List of Accepted Lectures and Papers for the 10th Biennial Iranian Chemometrics Seminar

Oral presentation	
Speech Topic	**Presenter**
Application of multivariate tools in the discrimination of geographical origin of Iranian polyfloral honeys by analysis of physicochemical and biochemical characterization	***Saber Amiri***
Comparative Study of Nonlinear Hard and Soft Discrimination in Genomic Cancer Classification	***Somaye Vali Zade***
A transfer learning workflow based on MCR and CNN to overcome limitations in Vis-NIR HSI data modeling: a case study	***Fatemeh Sadat Hashemi-Nasab***
Multivariate Calibration Models for ATR-FTIR Spectroscopy Analysis of Olive Oil Adulterated with Corn, Sunflower, and Palm Oils	***Esra modares Askari***
AI-Driven Design and Optimization of Novel Carbon Allotropes via Crystallographic Space Group Exploration and Machine Learning Potentials	***Ebrahim Nemato-Kande***
Machine Learning Empowered Sensor Array for Dopaminergic Agents' Discrimination	***Reza Koohsar***
Moving toward Smart Sensors for eDiagnostics and eMonitoring	***Hamed Golmohammadi***

Identification and Measurement of H2S, COS and SO2 in Natural Gas Using a Machine Learning Empowered Colorimetric Sensor Array	***Ahmad Moslehipour***
A Deep Learning Workflow Based on Convolutional Neural Networks for GC-IMS Feature Extraction and Classification	***Farbod Bayat-Afshary***
Multi-Class Classification of Odor Perception Using Graph Neural Networks and Molecular Graph Representations	***Mahia V. Solout***
Biologically Informed Prediction of Drug Synergy: A Transcriptomic Resistance Signature Approach	***Sajjad Gharaghani***
Application of support vector machine in predicting potentiometric selectivity (Mg2+/Ca2+) of some amide ligands	***Reza Mahmoudzadeh Laki***

Poster presentation	
Topic	**Presenter**
Focused Molecular Docking Study of Minocycline and Doxycycline with Selected Cyclodextrins: Toward Efficient Host–Guest Complexation	***Melika asadian***
Harnessing γ-Cyclodextrin for Enhanced Macrolide Antibiotics Delivery and Environmental Mitigation: A Computational Perspective	***Melika asadian***
Prediction of lipid/water distribution coefficient of the organic compounds using the Monte Carlo approach and hybrid optimal descriptors	***Shahram Lotfi***
QSPR modeling of chromatography retention indices of plant essential oils using SMILES and graph invariants	***Shahram Lotfi***
Monte Carlo algorithm in the prediction of Value of Binding Constants of Organic Ligands to Beta-Cyclodextrin	***Shahram Lotfi***
Simultaneous analysis of four cardiovascular drugs in synthetic mixtures and polypill tablets using triple devisor mean centering and derivative spectrophotometric techniques	***Maryam Maghfourian***
Artificial neural networks coupled Grey wolf optimizer for modeling of reactive red 198 adsorption onto novel poly(o-toluidine) / strontium hexaferrite /analsim nanocomposite	***H. Alijani***

SPA-PL-MARS QSAR Modeling of Xanthenone Derivatives as HCT-15 Colorectal Cancer Inhibitors: An Integrated Variable Selection and Nonparametric Regression Approach	***Maryam Allahverdi***
Classification of Extra Virgin Olive Oil Adulteration Using FTIR Spectroscopy and Machine Learning Algorithms	***Esra modares Askari***
Alternative Conditional Expectation Method for Modeling the QSAR (IC50) of Oxazolidinone Derivatives as 17β-Hydroxysteroid Dehydrogenase Type 3 Inhibitors	***Mohaddeseh Habibi***
Comparison of Regression Methods (ACE, SVR, PLS, MLR) in QSAR, a Kinesin-5 Inhibitor Case Study	***Mohammadreza Pourmohammad***
QSAR Modeling and Prediction of the Hallucinogenic Potency of Amphetamine Derivatives Using a Docking-Guided QSAR Approach	***Zahra Imanikia***
Predicting the Viscosity of Magnesium Oxide-Based Nanofluids in Deep Eutectic Solvents Using Quantitative Structure-Property Relationship Modeling	***Mohammad Hossein Hajian***
Discrimination of Iranian black teas through volatile compound fingerprints and chemometric modeling	***Adineh Aminianfar***
Selective Tankyrase Inhibitors for Wnt-Driven Cancers: QSAR, Docking, Virtual Screening, and ADMET-Based Selection	***Narjes Najafi***
Development of a chemometrics classification model in order to identification of diabetic patients for their saliva infrared spectrum	***Sepideh Khodkavandi***

