10th Iranian Biennial Chemometrics Seminar Timetable

Seminar Venue: International Campus, Urmia University – Shahid Beheshti Street

Tuesday, October 14, 2025	
Program Section	**Time**
Registration & Welcome	14:00-20:00

Wednesday, October 15, 2025	
First section	
Program Section	**Time**
Opening Ceremony	08:00 – 09:30
Speech: Prof. Hamid Abdollahi (Chemometrics Education in the Era of Digital Chemistry)	09:30 – 10:00
Break and poster presentation	10:00 – 11:00

Wednesday, October 15, 2025		
Second section		
Speech Topic	**Presenter**	**Time**
From Latent Structure to Neural Networks: Bridging Chemometrics and Deep Learning in Chromatography and Imaging	*Dr. Hadi Parastar*	11:00 – 11:30
Comparative Study of Nonlinear Hard and Soft Discrimination in Genomic Cancer Classification	*Somaye Vali Zade*	11:30 – 11:50
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*	11:50 –12:10

Multivariate Calibration Models for ATR-FTIR Spectroscopy Analysis of Olive Oil Adulterated with Corn, Sunflower, and Palm Oils	***Esra modares Askari***	**12:10 –12:30**
Lunch & Prayer		**12:30 – 14:30**
Third section		
Speech Topic	***Presenter***	***Time***
The Functions of Chemometrics Integrated with the Emerging Paradigm of Machine Learning and Artificial Intelligence in Pharmaceutical Sciences	***Dr. Somaieh Soltani***	**14:30 –15:00**
AI-Driven Design and Optimization of Novel Carbon Allotropes via Crystallographic Space Group Exploration and Machine Learning Potentials	***Ebrahim Nemato-Kande***	**15:00 –15:20**
Machine Learning Empowered Sensor Array for Dopaminergic Agents' Discrimination	***Reza Koohsar***	**15:20 –15:40**
Moving toward Smart Sensors for eDiagnostics and eMonitoring	***Hamed Golmohammadi***	**15:40 –16:00**
Break and poster presentation		**16:00 – 17:00**
Fourth section		
Speech Topic	***Presenter***	***Time***

Recent Developments in Multivariate Curve Resolution	***Prof. Roma Tauler***	**17:00 –17:30**
Identification and Measurement of H2S, COS and SO2 in Natural Gas Using a Machine Learning Empowered Colorimetric Sensor Array	***Ahmad Moslehipour***	**17:30 –17:50**
A Deep Learning Workflow Based on Convolutional Neural Networks for GC-IMS Feature Extraction and Classification	***Farbod Bayat-Afshary***	**17:50 –18:10**
Traditional Ashiq Live Music		**18:10 – 18:30**
Tour of Tabib House and Urmia University Central Laboratory		**18:30 – 20:00**
Dinner		**20:00 – 21:00**

Thursday, October 16, 2025		
Fifth section		
Speech Topic	***Presenter***	***Time***
Assessing Matrix Effects with Multivariate Curve Resolution	***Prof. Hamid Abdollahi***	**08:00 –08:30**

Multi-Class Classification of Odor Perception Using Graph Neural Networks and Molecular Graph Representations	***Mahia V. Solout***	**08:30 –08:50**
Biologically Informed Prediction of Drug Synergy: A Transcriptomic Resistance Signature Approach	***Sajjad Gharaghani***	**08:50 –09:10**
Break and poster presentation		**09:10 – 10:30**
Sixth section		
From punch card to AI in chemistry	***Prof. J.B Ghasemi***	**10:30 –10:50**
Divergent Biological Conclusions: A Comparison of PLS-DA and MCR-ALS in Metabolomics	***Dr. Maryam Khoshkam***	**10:50 –11:10**
Application of support vector machine in predicting potentiometric selectivity (Mg2+/Ca2+) of some amide ligands	***Reza Mahmoudzadeh Laki***	**11:10 –11:30**
Application of multivariate tools in the discrimination of geographical origin of Iranian polyfloral honeys by analysis of physicochemical and biochemical characterization	***Dr. Saber Amiri***	**11:30 –11:50**
Closing Ceremony		**11:50 – 12:40**
Lunch & Prayer		**12:40 – 14:30**
Free Urmia City Tour		**15:00 – ------**

