THE 13ᵀᴴ WINTER SYMPOSIUM ON CHEMOMETRICS (ONLINE EVENT 2022)

SYMPOSIUM SCHEDULE

All times are in Moscow time (MSK = GMT+3)

MONDAY, 28 FEBRUARY: ONLINE SCHOOL ON CHEMOMETRICS

Time		Speaker	Talk title
9:25	9:30	Timur Labutin	Welcome address
9:30	11:30	Ivan Krylov	Basics of PARAFAC decomposition in fluorescence excitation-emission spectroscopy
11:30	12:00		*Coffee break*
12:00	14:00	Yulia Monakhova	Independent components analysis (ICA) in practice: tips and tricks
14:00	15:00		*Lunch*
15:00	16:30	Dmitry Kirsanov	Multisensor systems' data processing

TUESDAY, 1 MARCH: ONLINE SYMPOSIUM, DAY 1

Time		Speaker	Talk title
8:55	9:00	Timur Labutin	Welcome address
9:00	9:40	Hadi Parastar	There is plenty of gloom in quantitative mass spectrometry imaging: can deep learning help?
9:40	10:05	Ryland Giebelhaus	Region of Interest Selection for GC-MS Data with a Pseudo Fisher Ratio Moving Window
10:05	10:25	Anastasia Surkova	Aquaphotomics approach for cancer diagnosis and monitoring
10:25	10:45	Yury Zontov	Study of the applicability of modern machine-learning techniques to the task of similarity search of objects represented by series of images and metadata
10:45	11:05	Yuri Kalambet	Peak modelling using exponentially modified functions
11:05	11:13	Lyudmila Bratchenko	Recognition and classification of skin Raman spectra using convolutional neural networks analysis
11:13	11:21	Michael Armstrong	PARAFAC2×2: a PARAFAC Model for Drift in Two Modes
11:21	11:29	Dmitry Silaev	Spectrophotometric determination of active substances in ophthalmic formulation using chemometrics
11:29	11:50		*Coffee break*

TUESDAY, 1 MARCH: ONLINE SYMPOSIUM, DAY 1

11:50	12:30	Yulia Monakhova	Independent components analysis (ICA) at the "cocktail-party" in analytical chemistry
12:30	12:50	Daniil Anisimov	Electronic nose based on Organic Field Effect Transistors for food quality monitoring
12:50	13:10	Claudio Marchesi	MicroNIR and chemometrics for microplastics pollution
13:10	13:30	Nikolai Sushkov	Compositional features of zooplankton species as studied by laser-based analytical techniques
13:30	13:50	Ivan Trukhin	Application of cluster analysis to identify the breakthrough of injected water in oil wells
13:50	14:10	Anastasia Shuba	Primary and secondary data fusion from a sensor array for prediction of qualitative and quantitative indicators
14:10	14:18	Yevgeni Skorobogatov	Discrimination of plant samples using carbocyanine fluorophore additives
14:26	15:30		*Lunch*
15:30	16:10	Rasmus Bro	Using chemical insight and AI to automate untargeted GC-MS profiling
16:10	16:30	Andrey Bogomolov	Development of a Multispectral Fiber Probe
16:30	16:50	Polina Turova	Various machine learning methods in HPLC-MS datasets treatment
16:50	17:10	Jordi Cruz Sanchez	Quantitative determination of curcuminoids in turmeric powder in just 5 seconds
17:10	17:30	Rene Burger	Benchtop NMR versus High Field NMR: Comparison of Chemometric Molecular Weight Analysis of Lignin
17:30	17:38	Anna Shik	The use of artificial neural networks for the simultaneous determination of several analytes by the oxidation reactions of carbocyanine fluorophores
17:38	17:46	Ivan Plyushchenko	Application of gradient boosting machine for signal processing in LC-MS metabolomics

WEDNESDAY, 2 MARCH: ONLINE SYMPOSIUM, DAY 2

Time		Speaker	Talk title
9:00	9:40	Timur Madzhidov	Chemoinformatics and machine learning in synthetic chemistry: from data to models, from models to robots
9:40	10:00	Nadezhda Vladimirova	Prediction of potentiometric selectivity for carbonate-selective plasticized membrane sensors using QSPR modelling
10:00	10:20	Isabelle Viegas	Advanced coupled factorization of multi-way fluorescence data to assess the conjugation of quantum dots to proteins
10:20	10:40	Andrey Ferubko	Fluorescent determination of the total content of humic substances in waters using multidimensional calibration models
10:40	11:00	Rustam Guliev	Generalization and geometrical interpretation of N-FINDR algorithms for unmixing hyperspectral data
11:00	11:08	Yuri Ikhalaynen	Untargeted metabolomics study of *Humulus lupulus* brewing cultivars, for genetic origin classification task
11:08	11:16	Zahars Selivanovs	Nonlinear dimensionality reduction methods for multisensor system data analysis
11:16	11:24	Sergey Zaytsev	Stochastic optimisation of spectra of laser-induced plasma for plasma composition calculation
11:24	11:50		*Coffee break*
11:50	12:30	Paolo Oliveri	Is signal pre-processing a trivial step? A focus on pitfalls and challenges
12:30	12:50	Ivan Krylov	Modelling of scattering signal for direct PARAFAC decompositions of excitation-emission matrices
12:50	13:10	Simon Lindner	Is the Calibration Transfer of Multivariate Calibration Models Between High- and Low-Field NMR Instruments Possible?
13:10	13:30	Alexey Skvortsov	Grey modelling of absorption spectra of silver nanoisland films
13:30	13:50	Liana Zagitova	Voltammetric sensors in the analysis of enantiomeric mixture using PLS
13:50	13:58	Yekaterina Yuskina	Chemometric processing of the data from high-frequency inductor for chemical sensing
13:58	15:30		*Lunch*
15:30	16:10	Puneet Mishra	Deep learning for spectral data modelling in Chemometrics: the benefits and the hypes
16:10	16:30	Soraya Aidene	Correcting sample matrix effects in XRF data using chemometrics
16:30	16:50	Timur Akhmetzhanov	Direct analysis of lanthanides in REE-rich ores by Laser-Induced Breakdown Spectrometry coupled with Chemometrics
16:50	17:10	Cristina Malegori	A moving-block-PCA based approach for real time monitoring of a powder blending process using a miniaturized near infrared sensor

WEDNESDAY, 2 MARCH: ONLINE SYMPOSIUM, DAY 2

17:10	17:30	Nadan Kravich	Improving precision of potentiometric multisensor analysis using nonlinear regression methods: spent nuclear fuel reprocessing case study
17:30	17:38	Alexandra Yevseeva	Handling of optical multisensor data
17:38	17:46	Marat Nazyrov	Sensor system based on Cu(II) and Zn(II) amino acid complexes for recognition of atenolol enantiomers in racemic mixture using the partial least squares
17:46	17:54	Irina Matveeva	Decomposition of in vivo skin Raman spectra using multivariate curve resolution method
17:54	18:00	Timur Labutin	Closing remarks