



## 7<sup>th</sup> Iranian Biennial Chemometrics Seminar

### The posters' titles

#### *The 1<sup>st</sup> section: Wednesday, 30 Oct 2019*

ID No.	Title	Presenter
PN 001	The extraction and measurement of nickel metal ion in crab, shellfish and rice samples using magnetic silk fibroin - EDTA ligand and chemometric method.	Manijeh yekrangi
PN 003	Probing the binding mechanism of sorafenib to bovine $\alpha$ -lactalbumin using spectrometric methods, molecular docking	Fatemeh Bagheri
PN 005	Visualization of Component-wise Rotational Ambiguity Using Signal Contribution Function.	Jamile Mohammad Jafari
PN 007	Local Calibration Using Multivariate Curve Resolution Methods.	Ali Pahlevan
PN 009	Application of Box-Behnken design and response surface methodology in optimization of salting out assisted liquid-liquid microextraction of chromium species in environmental samples.	Mina Khodabakhsh
PN 011	Performance comparison of wavelet neural network and adaptive neuro-fuzzy inference system.	Mina Khodabakhsh
PN 013	Experimental and theoretical studies on interaction of some drugs with human serum albumin.	Fatemeh Mohammadnia

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PN 015	The experimental and theoretical studies of Biopartitioning Micellar Chromatography to mimic the drug-protein binding of some drugs	Fatemeh Mohammadnia
PN 017	Partial least squares- residual bilinearization for simultaneous determination of ten pesticides in milk using QuEChERS-dispersive liquid-liquid microextraction followed by gas chromatography.	Farnoosh Koleini
PN 019	Random Augmented Classical Least Squares: A Modified Calibration with CLS and ILS Advantages .	Saeed Khalili Ali Abad
PN 021	Combination of Multivariate Curve Resolution Alternating Least Squares Method and Experimental Design to Optimize the Simultaneous Photocatalytic Degradation of some Nitro phenols.	Javad Yousefi
PN 023	Comparison of molecular based modelling for predicting gas heat capacity of organic compounds.	Aboozar Khajeh
PN 025	The feasibility of applying hand-held NIR for speciation of beef, chicken, mutton and pork with Chemometrics.	Abolfazl Dashti
PN 027	QSPR study of linear retention indices of some organic compounds extracted from Lupinus Pilosus Murr plants.	Razieh.Hamidi
PN 029	Geochemometrics Analysis of Cr, As, Hg, Cd, Pb in Tarom soil samples by spectroscopic methods.	Somayeh Veyseh

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PN 031	The effect of random noise and spectral overlapping on the accuracy of the extracted profiles from spectroscopic data by soft modeling method.	Mahsa Zarei
PN 033	Discovery of New Inhibitors of AChE by Virtual Screening, Molecular Docking and Molecular Dynamics Simulations.	Pedram Bakhshi
PN 035	Multi-Stimuli Responsive Molecularly Imprinted Polymer Based on Chain Transfer Agent Modified Chitosan Nanoparticles for Microextraction of Capecitabine: An Experimental Design Study.	Saeedeh Ansari
PN 037	QSAR Study of Diarylpyrimidine Derivatives as HIV-1 Nonnucleoside Reverse Transcriptase Inhibitors by Particle Swarm Optimization Feature Selection-Multiple Linear Regression and Artificial Neural Networks.	Seyed Mohammadreza Motalebi Tabaei
PN 039	Combining chemometrics and the TOPSIS: a new approach to optimizing HPLC parameters using multiple-responses.	Leila Mousavi
PN 041	A QSAR Study of GC-MS Retention Indices of Essential Oils Extracted From Polygonum Minus Huds.	Shokoufe Khani
PN 043	Multivariate Methods Enhanced Nontarget LC-HRMS Assessment of the River Upstream and Downstream Water Pollution Impressed by Wastewater Treatment Effluents.	Reza Lotfi Khatoonabadi
PN 045	Quantitative structure activity relationship study of azine derivatives as NNRTIs using artificial neural network.	Mozhgan. Beglari

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PN 047	Optimization of process parameters for Paraquat and Diquat removal from binary solution by Angelica adsorbent using Box-Behnken experimental design.	Nasrin Mehmandost
PN 049	Modeling of Adsorption of Cr(VI) on chitosan-graphene oxide nanocomposite using RSM and ANN Techniques.	Mohammad Hossein Ahmadi Azqhandi