Untargeted Metabolomics Based on NMR Spectroscopy and Supervised Kohonen Network for Plasma Biomarker Identification in Early Breast Cancer Detection	***Maryam Kashi***
Deep Learning-Enabled Vis-NIR Hyperspectral Imaging for Fast and Accurate Detection, Classification and Quantification of Dimethoate Residues in Apples	***Parya Omrani***
Exploring Independence in Area of Feasible Solutions of Three-Component Systems: Calculations and Significance	***Fatemeh Sadat Hashemi-Nasab***
Divergent Biological Conclusions: A Comparison of PLS-DA and MCR-ALS in Metabolomics	***Maryam Khoshkam***
Design the ElectroSensor- Liquid Phase Micro Extraction chip for Morphine detection as a model drug in urine sample	***Maryam Mehrban***
A Hybrid NARX Neural Network and Metaheuristic Optimization Approach for Predicting the Galvanostatic Charge-Discharge Dynamics of Supercapacitors	***Hamed Azimi***
Application of Group LASSO as dimension reduction method in QSAR Studies using a novel descriptor grouping strategy	***Farzaneh Kia***
Application of Group Exponential LASSO and as bi-level feature selection method in QSAR Studies	***Farzaneh Kia***
Effect of Descriptor Grouping Strategies on Bi-Level Feature Selection and Predictive Performance in GEL-Based QSAR Modeling	***Farzaneh Kia***

Rapid Methanol Detection in Ethanol Solutions via Non-Linear Raman Spectroscopy Modeling	***Somaye Vali Zade***
Correlation between Lubricant Viscosity Index and Mooney Viscosity of Polymers: A Predictive Model using Artificial Neural Networks	***Mohammad Hossein Aghamohammadi***
Viscosity Enhancement of MWCNT/SiC Hybrid Nanofluids in SAE 20W50 Engine Oil: Experimental Analysis and Machine Learning Modeling	***Mohammad Hossein Aghamohammadi***
QSAR and molecular docking studies for a chemometrics approach to the investigation of pyrimidine derivatives as novel inhibitors of anticancer drugs	***Dariush Fathali***
Application of preprocessing methodes in image processing for simultaneous determination of three drugs	***Parisa Shakhsari***
Application of preprocessing methods in image processing in QSAR and drug design	***Parisa Shakhsari***
Quantitative structure activity relationship study of p38α MAP kinase inhibitors	***Maryam Nouri majd***
Three-dimensional QSAR study on XIa (FXIa) inhibitors and design of new compounds based on CoMFA, CoMSIA and molecular docking	***Ladan Kazemnezhad***
Three-dimensional QSAR study on iazolo-pyrimidine derivatives as WRN inhibitors for the treatment of MSI tumors and design of new compounds based on CoMFA and molecular docking	***Mobina Haji Abbasi***

