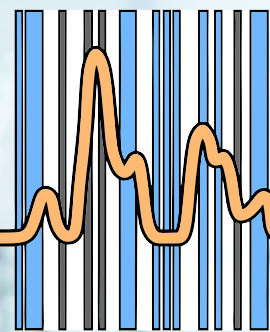# IMA-2021

12th International Conference on Instrumental Methods of Analysis
Modern Trends and Applications

20-23 September 2021 | VIRTUAL EVENT

BOOK OF ABSTRACTS
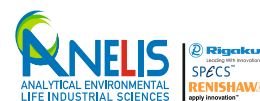
Organized by

ARISTOTLE UNIVERSITY OF THESSALONIKI

National Technical University of Athens

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CONFERENCE DETAILS

The 12th International Conference on "Instrumental Methods of Analysis" (IMA-2021) takes place between 20-23 September 2021 as a Virtual event organized by the Aristotle University of Thessaloniki and the National Technical University of Athens. IMA is a biannual series of conferences that started in 1999 and covers all areas of Chemical Analysis, including the development of new techniques, modern trends, and applications in a wide range of scientific disciplines. Up to date several leading analytical chemists from Greece and abroad have presented their research work at the previous IMA meetings. Considering existing pandemic conditions, the relevant uncertainty on international travelling and the difficulty of gathering large meeting groups, our decision to organize IMA-2021 with virtual presentations and attendance ensures safety for all participants while at the same time it provides the opportunity for high-level analytical scientists from all around the world to promote their relevant research.

For the 12th IMA conference (first time in Virtual format), it is our ambition to bring together some of the most talented and innovative analytical chemists from all over the world for an excellent scientific online conference. The scientific program consists of keynote lectures, oral and poster presentations, given by a wide mix of scientists and engineers, ranging from the established academics and world leaders in analytical chemistry to the dynamic and ambitious postgraduate students. Furthermore, contributions from companies, including presentations of new instrumentation, new applications, and assessment of future commercial trends and opportunities are also included.

TOPICS

- Spectrometric and Electrometric analysis
- Chromatographic, Mass Spectrometric and Microscopic analysis
- Thermal analysis
- Proteomics, Metabolomics, Metallomics and Elemental Speciation analysis
- Chemical- and bio- sensors
- Field analysis - Mobile analytical instruments
- Miniaturized analytical systems (Lab-on-a-Chip)
- Micro- and Nano- fluidics
- Immunoassays
- Electrophoretic separation techniques
- Sampling techniques and strategies
- Sample handling and preparation
- Robotics and Automation
- Quality control-quality assurance in analysis
- Metrology
- Environmental, Biomedical, Pharmaceutical, Food analysis

- Materials Analysis (Nanomaterials, Smart/Advanced Materials)Archaeometry
- Analytical chemistry markets and possibilities for commercialization

Special sessions on the following themes

- AEROSOL METROLOGY
- ADVANCED X-RAY TECHNIQUES
- VIRUS SPREAD ANALYTICS

AWARDS

The most outstanding presentations during IMA-2021 will receive one of the awards from the following categories:

- **Best presentation related to X-ray Spectroscopy.** The best oral presentation with X-ray Spectroscopy research will receive an award sponsored by the European X-ray Spectrometry Association.
- **Best poster award prize.** The best poster presentation will receive an award of 500 CHF sponsored by the new open-access journal MDPI Analytica. Apart from the significance and the originality of the poster, the presentation impact will be also evaluated through a short 3-min presentation of the work by the presenting author during the poster session. Therefore, participating with a short video or live presentation is a requirement to be included in the competition for this award.
- **Best oral presentation award in the field of sensors, instrumentation and multiphysics simulation.** The best oral presentation dealing with Chemical and biosensors, Multiphysics phenomena simulation, Field analysis—mobile analytical instruments, Robotics and automation, Miniaturized analytical systems (Lab-on-a-Chip), micro and nanofluidics, Multiscale modelling and characterization of materials and processes, Design and optimization of devices and systems with numerical approaches/techniques, will receive an award of 500 $ sponsored by the open-access journal MDPI Micromachines.

