



Advanced School of Mass Spectrometry

-On Mass Frontier-



Dear,

We would like to inform you that the Centre of Excellence of the Faculty of Chemistry, University of Belgrade organizes an advanced school of mass spectrometry, which will be held on 10 – 11 December 2014 at the Faculty of Chemistry.

The programme of lectures will include the topics in the area of the theory of mass analyzers, advanced setting during small molecules analysis, components identification using high-resolution screening, using a wide range of supporting application softwares in the area of mass spectrometry. The aim of these lectures are to get the participants introduced with possibilities and methodology of the operation of hybrid mass spectrometers as well as the implementation of a wide range of application softwares in processing and analysis of the acquired results. In fact, a constant evolution in the area of mass spectrometry enables that quantity and quality of the acquired data rapidly increase and, thereby, the time needed for their processing and analysis. Hence, choosing an adequate application software is of key importance and it largely facilitates the interpretation and extraction of useful data, acquired by the analysis. Robert Mistik, the owner and founder of software company HighChem and the creator of Mass Frontier software, will be one of the main lecturers at the advanced school. Robert Mistrik (48), HighChem, Slovakia, has a masters degree in chemistry from the Slovak Technical University, Bratislava, Slovakia and a Ph.D. from the University of Vienna, Austria. He held a postdoctoral position at the National Institute of Standards and Technology (NIST), Gaithersburg, MD, USA. Mr. Mistrik is the creator of Mass Frontier, a software for processing and interpreting mass spectral data in which the spectral tree concept was first introduced. He is the author of a precursor ion fingerprinting method that allows the identification of metabolites based on substructural identities of tandem mass spectra. In 2009, he was awarded the Head of the Year prize, a national award for exceptional achievement in science and technology. Mr. Mistrik has been a member of the scientific steering committee of the METAcancer consortium, aiming to identify small molecule biomarkers in breast cancer tissue. In 2012, he was elected - and in 2014 re-elected - to the Board of Directors of the Metabolomics Society. Currently, he is leading the mzCloud initiative which is a collaborative effort to build a comprehensive spectral trees' library for the identification of metabolic components utilizing molecular evolutionary patterns. On this occasion, Mr. Mistik will talk about the implementation of Massfrontier software during processing and interpretation of data and he will give the examples of high-resolution general unknown screening. Additionally, he will talk about mzCloud as a unique and innovative approach to creating an overwhole free online library and database for identification of small molecules and metabolic components.



New generations of high-resolution hybrid mass spectrometers as well as their possibilities and implementation depending on the application area where they are implemented in, will be also presented for the first time. It will be also discussed about a new generation of iontrap analyzers and innovative solutions in the area of mass spectrometry. Moreover, by direct operating on a hybrid mass spectrometer LTQ_XL-OrbiTrap the participants will have the opportunity to get to know the construction of one of a high-resolution hybrid mass spectrometers and the methodology of operating on it. Performing the analysis and setting up the experiment on the instrument in the example of multi-component analysis within chosen matrices as well as the software processing of acquired results will be shown.

School agenda :

Wednesday, 10.12.2014, Faculty of Chemistry

8:30 – 9:30 Registrarion of particpants

9:30 – 10:00 Welcome Prof. Zivoslav Tesić, Prof. Tanja Ćirković Veličković

10:00 – 11:00 **Mass analyzers**; *Silvio Kečkeš, Analysis, Serbia*

11:00 – 11:30 **Ion trap advance settings**; *Silvio Kečkeš, Analysis, Serbia*

11:30 – 12:00 Coffee break

12:00 – 13:30 **Orbitrap Fusion - An evolution in mass spectrometry**; *Luka Milivojević, Kobis, Slovenia*

13:30 – 15:00 Lunch- Italian restaurant " *Otimo* "

15:00 – 17:00 **Work Shop**

- LTQ_XL-OrbiTrap high-resolution hybrid mass spectrometer – introduction
- Instrument Seting for multicomponent analysis –creating instrument metod
- Injection of the samples

Thursday, 11.12.2014., Faculty of Chemistry

9:00 – 10:00 Result overview

10:00 – 11:30 **m/z Cloud : Freely accessible advanced mass spectral database of high resolution tandem spectra**; *Robert Mistik, HighChem, Slovakia*

11:30 – 12:00 Coffee break

12:00 – 13:30 **Advanced data processing and computer assisted structure elucidation using Mass Frontier software**; *Robert Mistik, HighChem, Slovakia*

13:30 – 15:00 Lunch- Italian restaurant " *Otimo* "

15:00 – 17:00 **Work Shop**

- Data procesing and structure elucidation using Mass Frontier software