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Document Abstract

The deliverable D2.9 “Final report of the different Advanced User Schools” is part of WP2, which includes the organization of several short courses and schools (for End Users and Advanced Users). This deliverable reports the overall course agenda, number of participants, location and logistic details of the 2nd Advanced Users School (AUS-2) that took place in Prague.



Table of Contents

1. Introduction	5
2. EU_FT-ICR_MS Advanced User School 2, Institute of Microbiology of the Czech Academy of Science, Prague - Czech Republic, September 26-30, 2021	6

Abbreviations (if any)

AUS Advanced Users School

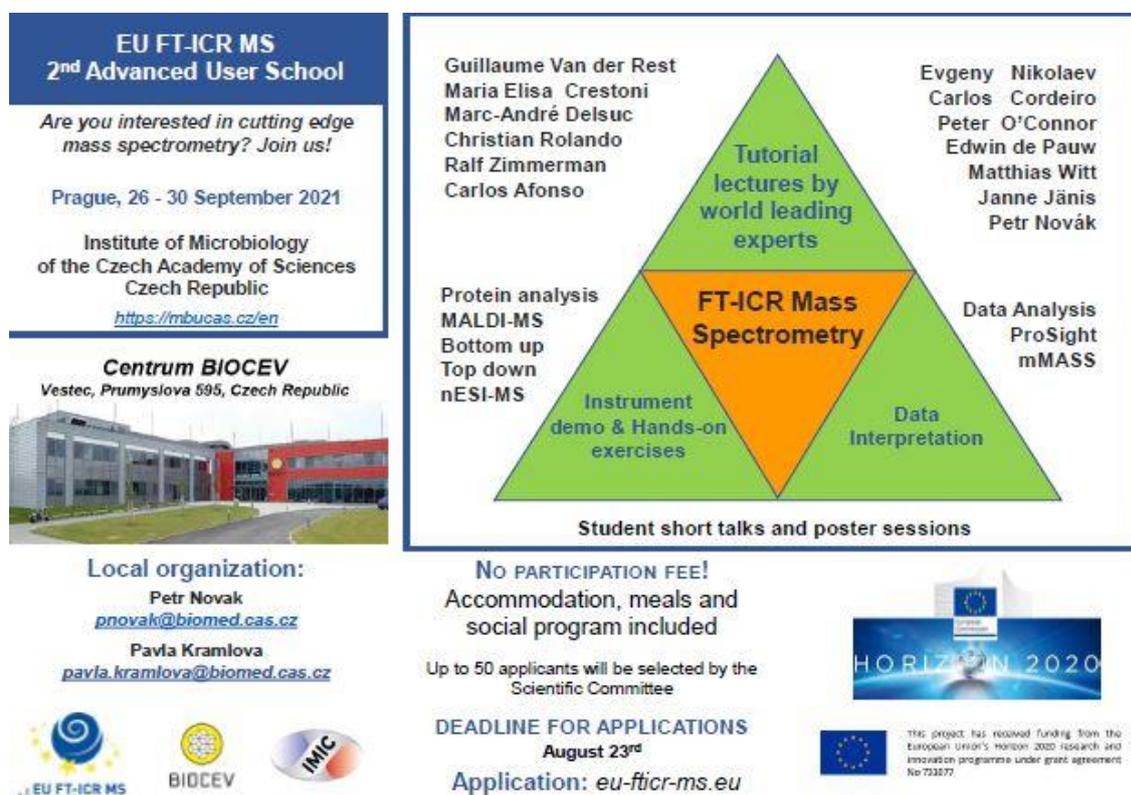
1. Introduction

One of the objectives of the EU FT-ICR-MS consortium is to provide training and advanced education in the field of FT-ICR MS. For this purpose, several courses and schools are planned with the participation of the whole EU FT-ICR MS network. These training courses aim to: i) contribute to the research work performed by graduate and postgraduate (PhD) students, post-docs and early-stage researchers, by exposing them to FT-ICR MS and its applications; ii) share newly developed state-of-the-art procedures for experiments and data analysis; iii) train qualified and highly skilled FT-ICR specialists (engineers and scientists); iv) extend and reinforce the contribution of FT-ICR MS to the current and future applications in many research fields; v) attract both FT-ICR data end-users and scientists from other disciplines required for further development of the FT-ICR technique (especially physicists, applied mathematicians and computer scientists). The Advanced User Schools (AUS) are mainly intended for researchers from both academia and industry who are already experienced in the use of FT-ICR MS and want to expand their knowledge and skills in terms of the more advanced methodology or specific applications of the technique. Thus, the main objective of AUS is to allow participants to gain a state-of-the-art expertise in FT-ICR MS and to provide incentive towards novel developments and applications.