Poster presentation Wednesday, October 15, 2025		
Topic	**Presenter**	**ID No.**
A Comprehensive FTIR Spectral Database for Authentication and Quality Control of Edible and Essential Oils	***Niloofar Rahmani***	**P1**
Machine Learning Enhanced Discrimination of Biothiol and Thiol Ratios Using Gold Nanorod Amalgamation	***Golara Akhondi***	**P2**
Application of Central Composite Design in Modeling and Optimization of a Bio-Based Time–Temperature Indicator Using Fatty Acids	***Maryam Safari***	***P3***
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***	***P4***
Chemometric Desgin of Experiments for the Optimization of conditions in HS-SPME-GC detection of Menthol	***Raziyeh gholami***	***P5***
Optimizing Anthocyanin Extraction from Prunus domestica Flesh Using Experimental Design	***Zahra Valizadeh***	***P6***
Design of Experiment for Optimized Ultrasound-Assisted Extraction of Natural Pigments	***Zeynab Rasuli***	***P7***

Optimized Extraction of Pectin from Apple Pomace Using Response Surface Methodology for Sustainable Industrial Applications	***Elham Teymorirad***	***P8***
Machine Learning Classification of Solid-Phase Microextraction (SPME) Types Based on Operational and Analytical Parameters from Experimental Data	***Erfan Hashemi***	***P9***
Molecular docking and DFT studies of a series of tetrazole derivatives and computational studies of Fe3O4@Phenyl phosphate creatine	***Fatemeh Mohsenzadeh***	***P10***
Multivariate image – QSAR of phenyl piperidine derivatives as potent dual NK1R antagonists/serotonin transporter (SERT) inhibitor	***Neda Ladooni***	***P11***
Design of Colorimetric Sensor Based on Anti-etching of Gold Nanorods for Discrimination and Detection of Dopaminergic Agents	***Zahra Hozhabr***	***P12***
PH-Dependent Sensor Array Based on Carbon Quantum Dots for Detection and Discrimination of Amines	***Tahereh Rasoulizadeh***	***P13***
Solvent-tuned Sensor Arrays Based on colored Carbon Quantum Dots for Discrimination of Multiple Metal Ions	***Tahereh Rasoulizadeh***	***P14***
Experimental design for optimization of the removal of Rhodamine B using a novel GQD incorporated Hydrogel	***Reza Dadashi***	***P15***
Rank Annihilation Factor Analysis for Kinetic Spectrophotometric Determination of MCPA herbicide in Unknown Samples	***Nima Karimnejad***	***P16***

Application of artificial neural network for the simultaneous determination of two rizatriptan and sumatriptan drugs via gold nanoparticle aggregation-based colorimetric sensing	***Masoud Esmailpak***	***P17***
Chemometric modeling of an electrochemical aptasensor for gluten detection using simulated electrochemical sensor data and comparison with experimental results	***Masoumeh Yousef-Zadeh***	***P18***
ComplexGNN: Hybrid Graph and Descriptor Learning for Interpretable Bandgap Prediction in Inorganic Crystals	***Dorsa Benvan***	***P19***
Machine Learning–Driven Discovery of a Potent Lead Compound for GPR17 via Graph Neural Networks and Multistage Structural Validation	***Noushin Agh Babaie***	***P20***
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***	***P21***
Spice Adulteration Detection Using Hyperspectral and Multispectral Imaging	***Mahshid Ziaee jazi***	***P22***
Seed quality assessment using hyperspectral and multispectral imaging techniques	***Yeganeh Nazari***	***P23***
AI-Driven Design of PCSK9 Allosteric Inhibitors for Atherosclerosis via Graph Neural Networks and Structure-Based Validation	***Behnaz Horri***	***P24***

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***	***P25***
Enhancing pH Measurement Accuracy Using Hyperspectral Imaging and commercial pH Strips	***Arshia Rostampour***	***P26***
Comparative investigation of BORGEN norms	***Hamideh Bakhshi***	***P27***
Multi-criteria evaluation of combined preprocessing techniques for first-order spectroscopic calibration	***Mohammad Khademloo***	***P28***
Feasible band boundaries computation in bilinear matrix decomposition using essential data	***Somaye Vali Zade***	***P29***
Evaluation of Classical and Statistical Mechanics-Based Models for Adsorption Data: Insights into Accurate Fitting and Physical Interpretation	***Fatemeh Khabbazi***	***P30***
Machine Learning Bases Optimal Design of Carbon Nanosheets	***Ebrahim Nemati-Kande***	***P31***
Oriented Hyper-Cyclic Geometry with Curvature: A Weighted Directed Graph Model for Molecular Asymmetry and Chirality	***Khalil Shahbazpoor***	***P32***
A Fluorescent Concentration-Based Sensor Array Utilizing Hydrogen Peroxide-Etched Sulfur Quantum Dots (SQDs-H_2O_2) for Simultaneous	***Sima Mojarrad***	***P33***

