells [2,3]. This spike protein has two functional subunits that mediate cell attachment and fusion of viral and cellular membrane [4]. The spike proteins of SARS-CoV-2 commonly bind to human angiotensin converting enzyme 2 (ACE2) protein as a host receptor [5]. Nanobody refers to a group of the single-domain antibody (sdAb) that were first engineered from heavy-chain antibodies naturally found in camelids and overcome many application problems of monoclonal antibodies in molecular imaging, diagnostic kits and therapeutic medicines [6-7]. Blocking ability of spike receptor binding domain (RBD) of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) theoretically was checked with some nanobodies. Firstly, 21 of Lama glama VHH that neutralized the viral glycoprotein of Severe acute respiratory syndrome coronavirus 1 (SARS-CoV-1), Middle East respiratory syndrome (MERS), Human immunodeficiency viruses 1 (HIV-1) or respiratory syncytial virus (RSV) was selected from structural antibody database (SAbDab) [8]. Then, ACE2 and each nanobody complexes with RBD were verified using CoDockPP Server [9] which provide a multistage protein-protein molecular docking based on shape complementarity that knowledge-based scoring function and site constraint. In the following, best conformation and binding energy of ACE2-RBD and VHH-RBD complexes were obtained by COVID-19 Docking Server [10]. The binding energy of RBD-ACE2 complex was recognized when RBD (6LZG (B)) and ACE2 (6LZG (A)) respectively was defined as target and ligand proteins and vice versa. It was seen, *JM4*, *F-VHH-L66*, *VHH-72*, and *VHH A12* respectively was proposed for neutralization of spike RBD with an estimated binding energy greater than -792.4 (kcal/mol) for ACE2. The PDB ID (VHH chain name) of proposed are *4LAJ (H)*, *6WAQ (A)*, *5TOK (E)*, *5TOK (D)*, *4LAJ (L)*, *6WAQ (C)*, *4LAJ (M)* and *3RJQ (B)*. It should be noted that the different crystallography structures of *F-VHH-L66* (*5TOK (E)*) and (*5TOK (D)*) could be due to various experimental contact region of spike glycoprotein that experimentally was involved. The estimated binding energy for these VHH respectively -341.45, -333.08, -332.49, -321.6, -320.98, -320.39, -317.03 and -312.29 (kcal/mol). This study provide a molecular basis for the blocking of RBD of SARS-CoV-2 with 13 proposed natural nanobody that suggest for therapeutics aim of the SARS-CoV-2.

Keywords: SARS-CoV-2, Receptor binding domain (RBD), covid-19 docking server, Nanobody, VHH.

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Ligand-based virtual screening for isoform-selective histone deacetylase inhibitors (class I)

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ABSTRACT

As one of the hot topics in the epigenetic studies, histone deacetylases inhibitors (HDACIs) have been introduced to treat a variety of diseases such as cancer, immune disorder and neuronal diseases [1]. Due to their effective roles in the onset of cancer and its progression, HDAC Class I isoforms (HDAC 1, 2, 3 and 8) were considered in this study. Herein, our objective is to determine the important isoform-selective and isoform-active structural features of HDACIs using the valid classification models. For this purpose, five datasets including 8224 molecules of HDAC1, HDAC2, HDAC3, and HDAC8 together with their corresponding biological activity (in terms of IC₅₀ (nM)) were collected from the Binding Database. Five classification models based on Support vector machine (SVM), and Supervised Kohonen network (SKN) methods were established to identify key features of isoform-selective and isoform-active HDACIs. The variable importance in projection (VIP) [2] method was used to select the suitable set of molecular descriptors from 3224 molecular descriptors that were calculated by DRAGON software ver. 5. The statistical evaluation of the developed classification models was implemented by parameters derived from confusion matrix. The descriptor analysis show that physicochemical properties, such as hydrogen bonding, number of branches, size, flexibility, polarity and sphericity in the structure of molecules, were closely related to the bioactivity of HDACIs. The reliability and predictive ability of the conducted models were evaluated using the tenfold cross-validation techniques, test sets and applicability domain analysis. All of the obtained classification models represented high statistical quality and predictive ability with accuracy greater than 85% for the test sets. The proposed strategy and the selective patterns represented in this paper can be applied by researchers in the pharmaceutical sciences who aim to use the same idea for the design of drugs with improved anticancer properties.

Keywords Isoform-selective HDAC inhibitors, Ligand-based virtual screening methods, Supervised Kohonen network, Support vector machine, Anti-cancer agents

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QSAR study & Molecular docking of matrix metalloproteinases inhibitory activity of hydroxamate derivatives by MIA-QSAR & using OSC-GA-PLS

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ABSTRACT

The quantitative structure-activity relationship (QSAR) is an important part of computer aided drug design. the design and model programs of a QSAR analysis base on MIA-QSAR analysis were presented. In this QSAR study, the compounds of matrix metalloproteinase inhibitors (MMP-2 and MMP-9) on anticancer activity were investigated by various chemometrics methods. Predicting its anti-cancer activity in this method is particular importance. The detailed application of the multivariate image analysis (MIA) method to the evaluation of a quantitative relationship between molecular structure and inhibitory activity of hydroxamate derivatives as inhibitors of matrix metalloproteinase (MMP-2 and MMP-9) as anticancer agents was discovered. MIA is a type of data mining method based on data sets obtained from 2D images (descriptors). The purpose of this research is to construct a relationship between pixels of images of studied compounds as independent variables and their inhibitory activities as a dependent variable. The resulted descriptors were exposed to principal component analysis (PCA) [1,2]. The pixel descriptors have been used for modeling using MIA and the effect of correcting vertical and coupled signals by genetic algorithm has been discussed. the modeling stage have been compared using the partial least squares (PLS) methods and the orthogonal signal correction (OSC) method was combined with the partial least squares (PLS) method. the results of PLS, GA- PLS, OSC- PLS, OSC-GA- PLS methods have been compared with using statistical results. the resultant OSC-GA-PLS model had a high statistical quality ($R^2=0.98$) for predicting the inhibitory activity of the compounds [3]. MIA-QSAR (multivariate image analysis-quantitative structure activity relationship) proved to be a highly predictive approach. It also showed that the OSC-GA-PLS method is better than the traditional PLS method. It can also be used to predict the inhibitory activity of new compounds. Finally, molecular docking was performed for the selected compounds in QSAR with the appropriate receptor and acceptable results were obtained. These results are suitable for predicting compounds with better properties.

Keywords: MIA-QSAR, Molecular docking, PLS, PCA, OSC, OSC- PLS, GA- PLS, OSC-GA-PLS method

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Discriminating between patients with endometriosis and healthy women using gas chromatography-mass spectrometry and chemometrics techniques

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ABSTRACT

Chromatographic fingerprinting is a common method for diagnosis of complex and rare diseases [1]. In this regard, gas chromatography –mass spectrometry (GC-MS) is one of the best options for fingerprinting and identification of chemicals in biological samples [2]. On the other hand, due to the complexity of serum sample matrices and lack of selectivity in analytical instruments, multivariate chemometrics methods have been largely applied to extract maximum useful information from chromatographic data [1]. In the present contribution, a chemometrics-based strategy is proposed for GC-MS fingerprint analysis of endometriosis women. In this study, the blood serum of women with endometriosis (referred to Ibn Sina Infertility and Recurrent Abortion Treatment Center, Endometriosis Clinic) whose disease and severity were confirmed by laparoscopic surgery in 18 samples (three samples related to stage 1 and 2 and 15 samples related to stages 3 and 4 of the disease) were prepared. Also, blood serum of healthy women (confirmed by laparoscopic surgery that they do not have endometriosis) was prepared as a control group for 13 samples. Extraction of polar metabolites and derivation of polar metabolites for sample injection into gas chromatography-mass spectrometry were performed. The GC-MS signals were recorded by taking three scans per sample. GC-MS together with pattern-recognition methods such as principal component analysis (PCA), linear discriminant analysis (LDA) and sparse partial least squares Discriminant Analysis (sPLS-DA) were used to discriminate healthy women and women with endometriosis. The results showed excellent discrimination between the healthy women and women with endometriosis. The obtained results were encouraging and showed a promising potential of GC-MS and chemometrics methods for detecting healthy women and women with endometriosis type. The proposed approach in this work could classify more than 85% of the samples correctly, in each group.

Keywords : Endometriosis, Classification, GC-MS, PCA, LDA, sPLS-DA

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A Colorimetric Chemical Nose with Unmodified Gold Nanoparticles for Multiplexed Detection and Discrimination of Catecholamine Neurotransmitters

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Abstract

Catecholamine neurotransmitters, specifically, dopamine, epinephrine, and norepinephrine, are known as substantial indicators of various neurological diseases. Developing rapid detection methods capable of simultaneously screening their concentrations is highly desired for early clinical diagnosis of such diseases [1-2]. In contrast to single probes, sensor arrays are capable of discriminating different analytes that may possess similar structures and/or exist in complex mixtures [3-5].

We have designed an optical sensor array using gold nanoparticles (AuNPs) with four distinct particle sizes as sensing elements for discrimination and semi-quantitative determination of DA, EP, NE and L-dopa. The aggregation of AuNPs produces changes in both the color and UV-vis spectra of nanoparticles generating a visual molecular fingerprint of each analyte. Using this chemical/nose strategy, four catecholamines can be differentiated by chemometric methods including PCA, HCA and even baked-eye. The proposed array could successfully differentiate the four target analytes in urine samples, suggesting the potential applicability of the nanoarray for analysis of real biological specimens.

Keywords: Optical sensor array; Catecholamine Neurotransmitters; Gold nanoparticles; Chemometric methods

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Prediction of RT-PCR results using multivariate investigation of important blood biomarkers in patients with covid 19

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ABSTRACT

Coronavirus disease 2019 (COVID-19) infection has affected many people and has reached to pandemic state in the world nowadays (1). Clinical studies demonstrated that altered levels of some blood markers might be related to Results of RT-PCR and degree of severity and mortality of patients with COVID-19 (2-9). Different biomarkers are considered to show their potential in prediction of severity and determination of prognosis in patients with COVID-19. In this study, Lab parameters of 111 patient with sever COVID-19 and 120 healthy people were used. The significance of each biomarker was tested using ANOVA followed by Duncan test and was observed a significant difference between levels of NEU, LYM, LDH and CRP among two groups. Then in order to evaluate predictive ability of each parameter ROC curve and AUC analysis was applied on among two groups. In the next step the correlation between parameters were studied. In the next step, in order to test the predictive ability of all parameters, multivariate data was loaded and analyzed to with PLS-DA method. *Univariate analysis show that* NEU, LDH, CRP and NEU/LYM ratio are good predictors in prediction of RT-PCR results. The correlation analysis show that as a result of disease, a significant correlation is appeared between WBC with NEU, LYM and LDH and between CRP and LDH parameters. Applying multivariate analysis showed that PLS-DA has a good predictive ability in prediction of RT-PCR results. The value of AUC equal to 0.86 shows that multivariate data is better than univariate data to predict the results of RT-PCR. Risk factor in severity of covid-19 are WBC, CRP, LDH, LYM and NEU. The correlation of these parameters is changed significantly during infection in severe cases and when using multivariate data, this correlation between parameters leads to better prediction Ability in comparison to individual parameters.

Keywords: Blood biomarker; COVID-19; Correlation analysis; severity

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Comparison of prediction uncertainty in first order multivariate calibration methods

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ABSTRACT

Most of the studies that are done in chemistry include measurements and numerical calculations and usually in these studies the results are reported quantitatively. Since no quantitative results are of any value unless they are accompanied by some estimate of the errors inherent in them [1], so calculating the error and its sources in these studies is very important. In every calibration a calibration diagram is obtained which is fitted by regression. The choice of regression method depends on the nature of the data. In this work, the three of the most important multivariate methods meaning Classical Least Squares (CLS), Principal Component Regression (PCR) and Partial least Squares (PLS), are compared based on their precision in prediction and various datasets, both simulated and real data, are used for this purpose. To do so, we needed equations for determining the concentration uncertainty in all three methods. In the literature we could only find these equations for PCR and PLS methods [2] and the ones for CLS were missing. So, we derived them ourselves. The simulated data include a series of diverse data in which the level of overlapping of spectrum of the components in chemical system is different and the effect of the intensity of the overlapping on the uncertainty of concentration prediction has been studied. The results showed that there is no significant difference in prediction uncertainties between mentioned methods and all methods had almost identical precisions. But also, one should consider the necessary conditions to perform methods and not only the prediction uncertainty or method simplicity.

Keywords: prediction, uncertainty, Regression, multivariate calibration.

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Application of Data Point Importance (DPI) Concept in Supervised and Unsupervised Pattern Recognition

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ABSTRACT

Nowadays, with the advent of big data from a variety of processes, variable selection (VS) has become an important research topic in academia and industry. Feature selection techniques are widely applied but the use of abstract variables may lose some important information. PCA is a linear modeling method which has been commonly used to explore the data sets. By performing PCA, the experimental data matrix D is decomposed into two matrices: scores, containing the information related to objects, and loadings, containing the information related to variables (spectral information). PCA, through feature reduction and visual display, allows us to observe the sources of variation in complex data sets. It is, however, possible to extract much more information from a PCA. The principal components (PCs) are called latent variables. The purest variables can identify by convex hull of the principal component scores. It was shown by removing all other data points; the data set can be reduced to a very sparse set of essential data points [1]. In this work, the recent introduced concept in our group, a data point importance (DPI) is used in order to sorting information and variable selection in the data set. The DPI defines an easily calculable value corresponding to each row or column of the data matrix (data point) to reflect its impact on keeping the pattern of the data structure. Usually, a lot of data points have DPIs equal or very close to zero that they do not carry on useful information about keeping the data pattern. DPI values for some of the data points are significant and they have been sorted regarding to their importances. In this regard, the applicability of the DPI information sorting of objects and variables is tested for the exploration and classification of the diabetic and healthy people dataset. This data contains the concentration values of 163 lipids that represent the differentiation of healthy people from diabetics for 30 healthy individuals and 30 diabetics [2]. DPI values have been used for discovering the relative importances of variables via DPI plot (figure 1a) and also the DPI information sorting has been incorporated in score plot (figure 1b) for fast visualization of relative impacts of variables in classifications applications.

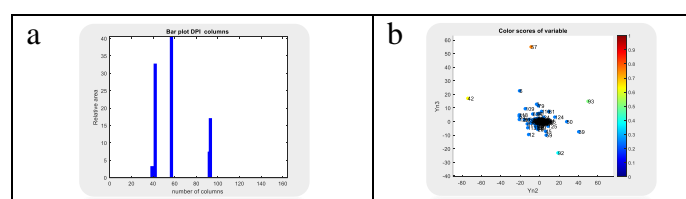


Figure 1. a) DPI plot, b) the colored latent variable plot.

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Comparison of embryo culture medium samples in IVF with infrared spectrometry using successive projections algorithm (SPA) - sum of ranking differences (SRD)

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ABSTRACT

Infertility is accepted as an essential health problem which vexes one per 6 couples. World Health Organization (WHO) defined it as the inability to succeed in a clinical pregnancy for 12 months or more of regular unprotected intercourse. In Iran, a meta-analysis has calculated infertility proportion of 10.9% [1]. In this work, the ATR-FTIR spectra of 16 embryo culture medium samples in IVF cycles, including 8 positive and 8 negative pregnancy results were compared and evaluated using several statistical methods such as cluster analysis and principal component analysis (PCA). Clinical pregnancy was validated by analyzing the serum β -Hcg levels, which was quantitatively examined after embryo transfer (ET) about 15 days later, in Imam Khomeini Hospital, Tehran, Iran (associated with Tehran University of Medical Sciences). Most signals in this region are related to carbohydrates and amino acids structure, at $1375\text{--}1385\text{ cm}^{-1}$ and 1455 cm^{-1} . In addition, these signals are related to the C-H bending vibrations (symmetric (sym)) in CH_3 and C-H scissoring in alicyclic $-\text{CH}_2$, respectively. The band at 1635 cm^{-1} is attributed to amide I due to C-O stretching vibration, which is a characteristic absorption band of β -sheet in proteins and amino acids structure. The band at 2920 cm^{-1} apporportioned with CH_2 stretching vibration of lipids, long-chain fatty acids and the band at 2952 cm^{-1} assigned to CH_3 stretching vibration of lipids, cholesterol esters, and fatty acids [2]. Principal component analysis (PCA) method was successfully applied to mid-IR spectra as outlier detection by application of Hotelling T^2 statistic procedure. Among the 1141 wavenumbers, 18 wavenumbers are selected which include the most spectral information by successive projections algorithm. The successive projections algorithm - sum of ranking differences approach for classification of the embryo culture medium samples exhibited the best performance and obtained accuracy, error rates, and non-error rate of 90%, 6% and 94% in the test set. Hence, the proposed method is rapid, simple and accurate for e discrimination of the embryo culture medium samples based on their morphology results.