Presented papers will be evaluated by the Award Committee according to the following criteria: Significance of the paper, Originality, Presentation impact, Young researcher. The winners of IMA-2021 awards will be announced during the closing ceremony of the conference.

PROCEEDINGS

A book of abstracts including submitted abstracts will be shared to the participants. In addition, all accepted abstracts will be published as open-access documents in the MDPI Applied Sciences (impact factor 2.679) Special issue dedicated to IMA-2021.

PUBLICATION IN JOURNALS

IMA-2021 provides several possibilities for the publication of presented studies in one of the collaborating peer-review journals.

Participants have the option to submit their full papers in the Special Issue "Selected Papers from the 12th International Conference on "Instrumental Methods of Analysis" (IMA-2021)" of the new open-access journal **MDPI Analytica**. All submissions through the conference will receive a full-waiver for article processing charges.

Participants have the option to submit their full papers in the Special Issue "12th International Conference on Instrumental Methods of Analysis - IMA-2021" of open-access journal **MDPI Applied Sciences** (Impact factor 2.679). All submissions through the conference will receive a 20% discount for article processing charges.

Selected works related to chemical and biosensors, multiphysics phenomena simulation, field analysis—mobile analytical instruments, robotics and automation, miniaturized analytical systems (lab-on-a-chip), micro and nanofluidics, multiscale modelling and characterization of materials and processes, design and optimization of devices and systems with numerical approaches/techniques will be published in the Special Issue related to IMA-2021 of journal **MDPI Micromachines** (Impact factor 2.891). All submissions through the conference will receive a 500 CHF discount for article processing charges.

Selected works related to the application of analytical techniques for sustainable water treatment will be published in the Special Issue "Sustainable Approaches in Water Treatment Practices, Presenting Minimum Environmental Impact "of journal **MDPI Water** (Impact factor 3.103).

CERTIFICATE OF ATTENDANCE

All registered participants are eligible to receive a certification of attendance at the end of the conference. The certificate will be sent electronically to online participants.
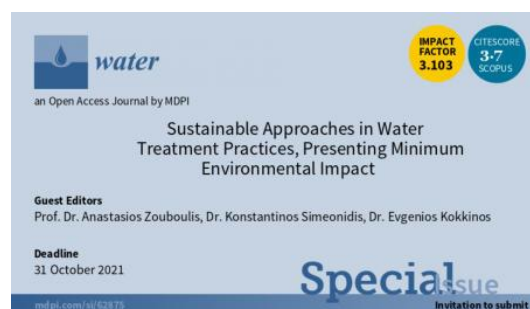
PROGRAM AT A GLANCE

Monday 20 September 2021

	09.30-10.00	Greetings
Session A1-Plenary	10.00-12.00	Virus spread analytics, Drug research
	12.00-12.15	Break
Session A2	12.15-14.00	Aerosol metrology, Advanced X-Ray techniques I
	14.00-14.30	Break
Session A3	14.30-16.15	Aerosol metrology, Advanced X-Ray techniques II
	16.15-16.30	Break
Session A4	16.30-18.30	Spectroscopy and applications

Tuesday 21 September 2021

Session B1-Plenary	09.30-11.30	Trends in analytical techniques
	11.30-11.45	Break
Session B2	11.45-12.30	Chromatography, Mass spectrometry I
	12.30-14.00	Virtual exhibition
	14.00-14.30	Break
Session B3	14.30-16.15	Chromatography, Mass spectrometry II
	16.15-16.30	Break
Session B4	16.30-18.15	Chromatography, Speciation, Bioanalytics, Bioseparation
	18.15-20.00	Poster session I

