

8th Iranian Biennial Chemometrics Seminar



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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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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Third section "scientific speeches"

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| 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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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 Neurotransmitters | 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

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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 |
|  Closing ceremony | | 16:30 -17:00 |
| Parto Afzar Sanaat Company workshop | | 17:00 -18:30 |

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