Keywords: Embryo culture medium; Infrared spectrometry; Successive projections algorithm (SPA); Sum of ranking differences (SRD); Principal component analysis (PCA)

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Area of Feasible Figures of Merit (AF-FOMs) for second-order multivariate calibrations in MCR methods

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ABSTRACT:

In recent years, powerful and widely used MCR techniques have been extensively used to study chemical systems in various scientific fields. In most cases, the main goal in all these fields is to extract quantitative information from the systems under consideration, which is basically possible using calibration methods that use second-order and higher-order multivariate calibrations as a more suitable alternative to univariate calibrations. As with any calibration, reporting the analytical figures of merit (AFOMs) is a requirement, but computation and extracting multivariate figures of merit (MFOMs) for this type of calibration is not simple and evident. But in the last decade, MFOMs have been reported completely and one by one for different analytical methods in multivariate calibrations [1 and 2]. When MCR is used to analyze complex systems, area feasible solutions (AFS) are found that result from the rotational ambiguity associated with the bilinear decomposition of the data matrix, in which case a unique solution is not possible even with applied appropriate constraints. Therefore, instead of having specific MFOMs (such as sensitivity, selectivity, LOD, LOQ and etc.), there should be an MFOM for each possible solution within the AFS, resulting in a range of MFOMs. In this report, we present that there is a range of FOMs due to rotational ambiguity, and we also show that the values of FOMs in the AFS range have variations with a fixed movement for each of the MFOMs that can be fully interpreted, and in this way, it can be predicted which MFOMs will have maximum or minimum values in which range of the feasible band, or even what kind of incremental or decremental changes will occur. Due to the rotational ambiguity in the bilinear solutions, the systematic grid search method was used to compute all possible solutions and then to calculate the MFOMs inside the feasible band. We support our proposal on several simulations for two-component systems (one calibrated analyte and one uncalibrated interferent in test sample) and demonstrate its application on two experimental data aimed at the determination of drugs in water and human urine samples and generalized this to the three-component simulated system. In the feasible band for simulated noise-free two-component chromatographic data in the concentration space, the maximum sensitivity and selectivity in the inner boundary of the band have the values 0.3643 and 0.5006 respectively, and their minimum in the outer boundary with the values 0.1747 and 0.1863.

Keywords: Multivariate Figures of Merit (MFOMs), Area of Feasible Solutions (AFS), Rotational ambiguity, Second-Order multivariate Calibration, systematic grid search method, Multivariate Curve Resolution (MCR).

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Measurement error structure estimation and confirmation in a smartphone-based diffuse reflectance spectrophotometer

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ABSTRACT

The goal of this study is to identify sources and error structures for a smartphone-based spectrophotometer. Here, we introduced a smartphone-based diffuse reflectance spectrophotometer (smartDRS) with the advantage of rapid, simple, and cost-effective to acquire spectral information from a Cadmium Sulfide (CdS) pigment. Using a grating containing accessory, and the camera of the smartphone a simple smartDRS, with a resolution of 5 nm, was manufactured in our lab [1]. Error structure information is important to identifying and minimizing error sources, as well as to separate chemical meaningful variance from noise variance [2]. To analyze the error structure of smartDRS, we used the error covariance and error correlation matrices obtained through replication [3]. Multivariate analysis techniques as maximum likelihood common factor analysis (MLCFA) and multivariate curve resolution alternative least square (MCR-ALS) methods were used to the analysis of experimental error covariance matrices (ECMs) and obtain the number and contribution of error sources. We analyzed experimental ECMs using the MLCFA and the MCR-ALS methods and obtained three correlated error sources and three independent error sources. Correlated error sources were included signal-proportional noise ($U_{p,s}$), first proportional noise similar to signal ($U_{p,1}$), and second proportional noise similar to signal ($U_{p,2}$). Independent error sources were included *iid* noise (V_{iid}), signal-proportional noise ($V_{p,s}$), and proportional noise similar to signal (V_p). Also, we applied the maximum likelihood criterion based on the Wishart distribution for fitting the calculated ECM to the experimental ECMs [4]. Obtained confidence intervals based on resampling, at the confidence level of 95% and regarding the distribution of the Wishart's objective functions, did not illustrate a considerable shift as the number of replicates to estimated experimental ECMs was increased. The results show that the difference between the calculated ECM and experimental ECM was negligible, and the error sources used for the calculation of ECM were all valid.

Keywords: Diffuse reflectance spectroscopy; Smartphone; Measurement noise; Maximum likelihood; MLCFA.

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Classification of Fluoroquinolones based on colorimetric sensor array using modified silver nanoparticles and Artificial Neural Networks

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ABSTRACT

Colorimetric sensor arrays are efficient, effective, and sensitive tools for quick detection and identification of a wide variety of chemicals based on the colorimetric or fluorimetric responses as measured by spectroscopic instruments[1]. Colloidal plasmonic metal nanoparticles, especially Au and Ag nanoparticles, show a very dense color in the visible region of the spectrum, which is due to the localized surface plasmon resonance (LSPR) phenomenon[2]. Plasmonic nanoparticle-based colorimetric sensor arrays are usually based on the changes in the optical properties of the nanoparticles due to their aggregation and change in morphology [3]. In this study, a colorimetric sensor array comprised of four different modified AgNPS was constructed for the classification of fluoroquinolones. The kinetic-spectrophotometric data for the aggregation behavior of the modified nanoparticles toward a specific analyte were collected, vectorized and augmented to form a 80160-element vector per sample and a big data matrix for all samples (90*80160). The obtained fingerprints for all of the samples were processed by the Discrete Wavelet Transform (DWT) with the Symlet mother wavelet and two decomposition levels to reduce the dimensionality and complexity of data which results in a set of approximation coefficients with the dimensions (90*12002). The reduced data were then introduced to a genetic-algorithm optimized XY-Fused neural network as a supervised pattern recognition technique for the classification of the drug samples. The resulting top map and the classification parameters indicate the good classification performance of the proposed method toward the analyzed fluoroquinolones.

Keywords : Classification, artificial neural network, silver nanoparticles, colorimetric sensor array

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The effect of experimental factors on quality of extracted essential oils from sweet fennel using GC-MASS with the aid of chemometrics

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ABSTRACT

Experimental design is a fundamental element in nearly all science domains, including analytical chemistry and chemometrics (1). ANOVA commonly uses univariate data and is one of the fundamental tools in many research domains. It is used to identify the impact on the variation in a data set of various experimental conditions (2). One method is to hyphenate Analysis of Variance (ANOVA) and PCA, resulting in a method that is applicable to multi-factor, high-dimensional data. This combination has resulted in a family of methods, the most well-known of which is ANOVA-Simultaneous Component Analysis (ASCA) (1). ASCA is a data analyst-friendly method that can be used to extract more information from a multivariate dataset from a defined experiment than existing methods (2). ASCA was found to be especially useful for analyzing the impacts of complicated data sets with a large number of variables to measure (3). The goal of this study is to see how reliable a multivariate statistical tool (ASCA) is for studying significant metabolites and affecting factors like: mesh size, distillation time, and ultrasonic effect (as well as their interaction) in order to determine the high quality of Foeniculi fructus oil and compared with results obtained from the D-optimal method and ANOVA in GC-Mass data. The essential oil Foeniculi fructus (sweet fennel) is extracted from the ripe and dried fruits of the plant Foeniculum vulgare Mill. Steam distillation of crushed sweet fennel fruits is the most common method for obtaining essential oil from sweet fennel fruits. Steam distilled oils of sweet fennel seeds commonly contain: trans-anethole, estragole, d-fenchone, and other compounds. Bitter fennel oil is thought to have more fenchone (12-25%) and less transanethole (55-75%) than sweeter fennel (4). The main purpose of this work was to compare two methods of chemometrics (ASCA and ANOVA) to identify and qualify essential oil from sweet fennel by examining important metabolites derived from GC-Mass data.

Keywords: ANOVA, ASCA, sweet fennel, GC-Mass, Anethole, Estragole, D-Fenchone.

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Spectrophotometric determination of Dexamethasone using dispersive liquid-liquid microextraction combined with chemometrics

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ABSTRACT

Optimization techniques are aimed to improve the performance of a system, process, or product for maximizing its benefits. Several variables in an analysis approach can influence the quality of the system analyzed and hence the amplitude of the responses obtained (1). Analytical methods are therefore required to be optimized. This is assessed by analyzing their variables, the assumable levels and responses yielded by changes in the experimental conditions of the system (2). RSM is a set of statistically useful approaches for designing experiments, simulation, and analyzing the effects of independent factors on response. It can be used to weigh the relative importance of numerous influencing factors. RSM is fundamental goal is to select the optimal operational circumstances for desirable responses (3). ASCA (ANOVA simultaneous component analysis) is a user-friendly method for extracting more data from a multivariate dataset from a specific experiment than previous methods (4). The major goal of this study was to apply chemometrics methods such as ASCA, RSM, and CCD (central composite design) to identify key parameters in Dexamethasone microextraction. So, the pre-concentration and determination of dexamethasone concentration are proposed in this work using dispersive liquid-liquid microextraction (DLLME) and spectrophotometry, in combination with chemometrics approaches. The extraction and dispersive solvents for the one-variable-at-a-time procedure were chloroform and acetonitrile. The volume of extraction and dispersion solvents, the amount of salt, and the incubation time were all optimized using the CCD. For more study, ASCA (a multivariate statistical tool) was used for studying affecting factors on microextraction and their interaction, then compared with results obtained from the central composite design method and RSM to achieved the optimum condition to be determined the trace amount of dexamethasone. Under the optimum conditions, a linear calibration curve with a detection limit of 0.092 ppm in the 0.1-10 ppm range.

Keywords: Dexamethasone, Dispersive liquid-liquid microextraction, ASCA, RSM, Central composite design, Spectrophotometry.

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The use of MCR-ALS to study the simultaneous release of combined drugs moxifloxacin and Pseudoephedrine based on spectrophotometric spectra obtained

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ABSTRACT

The importance of the intelligent drug delivery system is evident in cases such as: reducing the frequency of drug use by keeping its amount constant in the blood, reducing the destructive effects of the drug on excretion and persistence in the renal system and increasing the functional efficiency of the drug compared to traditional and older methods. nowadays The use of efficient drug delivery systems in the combinatorial or multi-drug treatment of complicated diseases for effective and target-specific delivery of therapeutic agents necessitates the use of fast and reliable analytical techniques to reveal the true release profiles of the investigated drugs. The use of mathematical models is very useful in the case of controlled drug delivery systems as this approach enables, the prediction of release kinetics before the release systems are to be realized, and also often, it can measurement of some important physical parameters, such as the drug diffusion[1,2]. In this work First, Moxifloxacin and Pseudoephedrine were loaded simultaneously on poly (acrylic acid-co2-hydroxyethyl methacrylate) copolymer crosslinked with butane Diol dimethacrylate, and then simultaneous release of two drugs from the polymer substrate in buffer and blood serum sample as a real sample. The results of simultaneous release of drugs were analyzed by MCR-ALS and finally, the obtained profiles with different mathematical models were analyzed by Microsoft Excel Solver. simultaneous release of these drugs was monitored in different pH by the UV-vis spectroscopy. pH=7.3 is chosen as the optimal pH. In order to study the release kinetics, experimental data obtained from in vitro drug release were approximated by several mathematical models including Korsmeyer-Peppas, Ritger-Peppas, zero-order, first-order and Hixson-Crowell to determine the kinetics of drug release from the polymeric substrate. The results obtained from fitting the curves separated by MCR-ALS with different mathematical models showed that the Korsmayer-Pipas kinetic model has the best results for both drugs and the mechanism of release of both moxifloxacin and Pseudoephedrine drugs from the polymer substrate is non-Fickian diffusion.

Keywords: Spectrophotometry” multy-Drug delivery” Chemometrics” Combination drug” MCR-ALS

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A new insight into a wide range of protease inhibitors for covid-19 therapy using consensus molecular docking

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ABSTRACT

Coronavirus disease 2019 (COVID-19) is an infectious cause that its rapid global prevalence threatened the public health at the beginning of the second decade of the twentieth century. The exceptional character of novel coronavirus is swift outbreak which lead to observed far away from where it was first observed in Wuhan, China [1]. Consensus molecular docking is a key topics in molecular docking for drug design which predict the binding mode and energy of protein-ligand complex with reasonable accuracy [2-4]. Over the presented protease inhibitors [5-7] antiviral properties of 40 studied drugs was surveyed in Drug bank and appeared their other antivirus therapeutic applications. The candidate drugs mainly were protease inhibitor of human immunodeficiency viruses (HIV), hepatitis or Ebola. Firstly, affinity based molecular docking was done using MGLTools (version 1.5.6) software. A grid box with $60 \times 60 \times 60$ points was defined in the inhibitory site of maine protease of COVID-19 (PDB ID: 6LU7). Then, the similarity based molecular docking was performed using Molegro Virtual Docker (MVD). The predicted both binding energy and similarity score of studied inhibitors was compared with native inhibitor of protease for COVID-19 [8]. *Darunavi*, *Simeprevir*, *Sofosbuvir*, *Dasabuvir*, *Etravirine* and *UC2* respectively suggested inhibitors based on similarity score for treatment of COVID-19. It should be noted that COVID-19 therapy application of some candidate drugs contains *Darunavir*, *Remdesivir*, *Lopinavir*, *Galidesivir*, *Favipiravir* underway the clinical trials. The more collaboration of individual molecular docking provided by define a consensus score that is a co-weight linear composition of standardized binding energy and similarity score. For achieving a balance consensus score, values of binding energy and similarity score for candidate drugs were standardized then their respective values for native inhibitor after normalization of both terms. Its evident the consensus score values for *Dasabuvir* and *Sofosbuvir* is greater than its respective value for the template ligand. This study concluded the inestimable insight about the affinity and similarity of six proposed antiviral drugs for covid-19 therapy.

Keywords: COVID-19, Consensus molecular docking, Inhibitor, Affinity, Similarity.