*The 2<sup>nd</sup> section: Thursday, 31 Oct 2019*

ID No.	Title	Presenter
PN 051	Adsorptive Removal of Phthalocyanine Using Nano-CoFe <sub>2</sub> O <sub>4</sub> as a Sorbent from Aqueous Solution; Optimization and Adsorption Characterization.	Mostafa Kazemi
PN 053	On MCR-BANDS and FACPACK under unimodality constraints.	Somaye Vali Zade
PN 055	Designing an IDA-based sensor array including a single indicator and receptor with multiple concentrations for quantitation of mixtures.	Vahideh Mahram
PN 057	Application of MIA-QSAR for design new protein P38 MAP kinase compounds with using Genetic Algorithm.	Atisa Yazdanipour
PN 059	Probing the binding mechanism of Nilotinib to bovine $\alpha$ -lactalbumin using spectrometric method, molecular docking.	Fatemeh Bagheri
PN 061	Analysis of residual moisture in a freeze-dried sample drug by multivariate fitting regression method.	Mahsa Akbari Lakeh
PN 063	Metabolomic study of the effects of parabens and pharmaceuticals in recycled water on metabolic pathways of lettuce using NMR and GC-MS followed by chemometric techniques.	Mahsa Seraj
PN 065	Response surface modelling by using principal component analysis followed by partial least squares for optimizing efficient factors in micro-solid phase extraction of polycyclic aromatic hydrocarbons in oil spills.	Nazanin Saburouh

*The 2<sup>nd</sup> section: Thursday, 31 Oct 2019*

PN 067	PLS-DA vs. Q/LDA for classification of isotope ratio mass spectrometry data: a new way for food authentication.	Ali Ghiasi
PN 069	Multiple response optimization of simultaneous biosorption of methylene blue and fuchsin acid by green alga <i>Ulva fasciata</i> .	Mina Khodabakhsh
PN 071	Principal component-adaptive neuro-fuzzy inference systems for the QSPR modeling of CMC of anionic gemini surfactants.	Mina Khodabakhsh
PN 073	QSPR model for adsorption of organic compounds by multi-walled carbon nanotube (MWCNT): Comparison between MLR and ANFIS.	Aboozar Khajeh
PN 075	Particle swarm optimization with various mutations for descriptor selection in QSPR studies.	Aboozar Khajeh
PN 077	Classification of three ground meat species using FTIR and chemometrics method.	Abolfazl Dashti
PN 079	Analysis of U and Th in Mahneshan soil samples by ICP-MS and Geochemometrics.	Somayeh Veyseh
PN 081	Modeling and Optimization of Electrical Conductivity of GO-Fe <sub>3</sub> O <sub>4</sub> Nanofluid by Using Experimental design and Artificial Neural Network.	Mohammad Hossein Ahmadi Azqhandi
PN 083	Analytical Figures of Merit for Feasible Solutions of Second-Order Calibration methods.	Fariba Norouz Yeganeh

*The 2<sup>nd</sup> section: Thursday, 31 Oct 2019*

PN 085	Preparation of Magnetic Molecularly Imprinted Polymer coated Multi-Walled Carbon Nanotubes for Ultra-Detection of Sotalol: An Experimental Design Study.	Saeedeh Ansari
PN 087	Application Constant center and Ratio difference Methods for Simultaneous Determination of m-nitroaniline and p-nitroaniline whit high overlapping spectra.	Fatemeh Mosayebi
PN 089	QSAR Study of New 1H-Pyrrolo [3, 2-c] Pyridine Derivatives against Melanoma Cell Lines by Firefly Algorithm-Support Vector Machine (FF-SVM).	Seyed Mohammadreza Motalebi Tabaei
PN 091	Hybrid QSPR models for the prediction of the linear retention index of volatile compounds in flour.	Zeinab Mozafari
PN 093	Chemometrics Study Of Dye-Surfactant Interaction By Spectroscopic And Conductometric Methods.	Anita Parsaei
PN 095	Quantitative structure activity relationship study of DAPY-like derivatives as NNRTIs using artificial neural network.	Mozhgan Beglari
PN 097	Discrimination of Iranian vegetable oils by coupling of colorimetric sensor arrays and chemometrics techniques.	Mahsa Chaharlangi
PN 099	A nanozyme-based colorimetric sensor array for discrimination of anions in water samples.	Hoda Sharifi