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Document Abstract

End Used School 2, as part of the activities of WP2 of the EU FT-ICR MS project, was held in presence at the University of Lille, Faculty of Sciences and Technologies on the Cité Scientifique Campus from Monday 12nd December 2022 to Friday 16th December 2022 . Altogether, 60 participants attended the school. The event consisted of tutorial lectures, short talks and poster sessions on principles and applications of FT-ICR MS as well as a daily social program for further discussions and participant networking. The school was successful with very positive feedback received from the participants during and after the event.



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1. Introduction

End User School 2 (EUS 2), as part of the activities of WP2 of the EU_FT-ICR_MS project was originally planned on M30. Due to COVID19 pandemic restrictions, End User School 2 has been postponed to M60 (Dec 2022) to be held in presence. End User School 2 (EUS 2) was held in presence at the University of Lille, Faculty of Sciences and Technologies on the Cité Scientifique Campus from Monday 12nd December 2022 to 16th December 2022. Altogether, 60 participants attended the school. The event consisted of tutorial lectures, short talks and poster sessions on principles and applications of FT-ICR MS as well as a daily social program for further discussions and participant networking. The school was successful with very positive feedback received from the participants during and after the event.

End User School 2 (EUS 2) constituted also the Closing ceremony of the EU_FT-ICR_MS project.

The announcement flyer is presented below in Figures 1.

EU FT-ICR MS

End User School
12 – 16 December 2022
Lille, France

The school will be focused on analytical applications and software tools developed by the sites of the EU FT-ICR MS network

See: <https://www.eu-fticr-ms.eu/>

Accommodation and meals for European participants are taken in charge by the EU (EU_FT-ICR_MS network, Grant Agreement 73107)

Register before the 5th of December by sending an email to Christian ROLANDO - christian.rolando@univ-lille.fr with the registration form (at the end)

Monday 12 December 2022

18:00-18:05	Welcome
18:05-18:45	FT-ICR MS: from signal to spectrum (C. Rolando, Lille, France)
18:45-18:55	Coffee break
18:55-19:30	Metabolomics: Creating life out of small molecules (C. Gondro, Lisbon, Portugal)
19:30-18:45	Short talks from EU_FT-ICR_MS staff and participants
19:55-21:00	Dinner

Tuesday 13 December 2022

9:00-10:15	How to deconvolve an MS (C. van der BEEK, Orsay, France)
10:15-10:45	Coffee break
10:45-11:00	From NMR, ESI, FT-ICR to metabolite identification (C. van Heijst, Ghent, Belgium)
11:00-11:30	Lunch break
11:30-11:45	Open house for FT-ICR MS data processing (M. A. Denis, Strasbourg, France)
11:45-18:00	Electrospray ionization, hybridization and related methods (C. Jentz, Jönköping, Sweden)
18:00-18:15	Coffee break
18:15-19:00	FT-ICR MS data visualization (M. Suter, Zürich, France)
19:00-18:00	Short talks from EU_FT-ICR_MS staff and participants
19:55-21:00	Dinner

Wednesday 14 December 2022

9:00-10:15	How to mine complex spectrum (C. Rigler, Herten, Germany)
10:15-10:45	Coffee break
10:45-11:00	Complex organic matter (C. Alouin, Rouen, France)
11:00-11:30	Lunch break
11:30-18:00	In a flash of light: Combining online MS with Every time detection (S. Jentz, Jönköping, Sweden)

Thursday 15 December 2022

9:00-10:15	2D FT-ICR & advanced MS/MS (P. O'Connor, Warwick, U.K.)
10:15-10:45	Coffee break
10:45-11:00	Better than your eyes: MS/MS imaging (C. de Pauw, Ugent, Belgium)
11:00-11:30	Lunch break
11:30-11:45	Genetics: From MS to FT-ICR (M. D. Irving, Ugent, Belgium)
11:45-11:55	Visit of the NMR (Including 1D and 2D NMR)
12:00-18:00	Travel by bus and surprise visit
19:55-21:00	Dinner

Friday 16 December 2022

9:00-18:00	Young EU_FT-ICR_MS PI: Maria von Aulhausen (Prague, Czech Republic)
9:00-18:00	Young EU_FT-ICR_MS PI: M. A. Denis (Strasbourg, France)
10:15-10:45	Coffee break
10:45-11:00	Young EU_FT-ICR_MS PI: Maria von Aulhausen (Prague, Czech Republic)
11:00-11:30	Young EU_FT-ICR_MS PI: M. A. Denis (Strasbourg, France)
11:30-11:45	EU_FT-ICR_MS closing ceremony
11:45-18:00	Lunch break

Figure 1. Flyer of EUS2.