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Molecular docking study and mapping the binding site of some antiviral nanobodies against receptor binding domains (RBDs) of SARS-CoV-2 B.1.617

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ABSTRACT

The B.1.617 lineage of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), has spread throughout India, displacing other pre-existing lineages [1]. The SARS-CoV-2 B.1.617 is case of Delta variant pandemic of coronavirus which there is no country in the worldwide is safe from its harm and consequences [2]. The neutralization ability of 51 antiviral nanobody toward RBDs of SARS-COV 2 B.1.617 against the human angiotensin converting enzyme 2 (ACE2) was repurposed using cluspro Server [3]. The candidate VHH selected from 1196 nanobodies that was available in structural antibody database (SAbDab) [4]. The 21 selected VHH experimentally was neutralized the member glycoprotein of Severe acute respiratory syndrome coronavirus 1 (SARS-COV-1), Middle East respiratory syndrome (MERS), Human immunodeficiency viruses 1 (HIV-1) or respiratory syncytial virus (RSV). Also, 15 candidate nanobodies were blocking the Nef and capsid protein p24 of human immunodeficiency viruses 1 (HIV-1) or capsid protein VP3 of poliovirus. Moreover, different conformations of nanobodies that are experimentally involved in the RBD of SARS-COV 2 were adapted from PDB. Regardless of the synthetic nanobodies blocking of spike glycoproteins RBD of SARS-COV 2, other natural VHH occurring in *Lama glama*, *Vicugna pacos* or *Camelus dromedaries*. The crystallography structure of RBD-ACE2 of SARS-COV 2 (6LZG) as well as delta variant mutant RBDs of SARS-CoV-2, T478K (7ORA) and L452R (7ORB) was taken from protein data bank (PDB). It was seen, *Sb23*, *SR4*, *VHH PVSS8A*, *VHH 17B*, *VHH PVSP29F*, *sdAb19*, *VHH PVSP19B*, *VHH-55*, *VHH A12*, and *VHH PVSP6A* respectively was proposed for neutralization of T478K RBD with an estimated binding energy greater than -792.4 (kcal/mol) for ACE2. Also, *VHH PVSP6A*, *Sb23*, *VHH PVSP29F*, *SR4*, *VHH-55*, and *VHH PVSP19B* are others proposed nanobodies according the estimated binding energy greater than -812.3 (kcal/mol) for ACE2- L452R. Overall, *Sb23*, *VHH PVSP29F*, *SR4*, *VHH-55*, and *VHH PVSP19B* are repurposing nanobodies for based on the censuses decision making for both against both T478K and L452R RBDs of SARS-CoV-2 B.1.617 strain.

Keywords: SARS-CoV-2 B.1.617, Nanobody, Molecular docking, T478K, L452R.

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Simultaneous determination of anti-breast cancer drugs in blood plasma by Excitation-emission Fluorescence Spectroscopy and N-Way Calibration Methods

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ABSTRACT

Breast cancer is the most common disease in women and chemotherapy is a major treatment of cancer [1]. Clinical evaluations, anti-cancer drugs (ACDs), and individualized medicine lead to safer treatment of patients with breast cancer [2]. In recent decades, various analytical methods were developed to analyze therapeutic drugs, especially in patients with need for advanced treatments. In many circumstances, simultaneous quantification of ACDs is vital to monitor the kinetics and metabolism of drugs in living organisms. Simultaneous determination three important anti-breast cancer drugs including capecitabine (CAP), paclitaxel (PAC), and vinorelbine (VIN) were considered, in this study. High sensitive excitation-emission fluorescence (EEF) technique was utilized to determine the analytes of interest. Due to intense overlapping between analyte peaks, the collected EEF data was non-selective. Moreover, interference overlapping cause difficulties for precise calibration of the analytes [3]. In this work, the collected EEF data was processed using N-way chemometric methods for alleviating the problem of spectral overlapping and unknown interferences. Multiway variable importance in projection (NVIP) and multiway partial least squares (NPLS) algorithms were used for variable selection and modeling steps, respectively. The obtained EEF data was huge and complex, so, data quality was increased by removing Rayleigh scattering, savitzki-golay smoothing, and multiway preprocessing methods such as centering and double slab scaling. The prediction ability of the NPLS model was improved after selection of the important variables using NVIP algorithm. Calibration and validation steps were performed in both aqueous and blood-plasma samples. The correlation coefficient (R^2) value for the validation set for CAP, PAC, and VIN are 0.896, 0.843, and 0.924 in aqueous samples, and 0.75, 0.698, and 0.713 in plasma samples, respectively. The suggested method is fast, sensitive, selective, low-cost, and can be used as an alternative and environmentally friendly approach for simultaneous determination of drugs in biological samples.

Keywords: Excitation-emission matrix fluorescence spectroscopy, Second-order advantage, Multiway partial least squares algorithm, Multiway variable importance in projection, Anti-cancer drug

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The use of handheld near-infrared spectroscopy combined with chemometric techniques for detecting adulteration in industrial lime juice samples

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ABSTRACT

The combination of chemometrics and near-infrared spectroscopy (NIRS) has been previously used for the detection of food adulteration in many cases [1]. The major advantage of NIRS is that usually no sample preparation is needed; hence the analysis is simple, cheap, and very quick. In addition, it can be carried out online employing handheld devices [2]. However, the knowledge of multivariate data analysis and chemometrics is necessary to magnify the relevant information and lessen the undesirable information in the spectra obtained from NIRS. Since handheld NIRS enables rapid screening of adulteration in food samples, this study was designed to determine the feasibility of handheld NIRS in combination with the chemometrics approach in the detection of citric acid adulterated industrial lime juice samples. In the current study, NIR spectra for 24 genuine and 168 adulterated industrial lime juices were recorded in triplicate in the reflectance mode using a handheld NIRS (Tellspec, 700 to 1900 nm) connected to a smartphone. Adulterated samples were prepared by means of dilution of genuine samples with water at different levels (10, 15, 20, 25, 30, 35, and 40%) and subsequently, adjusting the Brix number by the addition of exogenous citric acid. Sample outliers were removed using principal component analysis (PCA). Evaluation of the PCA scores plot revealed that PCA analysis can provide an estimation of the nature of lime juice samples based on their NIR spectra. In addition, one class modeling approach was employed for the detection of adulterated samples using MATLAB software [3]. On this matter, soft-independent modelling of class analogy (SIMCA) model by multiplicative scatter correction (MSC) preprocessing resulted in 89% sensitivity in the prediction of genuine samples and 99% specificity in the prediction of adulterated samples with an overall accuracy of 94%. Our findings demonstrate the potential of chemometrics in combination with portable NIRS for monitoring lime juice quality in terms of genuine or adulterated nature. However, further investigations using classification models (e.g., partial least squares-discriminant analysis, PLS-DA) and regression models (e.g., partial least squares regression, PLSR) are required to confirm the promising results of the current study.

Keywords: Adulteration, Lime, handheld Near-infrared, PCA, SIMCA

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Untargeted metabolomics based on gas chromatography-mass spectrometry and advanced chemometric tools for identifying responsible metabolites in lettuce exposed to emerging contaminants

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ABSTRACT

In a context of climate change and a burgeoning world population, the pressure on water resources will grow. A great number of integrated water resource management schemes are being implemented with focus on the 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 gas chromatography-mass spectrometry (GC-MS) and the huge amount of acquired data was analyzed by advanced chemometric techniques. For this purpose, seedlings of lettuce were planted in experimental units consisted of 4.5 L cylindrical amber glass pots ($\varnothing = 30$ cm and 25 cm high) fitted with a tubing outlet at the bottom connected to drainage tubing ($\varnothing = 1.5$ cm). Treatments consisted of direct application of 0 (control sample), 100 and 500 $\mu\text{g L}^{-1}$ of parabens (methyl, ethyl, propyl, and butyl-) and drugs (carbamazepine, mefenamic acid, diclofenac, gemfibrozil, and naproxen) per experimental unit (exposed samples with three replicates). Treatments were distributed among 10 experimental, starting 52 days after planting. After sampling, the leaves were comminuted with liquid nitrogen and stored at -20°C until analysis. The extraction of metabolites was performed using a solvent extraction procedure as reported elsewhere [2]. 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 into GC-MS. Then, two-way GC-MS data of control and exposed samples were arranged in a data matrix and analyzed by Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS) to recover the pure elution and mass spectral of the metabolites [3]. The identity of the resolved components was determined from the spectral profiles match with NIST MS library. Then, the peak areas of the identified metabolites were calculated and arranged in a new data matrix to be analyzed by Partial Least Squares-Discriminant Analysis (PLS-DA) to find a boundary between control and exposed samples and also to find responsible metabolites using variable importance in projection (VIP). Finally, the metabolic pathways were determined using KEGG database. The metabolic response indicates that exposure to CECs at environmentally relevant concentrations causes large metabolic alterations in lettuce (carbohydrate metabolism, TCA cycle, pentose phosphate pathway, and glutathione pathway).

Keywords: Metabolomics; Chemometrics; Gas Chromatography-Mass Spectroscopy; Lettuce; Paraben.

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Identification of important structural features for selective inhibition of cyclin-dependent kinase inhibitors using machine learning techniques

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ABSTRACT

Cyclin-dependent kinases (CDKs) are key regulators of the cell cycle that provides domains essential for enzymatic activity. To date, many kinase inhibitors have been approved for cancer treatment. Due to wide range of activities and functions for all kinases, there is a vital need for development of selective kinase inhibitors for targeting only some specific types of them for effective treatments. In the present contribution, we seek to find selectivity in structural patterns of inhibitor molecules for three important isoforms of kinases [2, 3]. In this regard, ~5086 molecules were loaded from the Binding database for CDK1, CDK2 and CDK5 enzymes. Referring to various articles and sources, the ranges of bioactivity (IC_{50}) for different receptors have been determined and the molecules were divided into two active and inactive categories in each class [4]. A wide range of molecular descriptors including, topological, constitutional, 2D- and 3D- descriptors were calculated for each molecule. The datasets were randomly split into 70% calibration (training) and 30% test sets. The best set of molecular descriptors were selected using variable importance in projection (VIP) algorithm. Counter propagation artificial neural network (CPANN), k-nearest neighbor (KNN), partial least squares-discriminant analysis (PLS-DA), supervised Kohonen networks (SKN), and support vector machine (SVM), were applied for modeling the activity of the molecules using the VIP-selected set of molecules. The performances of the models were evaluated by standard metrics derived from the confusion matrix and the values of sensitivity, specificity, precision and non-error rate were calculated for training and test sets. The accuracy values which refer to the ratio of correctly classified compounds were calculated to measure the overall performance of classifiers. The values of prediction accuracy in the test set for SKN and SVM methods were more than 80%. All of the optimized classification models represented high statistical quality and predictive ability with accuracy greater than 78% for the test sets. The high accuracy values of the obtained classifiers for the training and test sets demonstrate that the information provided is reliable for describing and predicting the activity of CDK inhibitors. It helps for designing molecules with better therapeutic potency and reduced side effects. The results in this work suggest some important molecular features that help medicinal chemists to develop selective inhibitors for different isoforms of kinases [2, 3].

Keywords: Chemical space, Data mining, Isoform, Kinase, Selective drug design

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Functionality of Rotational Ambiguity in Self-Modeling Methods to Signal Contribution of Chemical Component

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ABSTRACT:

Self-modeling curve resolution (SMCR) methods are a powerful tools in chemometrics, used for the decomposition of the measured data matrix to the product of two chemically meaningful matrices, containing the pure profiles. But, the results of these methods may be ambiguous. There are two types of ambiguities in SMCR methods, intensity and rotational ambiguities. Rotational ambiguity is the more difficult source than intensity ambiguity in SMCR methods. In The presence of rotational ambiguity, SMCR methods resolve data sets to a range of feasible solutions. Implementing the adequate information and constraints, eg, non-negativity for constituent concentrations and for spectral signals, unimodality for evolving signals such as those from chromatographic and zero regions where the contributions of certain components are known to be absent and etc, can reduce or remove the rotational ambiguity. In some special cases, the minimal information of the system, constraint of non-negativity is sufficient for obtaining unique solutions [1]. Tauler and et al, showed that the degree of rotational ambiguity depends on the selectivity and the similarities between the pure concentration and spectral profiles of components [2]. In this work we are showing that rotational ambiguity does not depend only on the selectivity. Increase or decrease of contribution of each component that present in the data matrix effects the rotational ambiguity of all species. Several simulated second-order chromatographic two-component systems are studied regarding the comparison of rotational ambiguity with increasing of contribution of each component, using computing volume of the area feasible solutions. Also the effect of contribution of components on accuracy of quantitative analysis was analyzed with experimental second-order excitation-emission fluorescence data sets. These data sets are several two component systems include Tyrosine as analyte and Tryptophan as interferent which is present in the unknown samples. Analysis of experimental data sets with grid search method and calculation the concentration range and evaluating the error prediction range showed that increasing or decreasing of contribution of components is effective on accuracy of quantitative analysis using SMCR methods.

Keywords: Self-modeling curve resolution, Rotational ambiguity, contribution of component

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Study the inhibitory effect of some antiviral flavonoids against main protease of COVID-19 by molecular docking

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ABSTRACT

Spread of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) pandemic across the worldwide causing global effort for discovery of vaccine or drug. SARS-CoV-2 is a members of coronavirus large family which are enveloped, positive-sense and single-stranded RNA (+ssRNA) viruses that termed as coronavirus disease 2019 (COVID-19) [1]. The potential of 39 antiviral flavonoid for inhibition of main protease of COVID-19 was investigated using molecular docking approach. The studied flavonoids were protease inhibitor of human immunodeficiency viruses (HIV), severe acute respiratory syndrome (SARS), hepatitis C virus (HCV) or Ebola virus. The both affinity and similarity based molecular docking approach was applied to improve the reliability of proposition. Firstly, the affinity based molecular docking approach was done using MGLTools (version 1.5.6) software. A grid box with $60 \times 60 \times 60$ points was defined in the inhibitory site while the crystallography structure of main protease of COVID-19 (6LU7) was taken from protein data bank (PDB). The predicted binding energy of flavonoids compare with co-crystallized inhibitor of protease for COVID-19 (N3) [2]. Then, the similarity screening was performed using Molegro Virtual Docker (MVD) against template N3 [2,3]. 6 hydrogen acceptor, 9 hydrogen donor, 9 steric criteria and 49 ring groups was considered as template group of native inhibitor N3 while a single atom may contribute to several centers in the several groups. The estimated binding energy proposed six flavonoids for COVID-19 therapy. The similarity screening arranged the candidate flavonoids respectively as *Quercetin 3-O-(2,6-digalloyl)-R-Larabinopyranoside* from *Acer okamotoanum*, *Tomentin D* and *Tomentin A* from *Paulownia tomentosa*, *Corylifol A* and *psoralidin* from *Psoralea* and *Ladanein* from *Lamiaceae* [4-7]. The values of similarity score for these phytochemicals respectively was -340, -225, -221, -213, -176 and -152 while the estimated binding energy was -9.52, -7.74, -7.67, -8.09, -8.58 and -8.02 (kcal/mol). Also, ligand map probing of native and six flavonoids was shown Phe 140, Gly 143, His 164, Glu 166, Gln 189, Thr 190, Thr 26, Cys 145 and Asn 142 amino acids of active site of main protease of Covid-19 commonly was in the hydrogen or steric interactions with these inhibitors. This study outstanding the inhibitor effect of some antiviral non-nutrient plant compounds against main protease of COVID-19.

Keywords: COVID-19, Molecular docking, Flavonoid, *Acer okamotoanu*, *Paulownia*, *Psoralea*, *Lamiaceae*.

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Application of vibrational spectroscopy tandem with chemometrics in the assessment of authenticity and adulteration of sport whey protein supplements

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ABSTRACT

Nowadays, one of the major concerns among athletes is finding authentic sports supplements following some illegal adulteration and contamination scandals. Whey protein powder is one of the most used supplements among athletes to build a muscular body which makes this supplement attractive for fraudsters. It could be adulterated by some cheaper materials such as milk powder. Hence, the determination of the authenticity of sports supplements has become a worldwide concern. This work aimed to propose near-infrared spectroscopy (NIR) as a fast and non-destructive testing tool for the detection of adulteration of whey protein supplements. After some investigations; we found out, whey protein powder could be adulterated with milk powder, maltodextrin, and milk whey powder in our country. These adulterants are used as bulking agents because of their lower price. Therefore, we made our adulterated samples in a range of 2% WW⁻¹ to 100% WW⁻¹ by each of these adulterants. NIR spectra were collected from samples in a range of 10000 cm⁻¹ to 4000 cm⁻¹ three times and the average of them was used for multivariate analysis. A variety of data pretreatments including first derivative, standard normal variate (SNV), multiplicative scatter correction (MSC) and combination of SNV-detrend, MSC-detrend, first derivative-SNV-detrend, and first derivative-MSC-detrend were examined after applying mean center. The best preprocessing method was selected according to the pattern of discrimination analysis which was principal component analysis (PCA) in this study. One hundred and ten sport whey protein supplements were purchased from the market and all these steps were repeated for them as a test set. The PCA results revealed a good pattern of classification after first derivative preprocessing. Thus, it seems NIR could be implemented as a rapid screening method for the detection of milk powder, maltodextrin, and milk whey powder in sport whey protein supplements.