2. EU_FT-ICR_MS Advanced User School 2, Institute of Microbiology of the Czech Academy of Science, Prague - Czech Republic, September 26-30, 2021

Final report

The second AUS was organized in Prague by Petr Novák (P3 – PRAG), in the period 26-30 September 2021, at the Institute of Microbiology of the Czech Academy of Science, Prague (Figure 1). This school brought together FT-ICR experts and students eager to learn together the tricks in the trade.



EU FT-ICR MS
2nd Advanced User School

Are you interested in cutting edge mass spectrometry? Join us!

Prague, 26 - 30 September 2021

Institute of Microbiology
of the Czech Academy of Sciences
Czech Republic
<https://imbucas.cz/en>

Centrum BIOCEV
Vestec, Prumyslova 595, Czech Republic

Local organization:
Petr Novak
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Pavla Kramlova
pavla.kramlova@biomed.cas.cz

NO PARTICIPATION FEE!
Accommodation, meals and social program included

Up to 50 applicants will be selected by the Scientific Committee

DEADLINE FOR APPLICATIONS
August 23rd
Application: eu-fticr-ms.eu

Tutorial lectures by world leading experts

FT-ICR Mass Spectrometry

Instrument demo & Hands-on exercises

Data Interpretation

Student short talks and poster sessions

Guillaume Van der Rest
Maria Elisa Crestoni
Marc-André Delsuc
Christian Rolando
Ralf Zimmerman
Carlos Afonso

Evgeny Nikolaev
Carlos Cordeiro
Peter O'Connor
Edwin de Pauw
Matthias Witt
Janne Jänis
Petr Novák

Protein analysis
MALDI-MS
Bottom up
Top down
nESI-MS

Data Analysis
ProSight
mMASS

HORIZON 2020

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Figure 1. Flyer of the 2nd AUS of the EU_FT-ICR_MS network.

Training was accomplished by a blend of lectures (14 tutorial lectures) and practical sessions, either in front of computers (1 computer session with demonstrations and data analysis) or in front of a real FT-ICR mass spectrometer (1 laboratory live demo sessions). The School programme is presented in Figure 2-5. All presentations from the teachers were uploaded into the portal <http://www.eu-fticr-ms.eu/>.



EU_FT-ICR_MS 2nd Advanced Users School

Prague, 26 - 30 September 2021



27th September, Monday

9:00 – 9:20	Opening
9:20 – 10:40	Carlos Afonso "The beautiful friendship of IMS and FT-ICR mass spectrometry for complex mixtures analysis"
10:40 – 11:00	Coffee break
11:00 – 12:20	Carlos Cordeiro "Metabolomics - Revealing the Biochemical Fingerprints of Life" (<i>on-line</i>)
12:20 – 13:20	Lunch
13:20 – 14:40	Guillaume Van der Rest "Combination of FT-ICR mass spectrometry and spectroscopy for the characterization of ion structures"
14:40 – 16:00	Maria Elisa Crestoni "Exploring the intrinsic properties of bioinorganic complexes by Ion-Molecule Reactions"
16:00 – 16:20	Coffee break
16:20 – 17:40	Christopher Rüger "Ionization schemes and techniques in FT-ICR MS: From commercial towards customized solutions" (<i>on-line</i>)
17:40 – 18:30	Short presentations of participants I
18:30 – 21:00	Dinner and poster section

Short presentations of participants I

Anthony Abou Dib "Pushing the capacity of the FT-ICR MS to a higher level"

Marc Haegelin "Super-resolution in FT-ICR MS by non-Fourier Transform genetic evolution signal processing"

Julie Guillemant "Sulfur compounds characterization using FT-ICR MS: towards a better comprehension of vacuum gas oils hydrodesulfurization process"

Davide Corinti "Open-shell Pt(III)-containing complexes characterized by IRMPD spectroscopy and quantum chemical calculations"

Nathaniel Terra Telles Souza "Analysis of solid and liquid samples in the context of SWIM using LDI FT-ICR MS"



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Figure 2. Programme of the 2nd AUS of the EU FT-ICR MS consortium (Monday).

28th September, Tuesday

9:00 – 10:00	Petr Novák “Structural Proteomics – From protein stable covalent labeling to chemical cross-linking”
10:00 – 11:00	Petr Man “Structural Proteomics – Hydrogen-deuterium exchange”
11:00 – 11:40	Coffee break and Guided tour (Structural mass spectrometry and Proteomics)
11:40 – 13:00	Petr Man, Zdeněk Kukačka and Petr Novák “Sample preparation, FT-ICR MS sample analysis / Top down of proteins / Data interpretation”
13:00 – 14:00	Lunch
14:00 – 17:30	Sightseeing tour “Karlštejn castle”
19:00 – 23:00	Boat trip and course dinner



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Figure 3. Programme of the 2nd AUS of the EU FT-ICR MS consortium (Tuesday).