Wednesday 22 September 2021

Session C1	09.30-11.30	Food analysis I
	11.30-11.45	Break
Session C2	11.45-12.45	Food analysis II
	13.00-14.00	Poster session II
	14.00-14.45	Break
Session C3	14.45-16.15	Chemistry associations
	16.15-16.30	Break
Session C4	16.30-18.30	Environmental analysis, Chromatography, Mass spectrometry
	18.30-18.45	Break
	18.45-20.00	Poster session III

Thursday 23 September 2021

Session D1	09.30-11.30	Materials analysis
	11.30-11.45	Break
Session D2	11.45-13.45	Electrochemistry, Sensors, Archaeometry
	13.45-14.30	Break
Session C3	14.30-15.30	Mobile analytical instruments, Robotics and Automation, Chemometrics
	15.30-16.15	Closing Ceremony-Awards

Tuesday 21 September 2021

SESSION B3

Chromatography | Mass spectrometry II

Chair: R. Lobinski, A. Hiskia

QSRR driven insight into retention in multimodal chromatography

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Liquid chromatography system in which several separation mechanisms are integrated in the composition of a single column is called multimodal or mixed-mode chromatography (MMC). MMC systems are classified based on combined separation mechanisms as bimodal (RP/HILIC, RP/IEX, HILIC/IEX) and trimodal (different combinations of RP/HILIC/IEX). The main benefit of MMC lies in widening the spectra of properties of analytes that can be simultaneously chromatographed (nonpolar, polar, organic, inorganic, ionized and / or non-ionized analytes). In this way, it is possible to reduce the number of required analyses for one complex sample compared to unimodal chromatographic systems. For that reason, the popularity of MMC has been growing fast in recent years. However, in line with this achievement, MMC is characterized by large number of intermolecular interactions governing separations which are related to the properties of the analyte (charge and polarity) and chromatographic conditions (ionic strength and the pH of the aqueous phase and the content of the organic solvent) [1]. In order to get insight into relative contribution of aforementioned factors to retention of selected group of analytes, preferred chemometric approach is Quantitative Structure Retention Relationship (QSRR) study. The QSRR models relate the physical-chemical properties of analytes reflected by assigned molecular descriptors with their retention behaviour in predefined experimental space described by the range of chromatographic conditions (instrumental and mobile phase composition related factors). Apart from its general purpose to assist in the characterization of observed chromatographic system, the reliable predictions of retention behaviour of so-called system blind analytes (analytes of known chemical structure but not subjected to experimentations) can also be derived from a QSRR model. In such way, the development of MMC based analytical method can be rationalized by saving time and other resources [2].

This research demonstrates the QSRR study performed on 31 pharmaceuticals covering wide range of polarities, acid-base properties and divergent retention in RP/WCX system (Thermo Acclaim Mixed Mode WCX-1 3 μm, 2.1x150 mm column). This system was subjected to variations of the mobile phase composition (30-50% (v/v) of acetonitrile; 3.8-5.6 pH value and 20-40 mM ionic strength of acetic buffer) and column temperature (30–38 °C) according to the plan of central composite design of experiments. The machine learning algorithm based on Artificial Neural Network was used for relating these independent variables to cube root transformed retention factors of analytes as observed responses. The network comprising of 11-7-1 topology was trained through 1200 cycles with learning rate set at 0.3 and momentum set at 0.5. Cross validation and external validation were used to prove good statistical performances of built model (Root Mean Square Error values 0.131 and 0.147 and Squared Correlation vales 0.963 and 0.944, respectively). According to the weighting scheme used, volume fraction of acetonitrile, pH of aqueous phase and descriptors related to hydrophobicity and molecule size demonstrated the greatest impact towards retention in MMC.

References
[1] D. Sýkora, P. Řezanka, K. Záruba and V. Král, Journal of Separation Science, 42 (2019) 89-129.
[2] P. Haddad, M. Taraji, R. Szücz, Analytical chemistry, 93 (2020) 228-256.