Keywords: Adulteration, Chemometrics, Near infrared spectroscopy, Protein, Supplements



A green approach for electrospun fiber-in-tube solid phase microextraction of acidic red dyes from juice samples

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ABSTRACT

Extra consumption of synthetic food dyes has some side effects such as DNA damage, allergy, and asthmatic reactions, carcinogenesis, and hyperactivity. So acceptable level of dyes must be controlled and is necessary to develop reliable analytical methods for extraction and determination of these chemicals in daily use products [1]. In this research, Fiber-in-tube solid phase microextraction (FIT-SPME) followed by HPLC-UV for extraction and determination of acidic red dyes (Amaranth, Ponceau 4R, Allura red, Carmoisine, and Erythrosine) in juice samples. There are some advantages in this device such as reduction of back pressure during extraction and desorption, higher surface area of the coating, and also smaller void volume of the extraction tube [2]. In this way, the fibers were fabricated with a composite of chitosan and polyvinyl alcohol by electrospinning method to achieve nanofibers with high surface area and porosity. Non-toxicity, biodegradability, biocompatibility, and hydrophilicity led to the use of chitosan in various fields. Moreover, there are amino and hydroxyl groups in its structure that make it as an inexpensive and recyclable bio sorbent for organic dyes by electrostatic interaction. Pure chitosan has a limited electrospinnability so to achieve the fine fibers, it should be blending with some co-polymers such as PVA. It is a synthetic polymer that is water-soluble, chemical resistive, non-toxic, biocompatible, and biodegradable [3]. The effective parameters on the extraction efficiency including desorption solvent type, extraction time, extraction flow rate, desorption flow rate, and desorption solvent volume were optimized by one variable at a time and experimental design approaches. Response surface methodology (RSM) is a statistical technique to display the coherency between variables, reduction of experiments number, materials, time and costs [4]. RSM based on an orthogonal and rotatable central composite design (CCD) in five levels was employed to optimize the quantitative factors. Due to the large number of experiments, they were divided into 3 blocks and carried out in 3 different days. Under the optimum conditions, the method showed good dynamic linearity in the range of 1.00-750.00 $\mu\text{g L}^{-1}$ with LODs in the range of 0.30-7.57 $\mu\text{g L}^{-1}$ and coefficient of determinations higher than 0.9943. The intra-day and inter-day RSDs were in the range of 2.5-9.5 % and 7.3-12.7 % respectively. Finally, this technique was applied for extraction and determination of analytes in beverages samples such as pomegranate, red grape, and sour cherry juices with acceptable and satisfying results.

Keywords: Acidic dyes, Chitosan, Electrospinning, Experimental design, Fiber-in-tube solid phase microextraction, Polyvinyl alcohol.

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Authentication of ink samples with ATR-FTIR spectroscopy associated with PLS-DA method

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ABSTRACT

Recently, adulteration and abuse in the production of industrial products with the aim of gaining more profit have caused the increase of consumers demand for supervision and authentication of these products. One of the strategic products used in different fields is ink. On the other hand, vibrational spectroscopic methods as a fast, strong and non-destructive tool provide useful and effective information on the chemical structure of the ink such as solvents and resins [1-3]. In this study, infrared (IR) spectroscopy and chemometrics statistical method were used to classify seven different brands of pen ink. Available samples were classified into 7 classes (5 original and 2 adulterated). Then, preprocessing methods were performed using mean centering (MC) and standard normal variate (SNV) method. In the next step, they were divided into two sets of 44 samples as training set and 19 samples as testing set by the Kennard-Stone algorithm, being analyzed by partial least squares discriminant analysis (PLS-DA) method. Error rate of these models with genetic algorithm (GA) and without it were 8% and 13% for the PLS-DA, respectively. Thus, it can be concluded that the presented method demonstrated the rapid, simple, without any chemical preparation and effectiveness classification method of ink samples by IR spectroscopy combined chemometric technique

Keywords: Inks; PLS-DA; Chemometric; Infrared spectrometry; GA

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A Poly(arylene ethynylene)-Based Microfluidic Fluorescence Sensor Array for Discrimination of Polycyclic Aromatic Hydrocarbons

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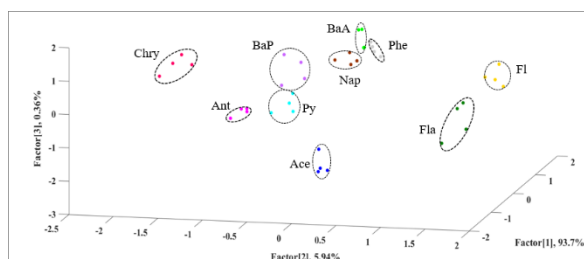
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ABSTRACT

Polycyclic aromatic hydrocarbons (PAHs) are mainly byproducts of incomplete combustion of coal/petroleum and pyrolysis of organic components. These components are listed as priority pollutants by the European Union and the U.S. Environmental Protection Agency due to carcinogenicity, teratogenicity, and mutagenicity. Hence, the identification and monitoring of PAHs as a worldwide concern has attracted great attention among researchers [1]. Recently, microfluidic paper-based analytical devices (μ PAD) have shown the high potential of paper as a substrate material in microfluidic technology it is easy to access, cheap, and chemically compatible for many applications [2]. Here, a simple microfluidic fluorescence paper-based sensor array designed for the rapid detection and simultaneous classification of ten PAHs (naphthalene (Nap), anthracene (Ant), phenanthrene (Phe), fluorene (Fl), pyrene (Py), acenaphthene (Ace), chrysene (Chry), benzo[a]anthracene (BaA), benzo[a]pyrene (BaP), fluoranthene (Fla)) using poly(arylene ethylene)s as sensing elements. Fluorescence intensity changes of the sensor array were recorded using a smartphone (irradiated by a UV lamp of 366 nm) and then linear discriminant analysis (LDA) is used as a pattern recognition method, analyzing the discrimination performance of the sensing array. This method offered accurate discrimination of 10 different PAHs at various concentrations in a range of 5-100 mgL⁻¹. 10 different PAHs were correctly identified using linear discrimination analysis. 100% classification accuracy was achieved for model training, validating LDA model by cross-validation resulted in 90% classification accuracy for 5 mg L⁻¹.

Keywords: Polycyclic aromatic hydrocarbons, Poly(arylene ethynylene)s, Fluorescence paper-based sensor array



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The Role of Metabolomics in Diagnosis of Covid-19 for Inhibition of Coronavirus Pandemic

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ABSTRACT

SARS-CoV-2 or covid-19 is a systematic virus infection has spread worldwide since 2019 (1). According to World Health Organization (WHO) the number of people, infected covid-19 is increasing rapidly. Coronavirus pandemic has become a global issue and the mortality rate is on the rise. This virus impairs the body's organ function and exerts a significant impact on metabolism but there is little information on how the virus affects metabolism. According to some researches, SARS-CoV-2 primarily causes lung infection through the binding of ACE2 receptors (2). Recognizing the virus characteristics and metabolism can help to provide a safe vaccine. Metabolites are small molecules that their amount in the body or the ratio of some of them change due to cellular metabolism and its disruption indicates the onset of disease and infection (3). The results of research showed metabolomics analysis revealed abnormal levels of some metabolites in the body, so checking the profile of metabolites and finding biomarkers play an important role in covid-19 faster diagnosis. Traditionally, biomarkers play a pivotal role in the early detection of disease etiology, diagnosis, treatment, and prognosis (4). Therefore, to understand the host response to covid-19 and to identify biomarkers in biological samples such as serum, plasma, urine, respiratory gases, saliva, etc. omics science such as transcriptomics, proteomics, and target and untargeted metabolomics (5) based mass spectrometry (6) and nuclear magnetic resonance spectroscopy (7) were used. Based on an article, Benzoate, β -alanine, and 4-chlorobenzene acid were first reported to be used as potential biomarkers to distinguish covid-19 patients from healthy individuals; taurochenodeoxycholic acid 3-sulfate, glucuronate, and N, N, N-trimethyl- alanylproline betaine are the top classifiers in the receiver operating characteristic curve of covid- severe and covid-nonsevere patients (8). Patients with serum levels of Galectin-3 above 35.3 ng/ml had increased risk for mortality (9). Non-invasive detection of methylpent-2-enal, 2,4-octadiene 1-chloroheptane, and nonanal in exhaled breath may identify patients with covid-19 (10). Metabolomics analysis in covid-19 patient reveals abnormally high levels of ketone bodies (acetoacetic acid, 3-hydroxybutyric acid, and acetone) and 2-hydroxybutyric acid, and the reduction in essential amino acids, tyrosine, and glutamine (11). According to literature, chemometric methods used to analyze obtained data from metabolite profiles. By using chemometric methods like PLS and PCA people classified into a healthy, mild patient and severe patients. In this article, some recent papers about the role of metabolomics in covid-19 reviewed and some metabolites and biomarkers in patients were reported.

Keywords: "Metabolite. Covid-19. Biomarker. Chemometrics. Omics science. SARS-CoV-2"

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Discrimination of original and fraud cigarette brands using a paper-based optoelectronic nose based on MoS₂ QDs and organic dyes

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ABSTRACT

The E-nose technique usually comprises two main components, the first being the sensory unit and the next is the data processing unit which comprises machine learning algorithms to predict and classify the outcome. The oxygen-functionalized compounds are oxidized to acids on the surface of MoS₂ QDs [1]. Here, combination of these catalytic properties of MoS₂ QDs with the colorimetric responses of organic reagents was investigated to design a portable paper-based colorimetric sensor array for discrimination of cigarette smoke VOCs, as a complex matrix. First, the designed sensor array was used for classification of fourteen different cigarette VOCs. Principal component analysis (PCA) and linear discriminant analysis (LDA) for classification of data were used as unsupervised and supervised methods, respectively. In PCA analysis, the accuracy was 96 and 86% for the training set and cross-validation set, respectively. The LDA analysis was also performed on the raw data (accuracy was 100% in both training and cross-validation sets). The raw data obtained from image analysis were used as input in LDA, the quality of the row databases was good enough that was no need to pre-processing steps. In the second step, the sensor was validated by discrimination of five cigarette brands, the accuracy was found to be 100% for training set and 82 % for cross-validation set. In the third step, four of the best-selling brands in the Iranian market (Bahman Kootah, Omega, Montana gold, and Williams), all of which also had fraud samples (eight in total), were studied by the developed sensor array. The accuracy of discrimination of these four brands and their frauds were all equal to 100%. Next, all original and fraud samples (126 cigarette) were analyzed in a matrix with dimensions of (126 × 27) by LDA. The accuracy of this LDA model was 98%. Finally, the results of the measurements compared to the results originating by a standard analytical technique. FTIR spectroscopy of cigarette smoke was only able to discriminate between original and fraud cigarette samples, but did not provide an acceptable answer for classification of different brands of cigarettes. The analytical procedure proposed here, is fast, cheap, user-friendly, and reliable. The selectivity the developed sensor array could make it a valuable tool to differentiate original cigarettes from counterfeit products crossing every day national borders around the world.

Keywords: E-nose, Chemometrics, Pattern recognition, Colorimetric sensor array, MoS₂ QDs, Cigarette.

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Determination of saffron adulteration thorough the package using Vis-NIR hyperspectral imaging and chemometric techniques

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ABSTRACT

Food authenticity is a very important field of research which enables consumers to get what they pay for and increases their overall level of trust of food. The occurrence of multiple widespread incidents of food fraud over the past decade has increased attention to issues of food authenticity as well as focus by both the food industry and regulatory agencies. Saffron is one of the most important spices with different properties ranging from food coloring and flavoring properties to health benefits. However, because of its limited production and high price, it is always a good candidate for adulteration [1,2]. Hyperspectral Imaging (HSI) has been proposed in recent decade as a reliable tool for food authenticity. This technique combines spectroscopy and imaging techniques, enabling the acquisition of hyperspectral images. These images are composed of reflectance pixel maps containing hundreds of channels, one per wavelength [3]. To the best of our knowledge, there is no study in the literature for saffron authenticity and adulteration detection with HSI and chemometric techniques. Therefore, the objective of the present study was combination of Vis-NIR HSI with chemometric techniques for saffron authentication and adulteration detection (safflower, calendula and style) in intact form thorough the package. Three different packages of thin and thick plastic envelope and poly-crystal were tested. For this purpose, HSI images of 38 intact authentic saffron samples were recorded in spectral range 400-950 nm. Then, multivariate curve resolution-alternating least squares (MCR-ALS) was used for obtaining pure spatial and spectral profiles of the components and then, principal component analysis (PCA) was applied to the resolved spatial profiles of saffron to find possible patterns of authentic samples. According to the PCA results, six authentic saffron samples were selected to make pooled sample for further analysis. Binary mixture of pooled saffron sample and safflower, calendula and style adulterants were prepared in five levels (5, 10, 15, 25, 35% (w/w)). Partial least squares-discriminant analysis (PLS-DA) algorithm was used for the classification of MCR-ALS resolved spatial profiles of saffron. The PLS-DA performance was evaluated using sensitivity (sen), specificity (spe) and accuracy (acc) which were 100 % for calibration, cross-validation and prediction sets using three different saffron packages. Finally, a dataset composed of pooled saffron samples and three adulterants in different levels was designed using D-optimal design and analyzed by MCR-ALS, PCA and PLS-DA methods. Again, the good values of sen, spe and acc for PLS-DA were obtained which confirmed the validity of the proposed method. It is concluded that the developed model can be used as a routine method to check the authenticity of intact saffron through the package.

Keywords: Saffron, Hyperspectral imaging, Chemometrics, Multivariate curve resolution, Adulteration.

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Hyperspectral Imaging System to Determine Volatile Oils Content of Medicinal Plants

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ABSTRACT

This study was conducted to non-destructively and rapidly determine total volatile oils and therefore the quality of *Nepeta Crispa* Willd samples using hyperspectral imaging system. *Nepeta Crispa* Willd is a medicinal plant with high nutritional and therapeutical properties. The plant samples were procured from different geographical origins and processed using different drying methods (sun, shade, microwave, oven, vacuum oven, and freeze dryer). Reflectance spectra (400-1000 nm) of the samples were collected and filtered using Savitzky Golay (SG) smoothing method. Principal Component Analysis (PCA) was used for a visual description of the samples and to select more effective wavelengths in order to do data reduction. Two artificial intelligence models (Radial Basis Function and Multilayer Perceptron Neural Network models) were created based on the total and more effective wavelengths (727-900nm) for volatile oils content prediction. Results indicated that the hyperspectral imaging system coupled with artificial intelligence models was capable to predict the total volatile oils content of the *Nepeta Crispa* plant with a high degree of accuracy.

Keywords: Geographical Origin, Herbal, Essential Oils, Quality



An efficient method for measuring the similarity of protein sequences based on physicochemical properties

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ABSTRACT

The graphical representation of protein sequence is a simple and common way to visualize protein sequences. In this study, a numerical descriptive vector for a given protein sequence is calculated based on twelve physicochemical properties of amino acids (AAs) and principal component analysis (PCA). Each entry of the descriptive vector corresponds to one AA in the sequence. By this vector, an intuitive spectrum-like graphical representation of protein sequence is proposed. Squared correlation coefficient as well as moving window correlation coefficient, as a new similarity/dissimilarity measure, were used to compare different sequences. Applicability of the proposed method is assessed by analyzing the nine ND5 proteins. The results revealed the utility of the proposed method.

Keywords: Similarity analysis, Protein sequence, Graphical representation, Principal component analysis, Physicochemical property, Moving window correlation coefficient.