Dispersive liquid-liquid microextraction for the extraction of ibrutinib drug from real samples using UV-Vis spectrophotometry and optimization by experimental design	***Sara Kharat Zabardast***
Dispersive liquid-liquid microextraction (DLLME) for extraction and preconcentration of Enzalutamide in real samples using the UV-Vis spectrophotometry	***Sanaz Saber Siyahpoush***
A Comprehensive FTIR Spectral Database for Authentication and Quality Control of Edible and Essential Oils	***Niloofar Rahmani***
Machine Learning Enhanced Discrimination of Biothiol and Thiol Ratios Using Gold Nanorod Amalgamation	***Golara Akhondi***
Application of Central Composite Design in Modeling and Optimization of a Bio-Based Time–Temperature Indicator Using Fatty Acids	***Maryam Safari***
Optimization of Aluminum Anodizing Conditions and Evaluation of Potassium Permanganate-Loaded Anodic Alumina for Ethylene Removal in Active Packaging of Fruits and Vegetables	***Saeid Golmirzaei***
Chemometric Desgin of Experiments for the Optimization of conditions in HS-SPME-GC detection of Menthol	***Raziyeh gholami***
Optimizing Anthocyanin Extraction from Prunus domestica Flesh Using Experimental Design	***Zahra Valizadeh***
Design of Experiment for Optimized Ultrasound-Assisted Extraction of Natural Pigments	***Zeynab Rasuli***

Optimized Extraction of Pectin from Apple Pomace Using Response Surface Methodology for Sustainable Industrial Applications	***Elham Teymorirad***
Machine Learning Classification of Solid-Phase Microextraction (SPME) Types Based on Operational and Analytical Parameters from Experimental Data	***Erfan Hashemi***
Molecular docking and DFT studies of a series of tetrazole derivatives and computational studies of Fe3O4@Phenyl phosphate creatine	***Fatemeh Mohsenzadeh***
Multivariate image – QSAR of phenyl piperidine derivatives as potent dual NK1R antagonists/serotonin transporter (SERT) inhibitor	***Neda Ladooni***
Design of Colorimetric Sensor Based on Anti-etching of Gold Nanorods for Discrimination and Detection of Dopaminergic Agents	***Zahra Hozhabr***
PH-Dependent Sensor Array Based on Carbon Quantum Dots for Detection and Discrimination of Amines	***Tahereh Rasoulizadeh***
Solvent-tuned Sensor Arrays Based on colored Carbon Quantum Dots for Discrimination of Multiple Metal Ions	***Tahereh Rasoulizadeh***
Experimental design for optimization of the removal of Rhodamine B using a novel GQD incorporated Hydrogel	***Reza Dadashi***
Rank Annihilation Factor Analysis for Kinetic Spectrophotometric Determination of MCPA herbicide in Unknown Samples	***Reza Dadashi***
Classification of some opioids using principal component Analysis	***Morteza Bahram***

Application of artificial neural network for the simultaneous determination of two rizatriptan and sumatriptan drugs via gold nanoparticle aggregation-based colorimetric sensing	***Masoud Esmailpak***
Chemometric modeling of an electrochemical aptasensor for gluten detection using simulated electrochemical sensor data and comparison with experimental results	***Masoumeh Yousef-Zadeh***
ComplexGNN: Hybrid Graph and Descriptor Learning for Interpretable Bandgap Prediction in Inorganic Crystals	***Dorsa Benvan***
Machine Learning–Driven Discovery of a Potent Lead Compound for GPR17 via Graph Neural Networks and Multistage Structural Validation	***Noushin Agh Babaie***
Using Machine Learning in the In-Silico Design of Selective Dopamine Receptor Ligands: Advancements in Targeted Therapies for Neurological and Psychiatric Disorders	***Melika F. Aghdam***
Seed quality assessment using hyperspectral and multispectral imaging techniques	***Yeganeh Nazari***
AI-Driven Design of PCSK9 Allosteric Inhibitors for Atherosclerosis via Graph Neural Networks and Structure-Based Validation	***Behnaz Horri***
Leveraging Machine Learning and Graph Neural Networks for the Discovery of JAK2 Inhibitors: Structure and Ligand-Based Approaches to Target Inflammatory and Autoimmune Diseases	***Shaghayegh K. Nezhad***