29th September, Wednesday

9:00 – 10:20	Peter O'Connor "Current capabilities in 2DMS on FTICR mass spectrometers" (<i>on-line</i>)
10:20 – 10:40	Coffee break
10:40 – 12:00	Marc-André Delsuc "Elements of data analysis in 1D and 2D FTICR-MS data"
12:00 – 12:30	Short presentations of participants II
12:30 – 13:30	Lunch

Short presentations of participants II: David Jurnečka "Acylation dictates the extent of activation of bacterial RTX toxins"; Cristina Dal Lago "Modification of Therapeutic monoclonal antibodies by Togni reagents"; Palasser Michael "FAST MS - An open-source software for automated and quantitative analysis of top-down mass spectra"

13:30 – 14:50	Maria Andrea van Aghoven "The Benefits of 2D-Mass Spectrometry for Protein Structural Characterization"
14:50 – 15:10	Coffee break
15:10 – 16:30	Janne Janis "Principle and practice of native mass spectrometry"
16:30 – 17:30	Short presentations of participants III
17:30 – 20:00	Dinner and poster section

Short presentations of participants III: Hynek Mácha "Visualization of Polyamines and Amino Acids Alterations in Neonatal Brain Hypoxic-Ischemic Injury in Rats by Mass Spectrometry Imaging"; Alessandro Maccelli "Untargeted metabolomic profiling of Goji berries and leaves (*Lycium barbarum* L.) by FT-ICR MS"; Rutuja Patil "Freeing *Aspergillus fumigatus* of Polymyovirus Infection Renders It More Resistant to Competition with *Pseudomonas aeruginosa* Due to Altered Iron-Acquiring Tactics"; Dominika Luptáková "Siderophore-based differentiation of *Aspergillus fumigatus* colonization and invasion"; Caterina Bordin "Oil paints: identification of siccative oil and cross-links from museum size sample by chemical depolymerization and ultra-high resolution mass spectrometer"; Bogdan Purcareanu "Application of MALDI-FT-ICR-MS for nanostructured thin films characterization"



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Figure 4. Programme of the 2nd AUS of the EU FT-ICR MS consortium (Wednesday).



EU_FT-ICR_MS 2nd Advanced Users School

Prague, 26 - 30 September 2021



30th September, Thursday

WHERE: Institute of Microbiology of the Czech Academy of Sciences (IMIC), Vídeňská 1083, 142 20 Prague 4

- | | |
|---------------|--|
| 9:00 – 10:20 | Evgeny Nikolaev “FT ICR cell: How to make the best” |
| 10:20 – 11:40 | Mathias Witt “Petroleomics – from crude oil to asphaltenes” |
| 11:40 – 12:00 | Coffee break |
| 12:00 – 13:20 | Christian ROLANDO “FT-ICR MS for Cultural Heritage” |
| 13:20 – 14:00 | Prize awards and Closing |
| 14:00 – 15:00 | Lunch |



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Figure 5. Programme of the 2nd AUS of the EU FT-ICR MS consortium (Thursday).

The second AUS was attended by 49 participants of which 12 participated online due to the SARS2 pandemic restrictions. The gender balance was 32 men / 17 women, coming from 13 different countries. Students presented their work either in the form of posters or in the form of oral presentations which is the best way to generate fruitful discussions and to discover yet unknown ways to solve difficult problems. There were 9 participant posters exhibited at the second AUS and 14 participants were selected for oral presentations (short talks) based on a selection of their topics. The best oral presentation and the best poster were awarded the MALDISAURUS statues printed in the Laboratory of structural biology and cell signaling at the Institute of Microbiology. Michael Palasser (University of Innsbruck, Austria) was awarded for the best oral presentation: "FAST MS - An open-source software for automated and quantitative analysis of top-down mass spectra" and Limei Han (Helmholtz Centre for Environmental Research, Germany) won the award for the best poster "FT-ICR MS hyphenated with liquid chromatography enables advanced characterization of DOM and DBPs". The winners were voted and selected by the jury comprised by the three consortium PIs. There were 2 social events during 2nd AUS: Orienteering in Kunratice forest ending with Welcome reception in a restaurant "On the green meadow; the Sightseeing tour "Karlštejn castle" and the boat trip on Vltava river with the dinner. The overall feedback was very positive. This 2nd AUS promoted the establishment of interesting and fruitful collaborations not only within the network, but also with the experts outside the consortium. Thanks to this 2nd AUS, one of the participants showed interest in working in our institute and participating in this project and he was hired to work in EU FT-ICR MS project at the Institute of Microbiology in Prague at the end of 2021.