Quality control of olive oils based on class discrimination methods

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ABSTRACT

Olive oil is associated with healthy food due to its high content of Vitamin E, antioxidants, and mono-unsaturated fatty acids (1). Olive oils are available in different qualities such as extra virgin, virgin, olive oil, and others. One of the most important problems is grade definition of olive oils in industry. Internationally, most countries use the International Olive Oil Council (IOOC) standards(2). The IOOC has a United Nations charter to develop criteria for olive oil quality and purity standards. There are different classical methods which they are used to define the grade of olive oils. However none of these method is sufficient individually and proposing an economic, comprehensive and easy method for grade definition of olive oil is very important (1). Metabolomics is the study and systematic quantification of small molecules in biological samples (cells, tissues, organs, biofluids, or whole organisms), and thus complements efforts from other high throughput omics platforms such as genomics, transcriptomics, and proteomics as an indispensable platform. Gas and liquid chromatography or capillary electrophoresis linked to mass spectrometry (GC-MS, LC-MS, and CE-MS) are common platforms for generating metabolomics data. In particular, polar primary metabolites (such as sugars, amino acids, amines, sugar phosphates, or sugar alcohols) and fatty acids are well-suited to gas chromatography mass spectrometry (GC-MS), which has excellent chromatographic resolution and thus lends itself to routine quantitative metabolomic applications (3). In this study PLS-DA, a multivariate based classification method, is suggested for grade definition of commercial olive oils in Iran. It has been shown that this method can be applied as a comprehensive method for grade definition of olive oils successfully. This method is easy and economic in grade definition of olive oils in industry.

Keywords: Olive oil, PLS-DA, Grade definition, extra virgin olive oil, virgin olive oil, Quality control

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An inexpensive analytical method based on colorimetric sensor array and chemometrics data analysis techniques for fraud detection in cherry seed oil samples

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ABSTRACT

Cherry seed oil is a high expensive and essential ingredient in cosmetics industries. due to the importance of this oil in cosmetic industries, there is an increasing potential for fraud in this oil products. one type of these adulterations including the replacement of this expensive oil with cheaper substitutes, could potentially be very lucrative for a vendor or raw material supplier [1,2]. Colorimetric sensor arrays(CSA) are example 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. Multivariate statistical techniques have been used for extraction of useful information from colorimetric sensor array patterns. Among this chemometrics techniques, pattern recognition and partial least square (PLS) regression methods have been found widespread application in sensor arrays [4]. In this work, we developed a cross-responsive colorimetric sensor array for determination of amount of adulteration in cherry seed oil, the sensor array was constructed from pH and redox indicators, these sensors were exposed to the vapor of oil samples and the difference in the color intensity of them was considered as a corresponding signal. the responses of the sensors were dependent on the amounts of canola oil, sunflower oil and sesame oil, as counterfeit that added to the cherry seed oil samples. Principal component analysis (PCA) as an unsupervised pattern recognition techniques was used for discrimination of different adulteration amount in the cherry seed oil samples, fitting accuracies of 95%, 86% and 82% were obtained for canola, sunflower and sesame oils and partial least square (PLS) regression as a multivariate calibration method was used to estimate the content of canola, sunflower and sesame oils in cherry seed oil samples through image analysis. A root mean square error for calibration of 0.31 8 for canola oil, 3.34 for sunflower oil and also 1.37 for sesame oil were obtained, respectively. This colorimetric sensor array demonstrates excellent potential for qualitative and quantitative control of cherry seed oil samples.

Keywords: Colorimetric sensor array, Cherry seed oil, Partial least squares (PLS) regression, Chemometrics, Multivariate statistical techniques, Principal component analysis(PCA).

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Peak Resolution in dual mode handheld Ion mobility spectrometry

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ABSTRACT

Overlapping dual mode handheld Ion mobility spectrometry peaks may occur and can really complicate the interpretation and analysis of data. Obtaining appropriate data analysis tools, which focus on the data to detect overlapped/embedded regions and to find the number of pure components that are hidden in these regions, is a problem in common analytical applications [1]. An algorithm based on Gaussian apodization factor analysis (GAFA) was applied to resolve different types of overlapped simulated and real complex data of dual mode handheld Ion mobility spectrometry. New algorithm for analyzing the structure of raw data based on discrete Gabor transforms combined with Gaussian apodization factor analysis (DGT-GAFA) was applied to find signal and noise components in frequency domain by applying Gaussian apodization factor analysis and remove unwanted components in frequency domain that lead to increase in signal to noise ratio (SNR) and preserve of weak signals. The DGT-GAFA method was applied to amplify significant information, detection of target signals [2]. This Peak Resolution algorithm finds spectra of pure component with GAFA one by one and eliminates obtained components from a data matrix and search for next pure component spectra until all the components are determined.

Keywords: ion mobility spectrometry, Gaussian apodization factor analysis discrete Gabor transforms, signal denoising, Signal-to-Noise Ratio, spike removal algorithm

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Combining NMR and LC-MS Using Hierarchical Modeling:

Untargeted Metabolomics Study of Opium Users and Healthy Controls

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ABSTRACT

Every year, a large number of people lose their lives due to opioid use, and a much larger number of people also suffer from opioid-related disorders. In addition to sedative effects, opioid use can have devastating effects on other parts of the body [1]. Identifying the metabolites that affect these lesions will be very valuable. Metabolic samples are very complex and their analysis requires a lot of information from the system. Both nuclear magnetic resonance (NMR) spectroscopy and mass spectrometry (MS) play important roles in metabolomics. Currently, the vast majority of metabolomics studies use either NMR or MS separately, and variable selection strategies that combines NMR and MS for biomarker identification and statistical modeling has not been well developed yet [2]. In this study, ultra-performance liquid chromatography (UPLC) high-resolution mass spectrometry (UPLC-HRMS) and NMR data obtained by the analysis of urine samples of Golestan Cohort opium users were fused hierarchically for identification of biochemical perturbations in opium users [3]. Here, principal component analysis (PCA) is applied separately to LC-HRMS and NMR data (lower-level stage). Then significant scores for each data are extracted from the PCA results and merged. Finally, partial least square discriminant analysis (PLS-DA) applied to fused data (higher-level stage). Consequently, the discriminating biological markers between healthy and addicted samples were uncovered. We demonstrated that variable selection is vitally important in fused NMR and HRMS data. The combined approach was more reliable than each individual modeling of NMR or LC-HRMS data with significantly improved prediction accuracy. Using this approach, a subset of metabolites (180 and 120 features from LC-HRMS and NMR data, respectively) responsible for an improved binary class separation was selected and investigated.

Keywords : Opioid, Metabolomics, PCA, PLS-DA, Data Fusion, Hierarchical modeling

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Application of PLS, OSC-PLS and GA-PLS for a QSAR study of inhibitory activity of p38MAP derivatives and design new compounds for kinas using image processing

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ABSTRACT

The purpose of the Multivariate Image Analysis quantitative structure–activity relationship (MIA-QSAR) study is to obtain information from a set of descriptors that descriptors are in fact pixels of images of two-dimensional structures of molecules. The genetic algorithm application for selecting pixels and image processing was investigated in the QSAR study of protein P38 MAP kinase compounds. Using the information obtained, there is a Quantitative relationship between the structure and the IC₅₀. Protein P38 MAP kinase is used in the treatment of malignant tumors that act as inhibitors. In this study, the generation of a model for predicting IC₅₀ of these compounds was considered. To this end, the molecules were first plotted in the ChemSketch software and fixed in the same coordinates, and finally the images were processed in the MATLAB program. Quantitative models were obtained with PLS, OSC-PLS and PLS-GA methods, and IC₅₀ prediction was performed. The results of a series of statistical parameters such as RMSEP, RSEP showed the highest predictive power for the PLS-GA model.

Keywords : Multivariate image analysis; Genetic algorithms; Partial least squares.

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Detection of citric acid-adulterated industrial lime juices using portable Linksquare visible-near infrared spectrometer and class modelling approach

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ABSTRACT

Manipulation of lime juice composition undoubtedly has adverse effects on the quality of lime juice. Dilution of lime juice with water or a mixture of water and citric acid is a common adulteration type in the lime juice industry [1]. Although different methods such as chromatographic methods and biological methods have been previously used to detect lime juice fraud [2], finding a low-cost, quick, non-destructive and portable method will result in the quick screening of a large number of samples. Therefore, the current study aimed to evaluate the application of a portable visible-near infrared spectrometer (Vis-NIR; Link Square; 400-1000 nm) and chemometrics approach as a screening method for detection of lime juice adulteration. Twenty-four genuine industrial lime juice samples were used in the current study. These samples were authenticated based on the citric acid to iso-citric acid ratio as provided by the Association of the Industry of Juices and Nectars of the European Union (AIJN). All the genuine samples were diluted with water at different levels (10, 15, 20, 25, 30, 35, and 40%) and subsequently, the Brix number was adjusted by the addition of citric acid. A handheld NIR device connected to a smartphone was used to analyze each sample (three replicates) in the reflectance mode. Following principal component analysis (PCA), the samples were not thoroughly clustered concerning their groups in score plots. However, the soft-independent modelling of class analogy (SIMCA) model as a class-modeling approach following smoothing and mean centering of data resulted in 100% sensitivity and 83% specificity in the prediction of genuine and adulterated samples, respectively. The overall accuracy of the model was calculated to be 91%. This level of accuracy provided empirical evidence of the potential of handheld NIR and chemometrics approach for the detection of lime juice adulteration, further investigations using classification models (e.g., partial least squares-discriminant analysis, PLS-DA) and regression models (e.g., partial least squares regression, PLSR) are required to confirm the promising results of the current study.

Keywords: Adulteration, Chemometrics, Lime, Near-infrared, Portable

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Determination of 2, 4, 6 trinitrotoluene in soil samples by flow injection analysis followed chemometrics methods

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ABSTRACT

2,4,6-trinitrotoluene (TNT) is relatively water soluble compound which can be found in soil and groundwater around places associated with the manufacturing, handling, testing, and disposal of explosive and propellant materials [1, 2]. In the presence of acetone and a base, TNT can form the red-colored Janovsky complexes to produce 2,4,6-trinitrobenzyl anion (TNT^-) which can easily monitored in the visible spectrum [3]. Therefore, a rapid flow injection (FI) spectrophotometric method as an effective method involving automation, miniaturization, versatility, greater accuracy, higher speed, lower sample and reagent consumption (few tenths of microliters), lower risk of contamination or analyte loss and inexpensiveness have been attracted great attention, especially in forensic science [3, 5]. This method is developed for the selective determination of TNT in soil samples. The method was based on a derivatization reaction of TNT with sodium sulfite in a basic acetone medium through Janovsky reaction. Besides the many advantages of spectrophotometric technique, some analytes may be hard to measure due to overlapping their bands [4]. Due to the high amount of data obtained and the need of evaluate and interpret these data, chemometrics method using partial least square regression (PLSR) was utilized. PLSR is the one of the multivariate calibration methods that is performed by decomposition of concentration and absorbance matrices in order to identify the unknown variables of the model [6, 7]. Finally, an acetone-water medium of 80% (v/v) acetone was found to be optimal condition for the determination of TNT. The dynamic linear range and limit of detection were $5\text{-}100\ \mu\text{g g}^{-1}$ and $1\ \mu\text{g g}^{-1}$ for 200 mg soil samples. Quantitative results from the determination of TNT in contaminated soil samples showed the good recoveries in the range of 94.6-106.3%.

Keywords: “2,4,6 trinitrotoluene” flow injection analysis” chemometrics ” PLSR” soil” TNT.

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Experimental design optimization usage in pathogen detection utilizing green-synthesized re-generable nanocomposite

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ABSTRACT

One urgent need for global health, is fast detection of pathogens [1]. A rapid detection assay utilizing synthesized magnetic Ag/Fe₃O₄/Chitosan (Ag@IO@CS) nanocomposite, was developed for efficient preconcentration and fluorometric determination of trace amounts of gram negative bacteria via SPE method. Cinnamon as a bio reluctant and capping agent was used in the green synthesis procedure [2]. Prepared nanocomposite was characterized by TEM, FTIR and XRD measurements. The fluorescence intensity gradually increased by the prepared nanosensor as E. coli concentration increased from 10 to 10⁴ CFU mL⁻¹ (Fig. 1). Herein we utilized the robust design parameter optimization in the laboratory experiment for effective sensing of bacteria. A 5⁴ design using central composite (CCD) based response surface methodology (RSM) was applied to accommodate the four significant factors as pH, solvent, time of adsorption and time of desorption of bacteria (Fig.2). All in all, preference physical and chemical properties of the prepared nanocomposite besides magnetic separation capability and simultaneous optimization advantages make this nanobiosensor excellent scaffolds for the construction of the unique probe for gram negative pathogen.

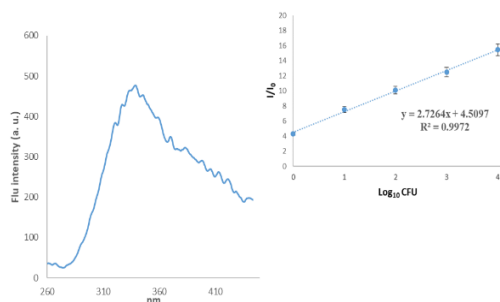


Fig. 1. Calibration curve for bacteria detection

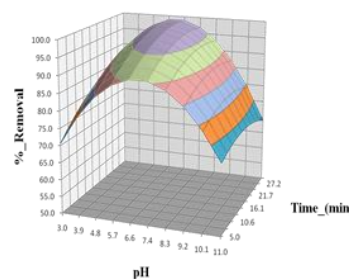


Fig.2. Typical response surface of full quadratic model

Keywords: Central composite design (CCD), Pathogen nanobiosensor, Ag/Fe₃O₄/Chitosan composite

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Quantitative Analysis of LC-PUFAs and Protein Content in Premature infant formula powders by ATR-FTIR Spectroscopy and Chemometrics

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ABSTRACT

Premature infant formula powder (PIFP) contains essential nutrients, such as protein and LC-PUFAs in which inadequate quantities of them may restrict the development of premature infants [1]. The aim of this study was to propose a quantitative analysis for evaluating these nutrients in PIFP. To achieve this purpose, an integrated methodology was developed by combining attenuated total reflectance Fourier-transform infrared spectroscopy (ATR-FTIR) with the chemometrics. ATR-FTIR was utilized to obtain the PIFP spectra in the wavenumber range of 4000-400 cm^{-1} . Principal component analysis (PCA) was employed to perform exploratory analysis of the spectra. *Partial least square regression (PLSR) and principal component regression (PCR) models were established for normal spectra, first, and second derivatives to quantitatively determine the protein and LC-PUFAs. The results showed that the PLSR model provided a better prediction than the PCR model with the coefficient of determinations (R^2) of 0.992 and 0.983 for calibration and validation, respectively. It also offers the best prediction for the PLSR model of protein considering the parameters such as R^2 (normal spectra) (Cal: 0.995, Val: 0.981). The results revealed that a combination of the ATR-FTIR spectroscopy and the chemometrics models creates a rapid, inexpensive, and non-destructive method for the quantitative analysis of PIFP.*

Keywords: ATR-FTIR spectroscopy, Chemometrics, LC-PUFAs, Premature infant formula powder, Protein

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Determination of heavy metal pollution (Pb, Ni and Cu) in groundwater by spectrometry –linear multivariate calibration

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ABSTRACT

Reliable access to safe and affordable water to meet human needs is a major challenge. Many countries around the world are currently facing water shortages or water pollution. Compounds that may enter water resources in various ways as industrial growth and human population increase are heavy metals. If the amount of heavy metals exceeds the standard, they can cause risks such as environmental problems, diseases, including cancer in consumers. The aim of this study was to determine the concentration of heavy metals lead, nickel and copper in groundwater of Qazvin province, which have many drinking, industrial and agricultural uses. At present, various methods have been used to determine heavy metals in water by instrumental methods such as AAS², ICP-AES³, ICP-MS⁴. In this study, accurate determination of heavy metals in water was performed using modern spectroscopic and chemometric methods. Fourier transform infrared spectroscopy provides a wealth of information on the molecular structure of water samples that can be used using linear regression methods to predict the concentration of elements in water samples. The proposed method was introduced as a fast, easy method without the need for sample preparation to measure elements in water samples. In modeling with partial least squares algorithm, orthogonal signal correction, mean center and *detrend* methods were used as preprocessing. The results of R^2 were obtained for lead, copper and nickel (0.99, 0.97 and 0.98), respectively. The square root of the predicted mean error squares (RMSEP) was 1.3346, 1.7350, 1.5550 for the mentioned elements, respectively, and the results of the calibration model for the data show the accuracy and value of the introduced model. Also, using the standard method of increasing the concentration of heavy metals in real samples was obtained.