Detection of Chromium(VI) and Bismuth(III) Ions via Multivariate Calibration		
Detection of Buffalo Milk Adulteration with Cow Milk Using NIR Spectroscopy and Multivariate Data Analysis	***Ghazaleh Alikbarzadeh***	***P34***
Molecular Modeling and Design of Novel Inhibitors for GABAA Receptors	***Farshad Jafari***	***P35***
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***	***P36***
Virtual screening study of some GSK-3 inhibitors, such as Benzamide, Pyrazolopyrimidine, and β-phenylalanine derivatives, as anti-diabetic agents	***M. Piria***	***P37***
The application of machine learning to identify the chemical features that affect the stability of low-dimensional perovskite layers	***Mahmoud Samadpour***	***P38***
Optimization of Cd Adsorption by Chitosan Using Response Surface Methodology (RSM) Based on Box-Behnken Model	***Marziyeh Piri***	***P39***
Explainable Artificial Intelligence (XAI) for Regulatory-Compliant Chemometric Models in Pharmaceutical Analysis	***Nastaran Bahadori***	***P40***
Prediction of blood-brain barrier penetration coefficient of some central nervous system drugs	***Pezhman Maghouli***	***P41***

using molecular docking modeling and quantitative structure-activity relationship		
FastCCS: A Deep Learning Framework for Accurate Collision Cross-Section Prediction from SMILES with Broad Applications in Cheminformatics and Omics	***Amir Aghajan***	***P42***
Enhanced Rhodamine B Removal by Green-Synthesized Cu/TiO_2 Adsorbent: Evaluation of Adsorption Isotherms	***Seyed Mehdi Sajjadi***	***P43***
Multiple Linear Regression and Radial Basis Function Neural Networks for Identifying Effective Parameters and Ensuring Robustness in LC–MS/MS Simultaneous Analysis	***Rabee Mahdavi***	***P44***
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***	***P45***
CCD-Based Integrated Extraction–Encapsulation of β-Carotene from Carrot: A Chemometrics Approach humanized	***Zahra Sadri***	***P46***
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***	***P47***
Explainable Machine Learning–Guided Optimization of µSPE-DLLµE for Phenol Extraction	***Marziyeh Hosseinchi***	***P48***

Detection of adulteration and rapid evaluation of food purity using electrochemical impedance spectroscopy and chemometrics methods	***Salar Khalili***	***P49***
Deep Learning-Enabled Vis-NIR Hyperspectral Imaging for Fast and Accurate Detection, Classification and Quantification of Dimethoate Residues in Apples	***Parya Omrani***	***P50***

Poster presentation ***Thursday, October 16, 2025***		
Topic	***Presenter***	**ID No.**
Focused Molecular Docking Study of Minocycline and Doxycycline with Selected Cyclodextrins: Toward Efficient Host–Guest Complexation	***Melika asadian***	***P51***
Harnessing γ-Cyclodextrin for Enhanced Macrolide Antibiotics Delivery and Environmental Mitigation: A Computational Perspective	***Melika asadian***	***P52***
Prediction of lipid/water distribution coefficient of the organic compounds using the Monte Carlo approach and hybrid optimal descriptors	***Shahram Lotfi***	***P53***
QSPR modeling of chromatography retention indices of plant essential oils using SMILES and graph invariants	***Shahram Lotfi***	***P54***