Enhancing pH Measurement Accuracy Using Hyperspectral Imaging and commercial pH Strips	***Arshia Rostampour***
Comparative investigation of BORGEN norms	***Hamideh Bakhshi***
Multi-criteria evaluation of combined preprocessing techniques for first-order spectroscopic calibration	***Mohammad Khademloo***
Feasible band boundaries computation in bilinear matrix decomposition using essential data	***Somaye Vali Zade***
Evaluation of Classical and Statistical Mechanics-Based Models for Adsorption Data: Insights into Accurate Fitting and Physical Interpretation	***Fatemeh Khabbazi***
Machine Learning Bases Optimal Design of Carbon Nanosheets	***Ebrahim Nemati-Kande***
Oriented Hyper-Cyclic Geometry with Curvature: A Weighted Directed Graph Model for Molecular Asymmetry and Chirality	***Khalil Shahbazpoor***
A Fluorescent Concentration-Based Sensor Array Utilizing Hydrogen Peroxide-Etched Sulfur Quantum Dots (SQDs-H_2O_2) for Simultaneous Detection of Chromium(VI) and Bismuth(III) Ions via Multivariate Calibration	***Sima Mojarrad***
Detection of Buffalo Milk Adulteration with Cow Milk Using NIR Spectroscopy and Multivariate Data Analysis	***Ghazaleh Alikbarzadeh***

Molecular Modeling and Design of Novel Inhibitors for GABAA Receptors	***Farshad Jafari***
Spice Adulteration Detection Using Hyperspectral and Multispectral Imaging	***Mahshid Ziaee jazi***
Artificial neural networks coupled Grey wolf optimizer for modeling of reactive red 198 adsorption onto novel poly(o-toluidine) / strontium hexaferrite /analsim nanocomposite	***H. Alijani***
Virtual screening study of some GSK-3 inhibitors, such as Benzamide, Pyrazolopyrimidine, and β-phenylalanine derivatives, as anti-diabetic agents	***M. Piria***
The application of machine learning to identify the chemical features that affect the stability of low-dimensional perovskite layers	***Mahmoud Samadpour***
Optimization of Cd Adsorption by Chitosan Using Response Surface Methodology (RSM) Based on Box-Behnken Model	***Marziyeh Piri***
Explainable Artificial Intelligence (XAI) for Regulatory-Compliant Chemometric Models in Pharmaceutical Analysis	***Nastaran Bahadori***
Prediction of blood-brain barrier penetration coefficient of some central nervous system drugs using molecular docking modeling and quantitative structure-activity relationship	***Pezhman Maghouli***

FastCCS: A Deep Learning Framework for Accurate Collision Cross-Section Prediction from SMILES with Broad Applications in Cheminformatics and Omics	***Amir Aghajan***
Enhanced Rhodamine B Removal by Green-Synthesized Cu/TiO_2 Adsorbent: Evaluation of Adsorption Isotherms	***Seyed Mehdi Sajjadi***
Multiple Linear Regression and Radial Basis Function Neural Networks for Identifying Effective Parameters and Ensuring Robustness in LC–MS/MS Simultaneous Analysis	***Rabee Mahdavi***
Presenting a rapid and inexpensive spectroscopic/chemimetric method for the simultaneous determination of drug mixture used in the treatment of infectious diseasesusing artificial intelligence based on fuzzy inference system and support vector machine	***Zeynab Abootorabi***
CCD-Based Integrated Extraction–Encapsulation of β-Carotene from Carrot: A Chemometrics Approach humanized	***Zahra Sadri***
A CCD-based two-stage DOE framework for the extraction and stabilization of lycopene from tomato pomace using ultrasound-assisted extraction and solid lipid encapsulation	***Fariba Abdi Saray***
Explainable Machine Learning–Guided Optimization of µSPE-DALOµE for Phenol Extraction	***Marziyeh Hosseinchi***
Detection of adulteration and rapid evaluation of food purity using electrochemical impedance spectroscopy and chemometrics methods	***Salar Khalili***