² Atomic Absorption Spectrometer

³ Inductively Coupled Plasma–Atomic Emission Spectrometer

⁴ Inductively coupled plasma mass spectrometry

Probing molecular interactions and anti-corrosion performance of a group of drugs as green corrosion inhibitors in acidic Environment : Theoretical studies

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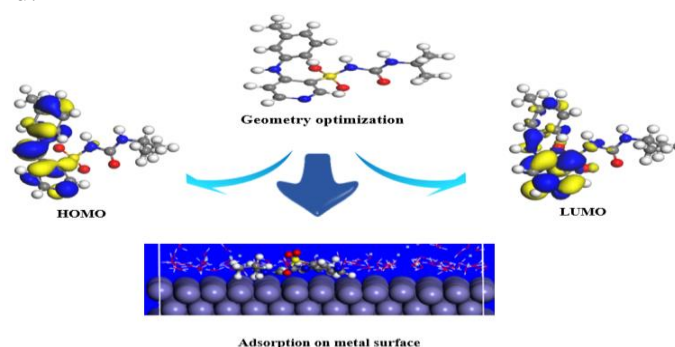
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ABSTRACT

The mineral acids are widely used in many industries for various metallurgical purposes like, chemical cleaning and descaling. It is a serious problem in industry. Thus results in increase in maintenance costs. Literature survey on green corrosion inhibitor suggest that the essential requirements for the selection of natural products include those containing phytochemicals, or isolated organic compound containing hetero atoms [1]. The purpose of this work is to understand the effect of molecular structure of a group of drugs on corrosion inhibition properties. In this study, the corrosion inhibitory performance of some drugs on mild steel in acidic environment was investigated using Quantum chemical calculation and Molecular Dynamics (MD) simulation. Quantum chemical calculations of Molecular electronic parameters such as Highest Occupied Molecular Orbital (E_{HOMO}) and Lowest Unoccupied Molecular Orbital (E_{LUMO}) energies, energy gap (ΔE), chemical potential (μ), electrophilicity (ω) and global hardness (η) and the correlation between the structure of inhibitors was determined by using Density Function Theory (DFT) method at the suitable basis set level. Quantum chemical calculations were explored by DMOL³ mode in Material Studio 2017. The GGA–PBE basis set in DFT was used to optimize the structure of drugs. Molecular Dynamics (MD) simulations was selected for exploring the adsorption ability of drugs on the target steel metal expressed by Fe (1 1 0) surface. The running of this dynamics simulations was done by the Materials Studio 2017 program. Classical simulations were based on COMPASS as an appropriate force field.



Keywords: Corrosion Inhibitor, Density Function Theory, Molecular Dynamics Simulation

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Determination of heavy metal pollution (Pb, Ni and Cu) in groundwater of Qazvin province by spectrometry –non-linear multivariate calibration

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ABSTRACT

In recent years, one of the main problems of human societies is the contamination of groundwater with heavy metals such as lead, nickel, copper, etc. In fact, the contamination of groundwater resources with heavy metals and the entry of these waters into the food cycle and health industries, etc., causes environmental problems and diseases such as cancer. Factors such as population growth, the creation of large industrial companies, excessive fuel consumption have caused environmental pollution. Heavy metals are among the pollutants that are present in soils, industrial wastewater, mines and rainwater that flows in rivers, etc. Heavy metals enter as a solution and cause pollution of surface water, groundwater and soil and they pollute them, causing the balance of the ecosystems that enter it to be compromised. In this study, the determination of metal ions by nonlinear chemistry-calibration (Artificial neural network) method is introduced. Fourier transform infrared spectroscopy provides a wealth of information on the molecular structure of water samples which can be used using nonlinear regression methods to predict the concentration of elements in water samples. A calibration model was presented for both training data and test data, and the correlation coefficient were acceptable for each element and 0.9879 for nickel, 0.9789 for copper and 0.9948 for lead, respectively. The root mean square error of the prediction for mentioned elements were 1.4511, 1.3626, 1.1302, respectively. Also, using the standard addition method for the heavy metal concentration was determined. And the correlation coefficient for the nickel in water related to the two wells of Rashtaghoon and Mahmoudabad were 0.9992 and 0.9966, respectively, and the copper was 0.9977 and 0.9997, the lead was 0.9770 and 0.9997, respectively. Also, the results related to the limit of detection in Rashtaghoon well for the three elements are 1.1, 0.30 and 0.12, respectively and the results of dynamic range are 4.3, 7.9, 0.62, respectively. In Mahmoudabad well, the lowest limit of detection related to lead was 0.12, and nickel and copper were 1.16, 0.62. The results of linear range of nickel, copper and lead were 4.4, 5.8 and 0.7, respectively.

Keywords: Heavy metal, Ground water, Non-linear multivariate calibration, Spectrometry

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MIA-QSAR Modeling and Molecular Docking Analysis of Some Cis- β -lactam Compounds with Antimalarial Activity

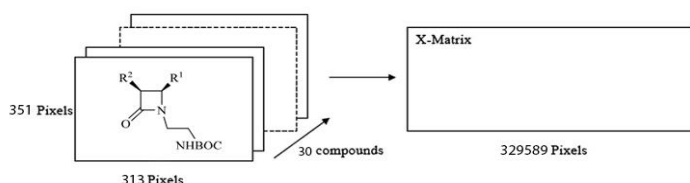
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ABSTRACT:

After years of efforts to fight and control of malaria, it is still a prevalent and deadly infectious disease, especially in the third-world countries in Africa, Asia, and South America. The major problem in the treatment of malaria is that *Plasmodium* parasites become resistant to antimalarial drugs. The most commonly used antimalarial drug, chloroquine, became ineffective due to rapidly spreading resistance of plasmodium falciparum to this compound; the newer antimalarial drugs, such as mefloquine or artemisinin also face to resistance problem. The other problem in control of malaria is the lack of an effective vaccine for this disease. Therefore, developing new antimalarial agents is a necessity and chemical modification of existing compounds is one of the strategies available [1]. β -Lactam derivatives with various functional groups have played an important role in antibacterial drugs and in medicinal chemistry [2]. β -lactam ring is an important structural element of the most widely employed β -lactam antibiotics family [3]. In this current research, Quantitative structure-activity relationship (QSAR) model was developed to predict the antimalarial activity of Cis- β -lactam agents by using multivariate image analysis (MIA-QSAR) methods. The created model showed acceptable and valuable result that used for molecular docking study of compounds and interaction of the selected compounds in QSAR with plasmepsin II as target (receptor) in human body was investigated. The result in this study showed that studied compounds exhibit good antimalarial activity and binding affinity. The final result are obtained, can be efficient and useful for design and development of stronger inhibitors against plasmodium falciparum.



2D images and unfolding step of the 30 chemical structures to give the X-matrix

Keywords: Cis- β -lactam, Antimalarial activity, Plasmodium falciparum, MIA-QSAR, Molecular docking, Binding affinity, Plasmepsin II.

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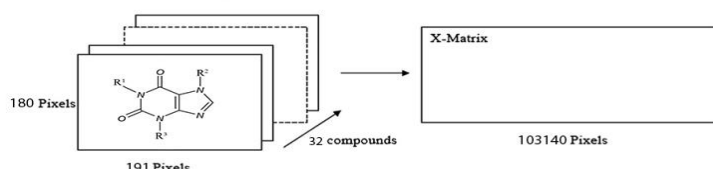
An In Silico Study of the Epithelial Anticancer Activity of Caffeine Derivatives by using MIA-QSAR methods and Molecular Docking

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ABSTRACT:

Epithelial tumors are a type of cancers that occur in epithelial cells in different part of the body and the most common of these is epithelial skin cancer, a malignant neoplasm of skin epithelial cells which is four times more common than other type of skin cancer [1]. Up to now, many studies on the mechanisms of antitumor initiating and antitumor promoting properties of potent drugs are currently being suggested for the prevention of skin cancer and other epithelial cancers in humans [2]. Caffeine is one of these compounds. Caffeine (1,3,7 trimethylxanthine) is an alkaloid compound belonging to the xanthine group. It contains in its composition nitrogen, oxygen, hydrogen and carbon [3]. In this study, inhibition activity of some caffeine derivatives (with specific amount of IC_{50}) against epithelial cancer, were studied by QSAR modeling and using application of pixel selection to predict the biological activity of caffeine and comparison with experimental data. In silico methods, such as quantitative structure activity relationship (QSAR), molecular docking and pharmacophore modelling by decreasing the time and cost of drug discovery play a significant role in the field of drug design and development [4]. The QSAR model showed satisfactory output validation parameters, which made the model acceptable, and molecular docking simulation were developed for considering interaction of selected caffeine derivatives with their receptors such as Chk1 and combination between their binding free energies. MIA-QSAR modeling and molecular docking studies showed valuable result that can help pharmaceutical researches to design and synthesis new compounds with more epithelial anticancer activity.



2D images and unfolding step of the 32 chemical structures to give the X-matrix

Keywords: Epithelial anticancer activity, Caffeine, MIA-QSAR, Pixel selection, Molecular docking, Chk1, Binding free energy

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Characterization of the volatile profile of Iranian tea using chromatographic fingerprint combined with multivariate curve resolution: Toward improving quality control and authentication

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ABSTRACT

GC-MS fingerprint analysis plays an outstanding role for characterizing and authenticating of unknown metabolites in complex natural products [1]. However, efficient acquisition of the required information about the components from a GC-MS-based dataset remains a challenging task because of fundamental problems including baseline drift, spectral background, various types of noises, peak shape deformation (non-Gaussian peaks), low S/N ratio and co-elution peaks that may mislead similarity searches in the standard mass spectral library, even under the best experimental conditions [2]. The main strategy for solving these problems is chemometrics approaches such as, multivariate curve resolution (MCR). The ultimate goal of curve resolution would be to be able to determine the number of components in an overlapping chromatographic peak as well as the spectrum and concentration profile of each compound [3]. In recent years, the multivariate curve resolution-alternating least squares (MCR-ALS) method, based on factor analysis, has been shown to be a powerful tool for the peak resolution of the screened TIC peaks to obtain the pure chromatographic profiles and pure mass spectra [4]. This study aimed to give a comprehensive characterization of volatile chemical constituents of Iranian tea using chemometric technique due to its ability for resolving the co-eluted peaks of the GC-MS-based data. The results indicated that the GC-Mass fingerprint combined with multivariate curve resolution–alternating least squares will open a more full-scale look at the volatile profile of Iranian tea and provide valuable guidance of its chemical constituents.

Keywords: Iranian tea, MCR-ALS, GC-MS

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A Study of antioxidant properties of some different species of the Malvaceae family using HPTLC and multivariate analysis technique

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ABSTRACT

The Malvaceae family contains at least 243 genera and 4225 species in the world and 11 genera and 70 species in Iran, which are seen as herbs, shrubs, and trees. This family has been not only economically but also medicinally considered in traditional medicine. This work was initiated with classification and determination of antioxidant properties of 9 species using high performance thin layer chromatography (HPTLC) and Principal Component Analysis (PCA) technique. Extraction was performed by soaking in ethanol solvent and placing it on a Stirrer magnetic. Then, different solvent systems were investigated. The hexane-ethyl acetate-acetic acid mobile phase (4: 5: 1) was selected. Free radical scavenging activity was evaluated by HPTLC with DPPH test and total phenolic content was evaluated by FeCl_3 test and vitamin E content of the species. Data analyzed using MATLAB software and PCA technique For classification. The results of DPPH test showed that, *Abutilon theophrasti*, *Malva sylvestris* , *Gossypium hirsutum* and *Alcea rosea* (Purple petals) were in one batch and had high free radical scavenging activity. According to the FeCl_3 test, samples of *Abutilon theophrasti*, *Malva sylvestris* and *Alcea rosea* (Purple petals) were in the same category and had a high phenolic content. According to the vitamin E test, *Abutilon theophrasti* and *Malva sylvestris* placed in the same category and presented a high amount of vitamin E. Antioxidant activity of *Abutilon theophrasti* and *Malva sylvestris* was higher than other samples. Therefore, *Abutilon theophrasti* and *Malva sylvestris* can be assumed as a rich source of compounds with antioxidant properties in the food and drug industry to maintain benefited human health. Also in this report, the extract of common *Alcea rosea* L. plant (white petals) was analyzed by GC-MS to identify phenolic compounds. The results of GC-MS showed that among the identified compounds, 8 are phenolic compounds, of which 4-Mercaptophenol (9%) has the highest percentage among phenolic compounds. This compound with the chemical formula $\text{C}_6\text{H}_6\text{OS}$ has antioxidant properties.

Keywords

Malvaceae, *Abutilon theophrasti*, *Malva sylvestris* and *Alcea rosea*, PCA, HPTLC



Classification of CC Chemokine Receptor Inhibitors: A Computational Journey Leading to Drug Discovery

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ABSTRACT

CC chemokine receptors are introduced as integral membrane proteins that particularly attach and respond to cytokines of the CC chemokine family representing one subfamily of chemokine receptors, a large family of G protein-linked receptors. CCR1 is broadly known as the first noticed CC chemokine receptor binding several inflammatory/inducible CC chemokines^[1], whereas CCR2 has been distinguished on the surface area of monocytes, activated memory T cells, B cells, and basophils in humans^[2]. Another indubitably vital member of CCR family is CCR4 that expressed on Th2 T lymphocytes^[3], whilst undoubtedly the most important CC chemokine receptor called CCR5 is expressed on multiple cell types including peripheral blood-derived dendritic cells, CD34+ hematopoietic progenitor cells to name but a few and it is patently defined as an essential coreceptor implicated in susceptibility to HIV-1 infection and disease^[4]. The given article illustrates the characterization of molecular features that induce selectivity for inhibition of CCR1, CCR2, CCR4 and CCR5, in which the number of 7294 molecules were collected from Binding Database and 3224 molecular descriptors for each molecule were calculated via Dragon Talete 5.5. Moreover, the best feasible subset of molecular descriptors were selected utilizing Variable Importance in Projection (VIP), providing the opportunity to classify the mentioned targets based on their therapeutic features and activities. Five various classification methods namely PLS-DA, SVM, SKN, KNN and CPANN were used so as to find the relationship amongst molecular structures of chemicals, their activities and selectivities. Generally, the performances of classified models were evaluated according to the statistical parameters derived from the given confusion matrices. Additionally, both dependability and predictability of the conducted models were estimated by the tenfold cross-validation techniques and test sets. The reliable statistical values of the obtained classified molecules can be not only meticulously found handful in order to design brand new drugs with selective inhibitory activities toward CCR1, CCR2, CCR4 and CCR5, but also much more efficacious in pharmaceutical aspects of miscellaneous medical treatments for inflammation, rheumatoid arthritis, cancer and infections resulted in HIV-1 virus.

