



# Seminar Programs

## Wednesday

- 7:30- 8:30, *On desk Registration and Reception*
- 8:30- 9:30, *Opening Ceremony*
- 9:30-10:00 *Coffee Break*
- 10:00- 12:10, *Lecture session 1*

**Chair: Prof. Abdollahi and Prof. Ghasemi**

Time	Lecturer	Title
10:00 – 10:35	Taghi Khayamian	Challenges in drug discovery and development
10:35 – 11:10	Marcel Maeder	Chemometrics and Chemistry
11:10– 11:30	Mahsa Akbari	An Investigation on Meaning and Reliability of Local Rank Constraint in Self-Modeling Curve Resolution of Chemical Data
11:30-11:50	Mohammad Ahmadvand	A systematic study on the effect of noise and shift on multivariate figures of merit of second-order calibration algorithms
11:50-12:10	Kobra Samghani	3D-QSAR studies of the inhibition efficiency of phenolic herbicides on photosynthesis by using CoMFA and CoMSIA

- 12:10-14:00, *Praying, Launch and Resting*
- 14:30- 15:50, *Lecture session 2*



**Chair: Prof. Maeder and Prof. Fatemi**

Time	Lecturer	Topic
14:00 – 14:35	Hamid Abdollahi	Calculation of Feasible Bands for Visualizing the Constraint Effects in Soft Modeling Methods
14:35 - 15:10	Hadi Parastar	How to Expand the Use of Independent Component Analysis in Analytical Chemistry?
15:10 – 15:30	Saeed Yousefinejad	Quantitative sequence activity relationship of bitter tasting threshold peptides: a comparison study between some two-way and three-way modeling methods
15:30-15:50	Elham Aghaei	Influence of bonded-phase density in chiral chromatography via molecular simulation

 **15:50 -17:00, Poster session 1 Numbers:1003-1065**

 **17:00 -18:50, Lecture session 3**

**Chair: Prof. Hemmateenejad and Dr. Vosough**

Time	Lecturer	Topic
17:00 – 17:35	Mohammad Hossein Fatemi	Present and future of QSAR methodology
17:35 – 18:10	Mehdi Mousavi	Novel feature selection methods and CAIS resolution software
18:10 – 18:30	Masoumeh Rashvand	Investigation of a sewage treatment plant for removal of selective pharmaceutical and personal care products using HPLC-DAD and second-order calibration
18:30-18:50	Zeinab Saberi Dehkordi	Design and construct a small fluoremeter with a smartphone as the detector associated with image processing



# Thursday



## 8:00 - 9:50, Lecture session 4

Chair: **Prof. Marini and Dr. Parastar**

Time	Lecturer	Topic
8:00 – 8:35	Knut Baumann	Defining the Applicability Domain for Classification Models by Hedging Predictions
8:35 – 9:10	Ali Niazi	Geochemometrics
9:10 – 9:30	Parisa Izadiyan	Metabolite profiling and chemometric classification of two varieties of Ocimum basilicum medicinal plant
9:30– 9:50	Samira Beyramysoltan	Analytical view on uniqueness

## 9:50-11:00, Poster session 2 Numbers:1068-1122

## Thursday, 11:00 - 12:30, Lecture session 5

Chair: **Prof. Bauman and Prof. Khayamian**

Time	Lecturer	Topic
11:00 – 11:35	Federico Marini	Applications of Particle swarm optimization in chemometrics
11:35 – 12:10	Maryam Vosough	Multi-way assisted chromatographic methodologies for analysing highly complex samples
12:10 – 12:30	Saheleh Sheykhizadeh	Introducing of invasive weed optimization as a new variable selection method

## 12:30-14:00, Praying, Launch and Resting

## 14:00 - 15:50, Lecture session 6



Chair: **Dr. Naseri and Dr. Mousavi**

Time	Lecturer	Topic
14:00 – 14:35	Saeed Masoum	Identification of potential antimicrobial and antioxidant constituents in some medicinal herbs using hephenated chromatograrhic methods and multivariate calibration techniques
14:35 – 15:10	Maryam Salahinezhad	Quantitative Nanostructure Activity Relationship Modeling (Nano-QSAR)
15:10 – 15:30	Akram Rostami	Using global and local sensitivity analysis for variable sorting and selection
15:30-15:50	Afsane Heidari	A theoretical approach to model and predict the adsorption coefficients of some small aromatic molecules on carbon nanotube

 **15:50-17:00, Poster session 3 Numbers:1123-1171**

 **17:00 - 18:50, Lecture session 7**

Chair: **Dr. Bahram and Dr. Masoum**

Time	Lecturer	Topic
17:00 – 17:35	Sajjad Gharaghani	Computational Chemogenomics: an emerging strategy for rapid target and drug discovery
17:35 – 18:10	Ahmad Mani	What is in Chemometrics for Chemoinformatics: Validating Classical Relativity in Chemical Space
18:10 – 18:30	Nematollah Omidikia	Direct Triadic Decomposition

 **19:00-20:00, Free Discussion Panel**