2. Final report of End User School 2

The school was intended for current and possible end users of FT-ICR MS, covering the most important theory and fundamental aspects of the technique as well as some of the key applications.

Altogether, 60 scientists attended the event, including 30 early-stage researchers (Bachelor, Master, PhD students), 12 post-doctoral researchers or senior scientists, 12 principal investigators (PIs) from the EU FTICR MS project, one company delegate (Bruker Daltonics) and 5 senior scientists. Among the participants, 11 countries were represented: Belgium, Czech Republic, Finland, France, Germany, Italy, Lebanon, Portugal, Syria, Sweden, United Kingdom. A female-to-male ratio in the event was approximately 60:40.

The school comprised of 12 tutorial lectures:

- MRMS: Ultra-high mass spectrometric technology (M. Witt, Bruker, Bremen, Germany),
- Metabolomics: Creating life out of small molecules (C. Cordeiro, Lisbon, Portugal),
- How to dynamite an ion (G. van der Rest, Orsay, France),
- The French National Infrastructure Infranalytics (NMR, EPR & FTICR) (C. van Heijenoort, Gif-sur-Yvette, France),
- Open tools for FTICR MS data processing (M.-A. Delsuc, Strasbourg, France),
- Biomix: biooils (pyro, hydrothermal) and natural extracts (J. Jannis, Joensuu, Finland),
- How to mine complex spectrum (C. Rüger, Rostock, Germany),
- Complex organic matter (C. Afonso, Rouen, France),
- In a flash of light: Combining native MS with X-ray free electron lasers (A. Kadek, Prague, Czech Republic & XFEL, Schenefeld, Germany),
- Search for site specific ion-molecule reactions (M.-E. Crestoni, Roma, Italy),
- The in and the out of a protein (P. Novak, Prague, Czech Republic),
- Better than your eyes: MALDI imaging (E. de Paw, Liege, Belgium),
- 2D FTICR & advance MS/MS (P. O'Connor, Warwick, UK),

given by the principal investigators (PIs) of the EU project or senior scientist, and 4 practical talks:

- FTICR MS data visualization (M. Sueur, Rouen, France),
- Processing of ICR transient with non-FT Genetic Algorithm (M. Haegelin, Lille, France),
- Software Tool for Uncommon Cross-Linking Chemistry (L. Dlabolova, Prague, Czech Republic),
- Kendrick's Plots for FTICR MALDI imaging (E. de Paw, J. Far, Liege, Belgium),

and 16 short talks given by the participants. The topics covered the following areas: fundamentals of FT-ICR, data acquisition and signal processing, dynamically harmonized

ICR cell, isotopic fine structure, quadrupolar ion detection, ion activation, analysis of chemically modified proteins, atmospheric pressure ionization for FT-ICR, glycomics, petroleomics, ion/molecule reactions, and mass spectrometry imaging. The short talks covered a wide range of interesting subjects, from fundamentals to more practical applications. The scientific level of all the talks was very high. A lot of time was also reserved during coffee and lunch breaks as well as evening dinners for a participant networking and further discussions. The participants have also the opportunity to visit of the NMR (including 1.2 GHz) and EPR centers.

A special session the Friday morning before the closing ceremony was dedicated to Young EU_FT-ICR_MS PI the Friday morning before the closing ceremony. The session was chaired by Christopher Rüger (Rostock, Germany), and included talks on "Two-dimensional Mass Spectrometry for Biomolecules" by Maria van Agthoven, Prague, Czechia, "HRMS and FT-ICR for experimental physical chemistry" by Joan Far, Liege, Belgium, "Metals elective affinities, an MS-based tale", by Davide Corinti, Roma, Italy, and "The wine tale told through FT-ICR-MS" by Maria Sousa Silva, Lisbon, Portugal). The lecture "When paleontology meets proteomics" by F. Bray, Lille, France was given earlier in the week.

The EU_FT-ICR_MS closing ceremony were given by Pr Yan Pennec, Vice-Dean for Research, Faculty of Sciences & Technologies, University of Lille, Pr Mehran Mostafavi, Deputy director, CNRS, Institute of Chemistry and Dr Christian Rolando, EU_FT-ICR_MS PI.

The social program of the school included a visit to a local craft brewery followed by a beer tasting event and a dinner on Thursday evening.

A course feedback was requested from the participants. The feedback was very good except for the temperature in Lille which was very cold...