Keywords: "chemokine receptor, protein, inhibitor, molecular descriptor, classification, model"

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Calibration updating Using Multivariate Curve Resolution Methods

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ABSTRACT

The normal process of building a spectral calibration model typically requires a large set of samples such that all variances are included in future predictions. However, once such a primary calibration model has been built, circumstances can cause the model to become invalid. For example, instrumental drift or uncalibrated spectral features appearing in new secondary samples can occur later in time. For these and other situations, the instrument must be recalibrated to accommodate new conditions. In theory, the remedy would be to include a large number of new calibration samples along with their reference measurements. In practice, though, the inclusion of such samples is often costly and lengthy in terms of laboratory time. Hence, mechanisms are needed to update the current model to include the new chemical, physical, environmental, and/or instrumental effects not spanning the current primary calibration domain. Calibration updating is an adaption process where models are updated from predicting in primary sample and measurement conditions to predict the analyte in new secondary conditions. Many calibration updating methods were used for the analyte quantitation in secondary situations and were compared with each other [1]. 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 [2, 3]. In this study we have used MCR first-order calibration for evaluating its ability to calibration updating in comparison with other updating methods. In order to evaluate our proposed strategy for calibration updating, the publicly available benchmark near-infrared spectra dataset consists of NIR spectra of 80 corn samples was utilized which were measured by different separate near-infrared instrumentals (M5, Mp5 and Mp6) [4]. The M5 instrument is considered as the primary condition and the Mp5 instrument is considered as the secondary condition and number of validation samples in the secondary condition is predicted with the updated model. The prediction error for the model that has not been updated (primary model) is RMSEV= 16.68 and the prediction error of the validation samples for the updated model is RMSEV= 0.54. The results show the ability of the MCR in calibration updating.

Keywords: "Multivariate Curve Resolution-Alternative Least Square (MCR-ALS)", "Primary calibration", "Calibration updating", "Primary instrument", "secondary instrument"

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Exploring the interactions of some PAHs with bovine serum albumin: spectroscopic method and chemometric approaches

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ABSTRACT

Polycyclic aromatic hydrocarbons (PAHs) have been listed by the International Agency for Research on Cancer (IARC) as possible carcinogens. Serum albumins serve as major transport proteins in the blood circulation system [1]. Thus, the study of binding affinity of a ligand to serum albumin determines its pharmacokinetic and pharmacodynamics behavior. The intrinsic fluorescence of bovine serum albumin (BSA) facilitated employing fluorescence spectroscopy as a selective and sensitive technique to explore the *in vitro* interactions between some PAHs and BSA. Therefore, the quenching mechanism, the quenching constant, the binding constant and the number of binding sites involved in the studied BSA-PAHs complex were clarified utilizing quenching study. Molecular docking, a computational tool, has been used to simulate the intermolecular interactions of a ligand with proteins, which visually disclose preferred binding mode of a ligand within active site of the protein at the molecular level [2]. Hence, experimental methods combined with molecular docking simulations provide comprehensive insight into complex interactions of small molecules with proteins. Attempts were made to reveal the specific binding sites and modes of some PAHs on BSA employing molecular docking simulation. The results of the present work should help predict the toxic effects of PAHs on organisms.

Keywords: PAHs, serum albumin, fluorescence spectroscopy, molecular docking.

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Sorting different types of rice using smartphone based multispectral images

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ABSTRACT

Spectral imaging techniques are 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. In spectral imaging techniques, a spectrum is measured per pixel and the sample can be scanned without any kind of preparation [1]. Hyperspectral images (HSIs) are often composed of large number of pixels because one usually aim to cover large scenes or/and to get sufficient spatial resolution. In addition, a large number of variables are usually measured, to get sufficient spectral resolution and chemical selectivity. As a consequence, large data sets are generated, their analysis is time consuming, and high-performance computers might be required [2]. In addition, measuring too many collinear variables might translate into error propagation and over-fitting issues in multivariate modeling. A multispectral image is one that captures image data within specific wavelength ranges. The wavelengths can be separated by filters or detected via the use of instruments that are sensitive to particular wavelengths. The size of the multispectral images can be very small but would carry more information than simple RGB image. Rice, as one of the popular nutritional products, is of high amount of thought to be classified by nondestructive methods [3]. In this study we utilized a simple set-up including a laptop's monitor and a smartphone to collect multispectral data so that the color of the laptop screen changed (9 colors) each time the object was photographed. Each image is taken in a separate spectral band in the visible spectral region. Then, multi-spectral images recorded from different Iranian rice were used in rice sorting using Partial Least-Squares Discriminant Analysis (PLS-DA). Specificity, precision and sensitivity for each class revealed that the discrimination model is adequate.

Keywords : Imaging, Multispectral images, Sorting, PLS-DA, smartphone

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Nonnegative matrix factorization in ASCA modeling of graphene oxide toxicometabolomics $^1\text{H-NMR}$ data

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ABSTRACT

Non-negative matrix factorization (NMF) has been shown to be a suitable decomposition method for multivariate data, to have a meaningful non-negativity physical interpretation [1]. The study is the employment of NMF to the calculation partitions variation and enables interpretation of these partitions in the ASCA model of metabolomics data set. ANOVA-Simultaneous Component Analysis (ASCA) is one of the most prominent methods to include such information in the quantitative analysis of multivariate data, especially when the number of variables is large [2]. The experimental dataset included $^1\text{H-NMR}$ spectra of mice serum samples exposed to three different doses (high, low and control) and at different time intervals such as 24 and 48 hours, 7 and 21 days post-injection of GO nano-sheets [3]. In this data, to analyze the effects of the specific factors like time, dose and their interaction, an ASCA model based on NMF was applied. P-values with confidence interval 90% for factors low dose with control, low dose with high dose, control with high dose, time and interaction between time and dose were obtained 0.049, 0.214, 0.365, 0.001, and 0.997 respectively. As it was clear from the results, low with control group and time factor were effective factors in creating variance in the data. For the other two cases, the factor dose did not play an effective role in the process of data variances. Loading corresponding to the factor time and low dose with control showed the chemical shifts and thus the compounds that are corresponding to the behavior observed in the scores, and can be used for biological interpretation. Scores corresponding to the factor interaction no trend related to dose was visible and none of the four measurement time-points showed an increasing or decreasing score value for differing graphene oxide doses. Also the scores of the second component do not show such a quantitative trend. Considering the complexity of the metabolic data, the use of NMF instead of PCA in ASCA is an important and more realistic strategy to obtain meaningful physical profiles for each effective factor.

Keywords : NMF, ASCA, Matrix decomposition, Experimental data, Metabolomics data, $^1\text{H-NMR}$.

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Development and optimization of microwave-assisted extraction of *Satureja bachtiarica* Bunge. essential oil using response surface methodology and its comparison with traditional method

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ABSTRACT

Essential oils are one of the most secondary metabolites in therapeutic herbs, rich in oxygenated compounds [1]. The proficiencies of traditional hydro-distillation (THD) and microwave-assisted steam hydro-diffusion (MSHD) techniques in extraction of Bakhtiari savory oil were evaluated. In order to obtain the golden yield and total phenol (TPC) in MSHD method, three factors were examined at 5 levels by applying central composite design under RSM technique: extraction time (15, 25, 35, 45, 55 min), microwave power (200, 400, 600, 800, 1000 W) and water volume to plant ratio (W/P) (0, 0.5, 1.5, 2.5, 3 ml/g) [2, 3]. The results of RSM in THD method showed, extraction time and (W/P) separately affected on yield and TPC without interaction. The best yield was 1.64 V/W% that collected at conditions [54.16 min, 872.42 W, 2.09 ml/g for extraction time, microwave power and (W/P)]. By using folin-ciocalteu method, the maximum of TPC was 344.07 mgGAE/g that was obtained at points [19.7 min, 1000 W, 3 ml/g for time, power and (W/P)] in MSHD technique. The highest amount of oxygenated fraction ($63.24 \pm 0.442\%$) were produced in the microwave method. The MSHD method is the economic technique for green extraction of essential oil from pharmaceutical and fragrant herbs [4,5].

Keywords: Microwave-assisted steam hydro-diffusion; *Satureja bachtiarica* Bunge. ; Essential oil; Response surface methodology; GC/MS.

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Comparison of variable selection methods to classification isoform selective Bcl-2 and Bcl-x_L inhibitors

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ABSTRACT

The variable selection is an important part of contemporary quantitative structure-activity relationship (QSAR) studies, which is often used as a preprocessing step in these approaches. The elimination of irrelevant and redundant information often improves the performance of learning algorithms as well as reduces the computational costs associated with model building and predictions tasks. Which variable selection method works well in QSAR study is still considered as a challenging question. To answer this question, we have examined the effects of 23 different variable selection methods on the performance of the SVM, SKN and PLS-DA techniques to classify Bcl-2 and Bcl-x_L selective inhibitors. These methods include Variable importance in projection, Feature selection via concave minimization [1], ReliefF [2], B2 and B4 algorithms [3], Non-iterative B2, Particle swarm optimization, Ant colony optimization, Centrality eigenvector feature selection, Infinite feature selection, Distributions of mutual information, Feature selection with adaptive structure learning [4], Fisher, Infinite latent feature selection, SVM recursive feature elimination, Least absolute shrinkage and selection operator, Simple pairwise correlation method, K Inflation factor (KIF) index and KIF non-iteration index method, First eigenvector and First eigenvector iterative method, Variance inflation factor (VIF) and VIF iterative, Genetic algorithm, Simulated annealing, Reshaped sequential replacement. The statistical evaluation of the developed classification models was implemented by parameters derived from confusion matrix. In addition, the predictive power of the created models was investigated by the 10-fold venetian blind cross-validation. Classification accuracy of more than 70% was achieved in all three machine learning techniques and for all variable selection methods in the evaluation series. No statistically significant difference can be seen in the results. This demonstrates that the only main factor to choose the best variable selection method is not the good statistical results from model building. Other parameters are also very important such as the information obtained from the selected variables and their relationship with the structural features and biological activities of the studied data.

Keywords: Variable selection methods, Bcl-2, Bcl-x_L, Classification, QSAR

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Development and validation of two handheld near infrared spectrometers to investigate water adulteration in bovine raw milk and comparison with Fourier transform infrared spectroscopy

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ABSTRACT

Food authenticity has been a major concern of consumers, producers and regulators all over the world [1]. Milk is wholesome nutritious dairy product, which has been confronted with various adulterations. Water is the most commonly added adulterant used in milk. This will not only reduce the nutritious quality of milk but also poses a threat to the health of consumers [2]. The presented study evaluates the performance of two handheld sensors (Wavelength range of 400-1000 nm for Linksquare and 900-1700 nm for Tellspec) benchtop attenuated total reflectance-Fourier transform infrared spectroscopy (ATR-FTIR) instrument combined with chemometrics methods to determine water adulteration in raw bovine milk. The adulterated samples were prepared in concentrations ranging from 0% to 30% water. No further preparation was required prior to analysis. All of the models developed were cross-validated and tested on a different set of data. Principal component analysis (PCA) was used to investigate and visualize the differences between authentic and adulterated milk samples and it could successfully discriminate authentic and adulterated ones. For quantification, two different models of partial least square regression (PLSR) and radial basis function-artificial neural network (RBF-ANN) [3] were applied on data and the best-established model was obtained from samples measured with the benchtop FTIR with the prediction regression coefficient (R^2_p) of 0.999 and the minimum root mean square of prediction (RMSEP) of 0.196%. Furthermore, the handheld sensors gained reliable results as Tellspec offered a R^2_p of 0.994 and a RMSEP of 1.116% and Linksquare showed a R^2_p of 0.920 and a RMSEP of 1.742%. To evaluate the applicability of the built models, ratio of performance to deviation (RPD) and range error ratio (RER) parameters were assessed. The optimal model based on FTIR instrument data obtained RPD=31.62 and RER=153.06, whereas the best models resulted in RPD=12.91 and RER=26.88 for Tellspec and RPD=4.34 and RER=6.21 for Linksquare. Taking into account the results, the studied handheld sensors revealed excellent capability for simple, economical, non-destructive and rapid measurements of water adulterated milk as screening and/or quality control technologies in the dairy industry.

Keywords: Milk; Handheld infrared spectrometer; Chemometrics; Adulteration; FT-IR.

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Documenting science: an initial formal experience

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ABSTRACT

Traditionally documenting in science has meant writing down any work carried out in either research or day-to-day settings on paper, if any, and keeping output from a variable number of software packages. However in today's scientific climate, documenting in science could (and should) include all aspects of the study that is from developing an idea, break down of tasks, project management, protocol and interactive recorded observations (such as spectroscopy, flowcytometry, and patient records) , audit trails, dashboards, collaboration inputs and ultimately to write up of reports and papers. An integrated formal documenting approach in science would be significant towards continuity of research, problem solving and resource management, handling legal rights disputes and fighting against plagiarism. In this study, it was intended to assess the perception and usage of users towards a cloud-based research platform with above functionalities, within a multi-disciplinary, multi-center setting during a pilot study over a 12 months period. The cloud-based research platform employed, has been designed and developed over several years without any reverse engineering, based on open source technologies and fully accessible via web browsers. Users came from diverse background, including pharmacy, pharmacology, molecular biology, biomaterials, tissue engineering, public health services and health policy. Therefore the chosen teams were involved in laboratory and non-laboratory based clinical and field studies environments. Following the initial selection of senior scientists (n=19), who appreciated the importance of formal documentation of their work, were interviewed and agreed to encourage their team members to take part in the pilot study. An online survey was carried to learn about their view of what core functions of such system might be. Later, citing increased ratio of foreign currencies to the Rial and of course the impact of COVID19 pandemic in everyday life, number of actual teams taking part in the pilot were reduced (n=4). During the year pilot, other teams (n=3) discontinued their efforts and recorded their views and ideas in a feedback online survey. Remaining one team (with a growing number of user base, n>30) completed the pilot and has continued since using the platform. One of interesting results of the study, admittedly not statistically significant, was that the last remaining team is not even involved in laboratory based research, but screening for mental health in children. It is hereby acknowledged that part of the study was financially supported by the National Institute of Medical Research of Iran, grant number: 978379.

Keywords: Electronic laboratory notebook, research document management, research continuity, quality control



Classification of Iranian rice varieties using FTIR spectroscopy and sparse Linear Discriminant Analysis

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ABSTRACT

Authentication and classification of rice varieties have attracted much attention in food science and technology for quality assurance and adulteration detection in recent years. In this study, FTIR spectroscopy was integrated with chemometrics techniques for discrimination of seven different ‘Iranian rice’ varieties. Herein, for the first time, the sparse version of Linear Discriminant Analysis (sLDA) was used for the development of the interpretable and reliable FTIR-based classification model to achieve the discrimination of rice samples. The development of the sLDA algorithm was done by applying an elastic net penalty to the discriminant vectors in the optimal scoring explanation of LDA, which could simultaneously perform classification and variable selection. A grid search technique combined with 5-fold cross-validation was used to tune the parameters and optimizing the model. The performance of the sLDA model was compared with LDA, and the accuracy of the validation set increased from 89.52% for the LDA model to 95.24% for the sLDA model. The results indicated that the sLDA outperformed the LDA in terms of interpretability and prediction accuracy, which is mostly due to sparse loading vectors in the sLDA method. The present work revealed that a tuned and optimized sLDA technique combined with FTIR data can be successfully applied as a robust and interpretable tool for authentication and classification of the rice samples in food industry [1, 2].

Keywords: FTIR spectroscopy, Iranian rice, sparse Linear Discriminant Analysis, food adulteration.

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Simultaneous determination of antiviral drugs in biological fluids using excitation-emission fluorescence spectroscopy and chemometrics

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ABSTRACT

This study presents a new method for simultaneous determination of antiviral drugs in biological fluids using excitation-emission fluorescence (EEF) spectroscopy and N-way partial least square (N-PLS) algorithm [1]. Several methods including high performance liquid chromatography (HPLC) and ion mobility spectroscopy (IMS) were previously proposed for simultaneous determination of drugs in biological fluids. These methods suffer from the need for large sample volumes, being time-consuming and a need for extensive pretreatment protocols. Despite extraction and chromatographic methods, EEF is fast, green and can be used for quantification of the analytes in the presence of uncalibrated interferences (i.e. second-order advantage) [3]. In this study, the central composite design (CCD) was used for construction of the calibration samples for ensuring orthogonality of the concentration of the analytes. We used an extension of the variable importance in projection (VIP) method to three-way arrays in order to select the most relevant wavelengths [2]. Three important antiviral drugs including Aciclovir, Valacyclovir and Ribavirin were used as model compounds to test the feasibility of the proposed method. The structural similarity of the studied molecules provides efficient study design for assessing the ability of the proposed method for calibrating molecules with intense overlapping peaks. The obtained statistical parameters in terms of regression coefficient (R^2) and root mean square error (RMSE) were satisfactory for the calibration and prediction sets. Table 1 shows R^2 and RMSE values for NPLS model before after selection of important variables. The given figures of merits reveal that the proposed method could nicely calibrate the studied molecules even with small set of selected wavelengths in both excitation and emission fluorescence modes. The results revealed the superiority of the VIP-NPLS algorithm compared to NPLS and the number of selected variables reduced about two orders of magnitudes. It extensively increases the interpretability of the models which is a vital for systematic investigations in such complex interacting systems.