Monte Carlo algorithm in the prediction of Value of Binding Constants of Organic Ligands to Beta-Cyclodextrin	***Shahram Lotfi***	***P55***
Simultaneous analysis of four cardiovascular drugs in synthetic mixtures and polypill tablets using triple devisor mean centering and derivative spectrophotometric techniques	***Maryam Maghfourian***	***P56***
SPA-PL-MARS QSAR Modeling of Xanthenone Derivatives as HCT-15 Colorectal Cancer Inhibitors: An Integrated Variable Selection and Nonparametric Regression Approach	***Maryam Allahverdi***	***P57***
Classification of Extra Virgin Olive Oil Adulteration Using FTIR Spectroscopy and Machine Learning Algorithms	***Esra modares Askari***	***P58***
Alternative Conditional Expectation Method for Modeling the QSAR (IC50) of Oxazolidinone Derivatives as 17β-Hydroxysteroid Dehydrogenase Type 3 Inhibitors	***Mohaddeseh Habibi***	***P59***
Comparison of Regression Methods (ACE, SVR, PLS, MLR) in QSAR, a Kinesin-5 Inhibitor Case Study	***Mohammadreza Pourmohammad***	***P60***
QSAR Modeling and Prediction of the Hallucinogenic Potency of Amphetamine Derivatives Using a Docking-Guided QSAR Approach	***Zahra Imanikia***	***P61***
Predicting the Viscosity of Magnesium Oxide-Based Nanofluids in Deep Eutectic Solvents Using Quantitative Structure-Property Relationship Modeling	***Mohammad Hossein Hajian***	***P62***

Discrimination of Iranian black teas through volatile compound fingerprints and chemometric modeling	***Adineh Aminianfar***	***P63***
Selective Tankyrase Inhibitors for Wnt-Driven Cancers: QSAR, Docking, Virtual Screening, and ADMET-Based Selection	***Narjes Najafi***	***P64***
Development of a chemometrics classification model in order to identification of diabetic patients for their saliva infrared spectrum	***Sepideh Khodkavandi***	***P65***
Untargeted Metabolomics Based on NMR Spectroscopy and Supervised Kohonen Network for Plasma Biomarker Identification in Early Breast Cancer Detection	***Maryam Kashi***	***P66***
Exploring Independence in Area of Feasible Solutions of Three-Component Systems: Calculations and Significance	***Fatemeh Sadat Hashemi-Nasab***	***P67***
Design the ElectroSensor- Liquid Phase Micro Extraction chip for Morphine detection as a model drug in urine sample	***Maryam Mehrban***	***P68***
A Hybrid NARX Neural Network and Metaheuristic Optimization Approach for Predicting the Galvanostatic Charge-Discharge Dynamics of Supercapacitors	***Hamed Azimi***	***P69***
Application of Group LASSO as dimension reduction method in QSAR Studies using a novel descriptor grouping strategy	***Farzaneh Kia***	***P70***

Application of Group Exponential LASSO and as bi-level feature selection method in QSAR Studies	***Farzaneh Kia***	***P71***
Effect of Descriptor Grouping Strategies on Bi-Level Feature Selection and Predictive Performance in GEL-Based QSAR Modeling	***Farzaneh Kia***	***P72***
Rapid Methanol Detection in Ethanol Solutions via Non-Linear Raman Spectroscopy Modeling	***Somaye Vali Zade***	***P73***
Correlation between Lubricant Viscosity Index and Mooney Viscosity of Polymers: A Predictive Model using Artificial Neural Networks	***Mohammad Hossein Aghamohammadi***	***P74***
Viscosity Enhancement of MWCNT/SiC Hybrid Nanofluids in SAE 20W50 Engine Oil: Experimental Analysis and Machine Learning Modeling	***Mohammad Hossein Aghamohammadi***	***P75***
QSAR and molecular docking studies for a chemometrics approach to the investigation of pyrimidine derivatives as novel inhibitors of anticancer drugs	***Dariush Fathali***	***P76***
Application of preprocessing methodes in image processing for simultaneous determination of three drugs	***Parisa Shakhsari***	***P77***
Application of preprocessing methods in image processing in QSAR and drug design	***Parisa Shakhsari***	***P78***
Quantitative structure activity relationship study of p38α MAP kinase inhibitors	***Maryam Nouri majd***	***P79***

Three-dimensional QSAR study on XIa (FXIa) inhibitors and design of new compounds based on CoMFA, CoMSIA and molecular docking	***Ladan Kazemnezhad***	***P80***
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***	***P81***
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***	***P82***
Dispersive liquid-liquid microextraction (DLLME) for extraction and preconcentration of Enzalutamide in real samples using the UV-Vis spectrophotometry	***Sanaz Saber Siyahpoush***	***P83***