Table 1 R^2 and RMSE for N-PLS model before and after using VIP for variable selection

Analytes	before selection of variables		after implementation of VIP	
	R^2	RMSE	R^2	RMSE
Acyclovir	0.93	0.0016	0.98	0.0013
Valacyclovir	0.94	0.0024	0.92	0.0014
Ribavirin	0.94	0.0026	0.98	0.0017

Keywords: Excitation-Emission Matrix Fluorescence, N-PLS, Variable Importance in Projection (VIP)

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Central Composite Design for Experimental Study and Statistical Modelling of Solubility Parameters of RDX and HMX in Solution of Diethylene Glycol and Ammonium Acetate

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ABSTRACT

In this study, for the first time, using the safe, inexpensive, non-volatile and low toxicity solution of diethylene glycol (DEG) and ammonium acetate salt, solubility and thermodynamic parameters of two energetic substances, cyclotrimethylenetrinitramine (RDX) and cyclotetramethylenetetranitramine (HMX) energetic materials were experimentally studied. The effect two main factors of temperature and weight percent of ammonium acetate in DEG on the solubility of RDX and HMX over a temperature range of 30 °C to 90 °C and 70.0 wt.% to 100.0 wt.% of ammonium acetate in DEG mixtures were determined and statistically modelled and optimized using a central composite design (CCD) of experiment with Minitab (ver. 19) software. Multiple regression analysis and analysis of variance (ANOVA) showed that the predicted results were in good agreement with the experimental data. Also, precision and accuracy of results were evaluated. The solubility coefficient, enthalpy of dissolution of the two substances in DEG solvent and its mixture with ammonium acetate were determined. The results show that with increasing the concentration of ammonium acetate in the solvent, the solubility of RDX increases while the solubility of HMX is low, with the solubility ratio of RDX to HMX near to 10 to 30-fold. This study indicates a much lower solubility of HMX in ammonium acetate /DEG mixture relative to RDX, thus separation of the two compounds, having similar structural and chemical properties, can be performed.

Keywords: Solubility, Diethylene glycol, Ammonium acetate, Explosive, Central composite design



Developing a novel biosensing system and investigation of interactions of acarbose with normal and glycated human serum albumin

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ABSTRACT

Tracking blood sugar, glycated human serum albumin (GHSA) and glycosylated hemoglobin (HbA1c) are critical keys for the analysis and checking of blood sugar levels for diabetics [1]. Researchers have revealed that the GHSA has a higher potential as a glucose blood indicator compare to HbA1c for patients with changing of blood sugar content, patients hospitalized for a short-term, and the pregnant women with hyperglycemia [2,3]. The methods for GHSA determination are including chromatography and immunology assays, Raman spectroscopy, capillary electrophoresis, and refractive index. Novel methods should be developed because these conventional methods are limited by time and cost. Hence, in this study, we tried to develop a novel method for GHSA determination using chemometric modeling of the experimental data in the presence of GHSA and human serum albumin (HSA) based on their binding with acarbose. The interactions of acarbose with GHSA and HSA was investigated by chemometric assisted electrochemical and spectroscopic methods. Afterwards, by recording second-order differential pulse voltammetric data, a monitoring system was developed for GHSA determination in the presence of HSA based on their binding with acarbose. The modified electrode was able to detect GHSA and HSA in linear ranges of 0.07-10 mg/mL, and 0.08-10 mg/mL respectively. Also, this method was successful of GHSA determination in spiked samples. Furthermore, the sensor response to GHSA was recorded during one month which confirmed 95% stability of the developed method.

Keywords: Biosensing, Glycated human serum albumin, Human serum albumin, Acarbose

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Statistical optimization of removal of Cr(VI) by *Pistacia Atlantica*-based activated carbon nanostructures using experimental design

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ABSTRACT

Pistacia Atlantica, an inexpensive and plentiful natural resource in Kermanshah province, was used to produce nanostructures of activated carbon (AC). The structural properties of AC nanostructure were characterized utilizing Fourier transform infrared (FTIR), Barret-Joyner-Halenda (BJH), X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). Chromium (Cr(VI)) is an extremely toxic and carcinogenic substance so its water pollution has become more and more serious. Its wastewater treatment is still a big problem because more than 96% of it is stockpiled on land, leading to environmental pollution and threatening human health [1,2]. This study used *Pistacia Atlantica*-based activated carbon nanostructures to remove Cr(VI) from aqueous solution and effective factors on the removal mechanism have been analyzed. In this work, a rapid/assisted adsorption method followed by ultraviolet-visible spectroscopy (UV/Vis) detection has been used for efficient short-time removal of Cr(VI). A combination of central composite design (CCD) and response surface methodology (RSM) has been applied to model and optimize the influencing variables on the Cr(VI) adsorption by produced AC nanostructure. More specifically, the effects of imperative variables such as adsorbent mass, Cr(VI) concentration, temperature, and stirring time have been investigated. The results show that the Langmuir and pseudo-second-order kinetic models fitted well to the adsorption experimental data [3,4]. Compared with the recently reported techniques for removing Cr(VI), the proposed technique has several advantages such as low cost, the abundance of raw materials, ease of production, fast adsorption kinetics, and high adsorption capacity.

Keywords: *Pistacia Atlantica*, Activated carbon, Experimental design methodology, Chromium, Central composite design

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Discrimination of Heavy Metal Ions using an Optoelectronic Tongue-Sensor Array on a Paper Device

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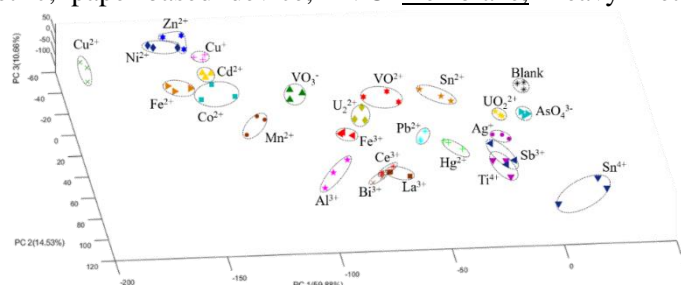
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ABSTRACT

Analyzing the hazardous metal concentration in water usually requires collecting samples on-site and then performing expensive laboratory analysis, which may take days to weeks to obtain results [1]. So, as an important goal of the research programs, the development of simple, rapid, sensitive, and inexpensive detection method for identifying and sensing the environmental pollutions has attracted considerable attention. Recently, paper-based assays have been widely applied in food analysis, environmental monitoring, and disease diagnosis due to flexibility, portability, easy to produce and use, low cost, low sample and reagent consumption, accessibility and biocompatibility [2]. Here, a simple colorimetric paper-based sensor array was developed by using six metal indicators immobilized into PVC membrane, which can quickly and accurately identify twenty-five kinds of heavy metal ions (Ce^{3+} , Ag^+ , Cu^{2+} , Co^{2+} , Ni^{2+} , Sn^{4+} , Cd^{2+} , Fe^{2+} , Fe^{3+} , Al^{3+} , Zn^{2+} , Hg^{2+} , Pb^{2+} , Mn^{2+} , Bi^{3+} , La^{3+} , U_2^{2+} , Ti^{4+} , VO_3^- , AsO_4^{3-} , Sb^{3+} , UO_2^{2+} , Cu^+ , Sn^{2+} , and VO^{2+}). These sensing elements were produced a unique colorimetric response pattern for each metal, all obtained patterns were investigated by chemometrics methods such as principal component analysis (PCA), hierarchical clustering analysis (HCA) and linear discriminant analysis (LDA), leading to generate a clustering map for classifying heavy metal ions at different four concentrations of 10.0, 5.0, 2.5, 1.0 mg L^{-1} . The proposed sensor array exhibited substantial capacity for the discrimination of individual metal ions with accuracies higher than 96% at concentrations of 10.0, 5.0 and 2.5 mg L^{-1} . Also, it could successfully discriminate between the binary and ternary mixtures of metal ions. Discrimination of metal elements of different oxidation state is another potential of this array. Beside to qualitative analysis, it represented quantitative analysis ability, e.g., in the concentration ranges of 0.10 to 10.00 mg L^{-1} ($R^2 = 0.99$) and 0.25 to 12.50 mg L^{-1} ($R^2 = 0.99$) for Zn^{2+} and Co^{2+} , respectively.

Keywords: Colorimetric; paper-based device; PVC membrane; Heavy metal ions; Chemometric methods



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Analyzing Imaging Mass Spectrometry Data by Using Matrix Decomposition Methods in Chemometrics

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ABSTRACT

In this work, the potential of data analysis methods in obtaining quantitative and qualitative chemical information from mass spectrometry imaging (MSI) data about biological tissue will be studied. In recent years, due to the increasing high-resolution power of mass spectrometers, the number of the mass-to-charge (m/z) of mass spectra has also become very high, which leads to the production of very large data [1]. So, in raw data, the amount of information obtained from the sum of all spectra is very more than the required value. Ignoring much of the data does not fully exploit the potential of MSI techniques [2]. Using this method, both spatial distribution and spectral information of analyzed samples can be obtained. However, these main MSI bugs are mostly dependent on the complexity of the real target samples and the huge size of the data generated by this method [3]. Therefore, chemometrical tools are used to solve this problem. The present contribution is about the implementation of sparsity constraint in multivariate curve resolution-alternating least square (MCR-ALS) technique for analysis of three-way MSI data arrays (two spatial and one m/z dimensions) [4]. In the present study, the L1-regularization paradigm has been implemented in each iteration of the MCR-ALS algorithm in order to force the algorithm to return sparser mass spectra. L1-regularization has been applied by using the least absolute shrinkage and selection operator (Lasso) instead of the ordinary least square [5]. The advantages of the application of this method are shown for several examples of different data consisting of two three-way simulated data with 3 components that each component has a specific pattern to examine its effect on their interactions with each other and the background and also on a real MS data image of a mouse brain thin layer that was obtained by MALDI-MSI at (NERSC) [6]. The simulated data in this work have been fabricated and studied in different background modes with and without overlapping m/z channels, which makes this study comprehensive. Finally, the effect of the "sparsity constraint" has been explored on the possible solutions in MCR methods is investigated. The results in this work showed that the implementation of this constraint reduces the extent of rotational ambiguity in MCR results and can be useful for solving MS data with overlapping in mass spectra and concentration profiles [4].

Keywords: imaging, mass spectrometry, matrix decomposition, chemometrics, lasso regression

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Comparing the performance of PLS, GA-PLS, and OSC-GA-PLS models for QSAR Study of Inhibitory Activity of Pyrazolone Derivatives and Design of New Compounds Using Image Processing

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ABSTRACT

Nowadays, Pyrazolone and its derivatives have gained a lot of attention due to their biological and medicinal applications. These compounds have antimicrobial, antifungal and anticancer properties. Therefore, using simple methods to prepare these compounds is of importance. Pyrazolone is one of the inhibitors of kinase domain containing receptor KDR or VEGFR-2. In this study, quantitative structure-activity relationship (QSAR) analysis was used to predict the inhibitory activity of new Pyrazolone derivatives. Bi-dimensional images were used to calculate pixels for QSAR modeling. Furthermore, the partial least squares (PLS) was used to establish a relationship between IC_{50} dependent variables and independent variables, i.e., pixels or hidden variables. In addition, genetic algorithm (GA) was used in PLS method (GA-PLS) to select the descriptors. In this method, the variables selected to form the calibration model had negligible errors with acceptable characteristics. Pre-processing methods such as orthogonal signal correction (OSC) were also used to provide a suitable input for modeling as well as to improve the results of the GA (OSC-GA-PLS). Finally, root mean squared error of prediction (RMSEP) was used to assess the performance of the models for predicting the pIC_{50} of the studied compounds, the value of which was obtained equal to 0.3, 0.22, and 0.19 for PLS, GA-PLS and OSC-GA-PLS models, respectively. Furthermore, the proposed QSAR model was developed with the OSC-GA-PLS method to predict the inhibitory activity of the new compounds.

Keywords: Quantitative structure-activity relationship, Orthogonal signal correction, Genetic Algorithms, Partial least squares, Pyrazolone.

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Application of Image Processing for QSAR Study of Quinolone Derivatives as Anti-malaria Agents using different Chemometrics Methods

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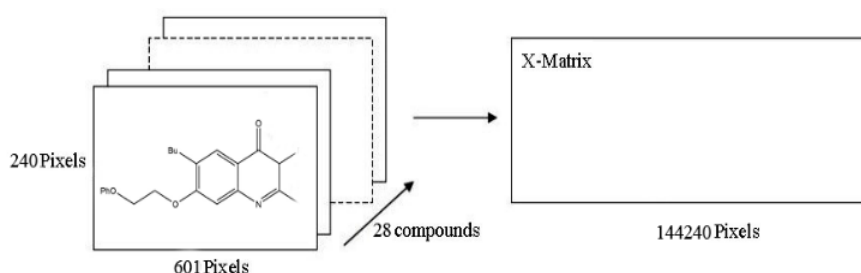
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ABSTRACT

A quantitative structure activity relationship (QSAR) study was performed using image processing method to obtain a model that best describes the anti-malaria activities (EC_{50}) of quinolone derivatives. In this study, pixel of molecular structures was considered as descriptors. Accordingly, a dataset of 28 quinolone derivatives was collected from literature [1]. Then structures were drawn in ChemOffice package and converted to pixels using MATLAB software. In order to have an appropriate selection of pixels, pre-processed methods such as mean centering and scaling were used. The useful descriptors were then selected using principal component analysis method (PCA) and genetic algorithm (GA) methods and the final model was developed by partial least squares (PLS) multivariate calibration method [2,3].



2D images and unfolding step of the 28 chemical structures to give the X-matrix

The QSAR model performance was evaluated and the agreement between computational and experimental values was investigated. The statistical parameters of all models were compared such as RMSEP (Best model, 0.0183), RSEP (Best Model, 0.246) and R^2 (Best Model, 0.9986). The developed model showed high ability to predict anti-malaria activities (EC_{50}).

Keywords: QSAR, Quinolone, Image processing, PLS, PCA

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QSAR Modeling for the In Silico Rational Design and Virtual Screening of Bioactive Peptides

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ABSTRACT

Predicting the bioactivity of peptides is an important challenge in drug development and peptide research. In this study, numerical descriptive vectors (NDVs) for peptide sequences were calculated based on the physicochemical properties of amino acids (AAs) and principal component analysis (PCA). The resulted NDV had the same length as the peptide sequence, so that each entry of NDV corresponded to one AA in the sequence. They were then applied to quantitative structure–activity relationship (QSAR) analysis of angiotensin-converting enzyme (ACE) inhibitor dipeptides, bitter-tasting dipeptides, and nonameric binding peptides of the human leukocyte antigens (HLA-A*0201). Multiple linear regression was used to construct the QSAR models. For each peptide set, a proper subset of physicochemical properties was chosen by the ant colony optimization algorithm. The leave-one-out cross-validation (q_{loo}^2) values were 0.855, 0.936, and 0.642 and the root-mean-square errors (RMSEs) were 0.450, 0.149, and 0.461. Our results revealed that the new numerical descriptive vector can afford extensive characterization of peptide sequence so that it can be easily employed in peptide QSAR studies. Moreover, the proposed numerical descriptive vectors were able to determine hot spot residues in the peptides under study.

Keywords: Bioactive peptides, ant colony optimization, Y-randomization test, BTT dipeptides, ACE tripeptides



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