



European Network of Fourier-Transform Ion-Cyclotron-Resonance Mass Spectrometry Centers

Grant Agreement n° 731077

Deliverable D1.4 **18-month report of the** **EU_FT-ICR_MS network – iteration #2**

Start date of the project: 1st January 2018

Duration: 54 months

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Document Abstract

The deliverable D1.2 “Annual activity report of the EU_FT-ICR_MS network” is part of WP1, dedicated to the trans-national access activities of the Consortium. This deliverable reports the networking activities of the Consortium during the first 3 years of the project (M36, 2018-2020), including trans-national accesses, staff-exchange, round-robin tests, short courses and the first end-user and advanced user schools.

Table of Contents

1. INTRODUCTION	5
2. TRANS-NATIONAL ACCESS	5
3. TRAINING, EDUCATION AND NETWORKING ACTIVITIES	8
4. JOINT RESEARCH ACTIONS.....	15
5. CONCLUSION AND PERSPECTIVES.....	15

Abbreviations

AUS	Advanced Users School
EUS	End-Users School
TNA	Trans-national access

1. INTRODUCTION

Networking activities are the cornerstone of the EU_FT-ICR_MS Consortium. These are centred on trans-national access to the FT-ICR-MS technology and know-how by academic, SME and industrial communities, staff exchange and joint research activities between the Consortium Centres, and advanced training in FT-ICR-MS and its applications through the organization of short, focused courses as well as end-user and advanced user schools.

2. TRANS-NATIONAL ACCESS

TNA is a key point of the EU FT-ICR MS network and is part of the Objective 1 of the Consortium: "Provide the EU academic, SME and industrial communities with access to world-class FT-ICR MS centers". All Centers agreed to offer the same number of TNA days (100 days for each Centre).

During the project's first year, trans-national access (TNA) started after May 2018. A total of 26 TNAs were completed in 2018 within the entire EU FT-ICR MS Centers (with an average of 3 per Center), from a total of 26 proposals, corresponding to a 100% success rate. The duration of the TNAs varied between 3 and 12 days. In most of them, samples were shipped to the selected Consortium Center, but in some cases, researcher and students benefited from the opportunity to visit and stay on site to follow the analysis, gaining experience in sample preparation, data acquisition and subsequent analysis. During the reporting period, the portal for TNA project management and evaluation was not fully functional and the projects were approved without external revision. After one and a half years (30/06/2019), 55 projects were submitted and successfully completed, 9 of which were a follow-up of the first submission. They were reviewed and approved either by the project coordinator or by the WP1 leader. The TNA distribution among the different Centers during the first 1.5 years is presented in Figure 1.

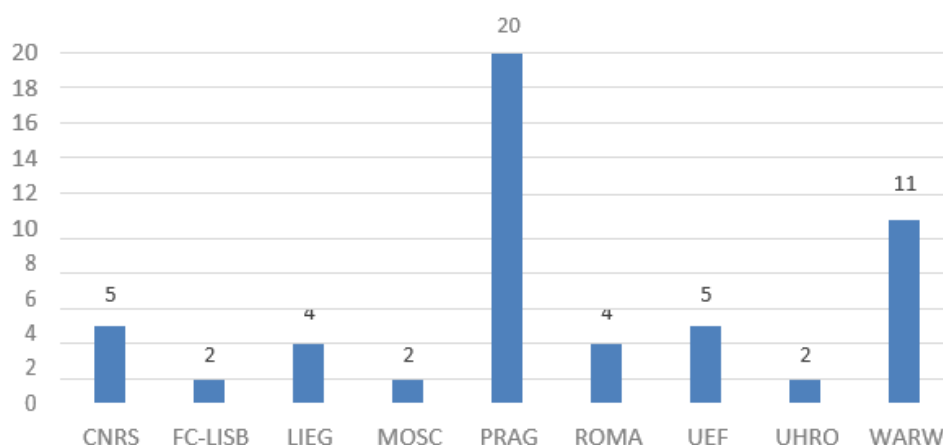


Figure 1: Trans-national accesses during the first 1.5 years (01/01/2018 to 30/06/2019) at the different Centers of the EU FT-ICR MS Consortium.



During the second 1.5-year period (01/07/2019 to 31/12/2020), 40 projects were successfully completed within the entire EU FT-ICR MS network, 6 of which were follow-up of the first submission. TNA accesses were submitted from 19 different countries. The TNA distribution among the different Centers during the second 1.5 years is presented in Figure 2.

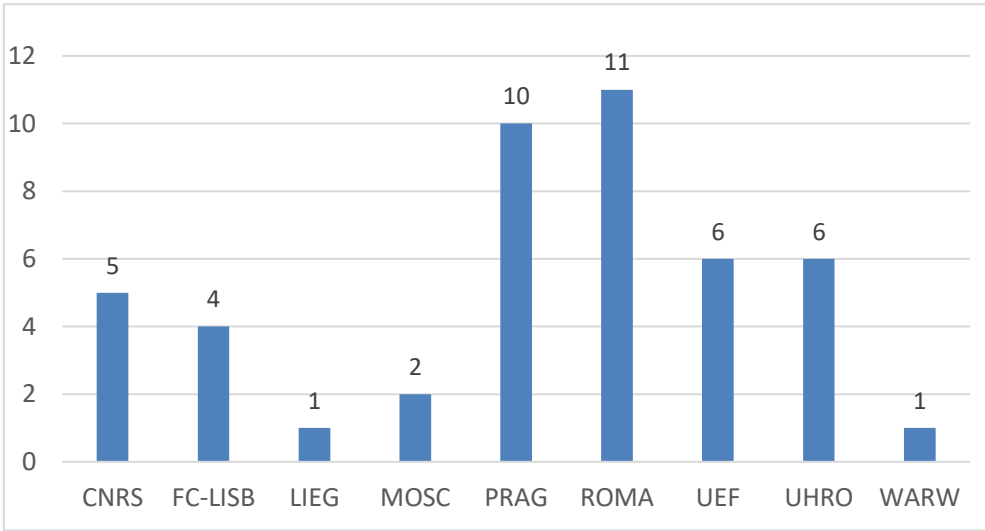


Figure 2: Trans-national accesses during the first 1.5 years (01/01/2018 to 30/06/2019) at the different Centers of the EU FT-ICR MS Consortium.

During the first 1.5 years, TNA projects were submitted mainly by researchers from universities or other higher education organizations. However, during the second period (2019-2020), there was a significant increase in accesses from national small and medium-sized enterprises (SMEs), (Figure 3).

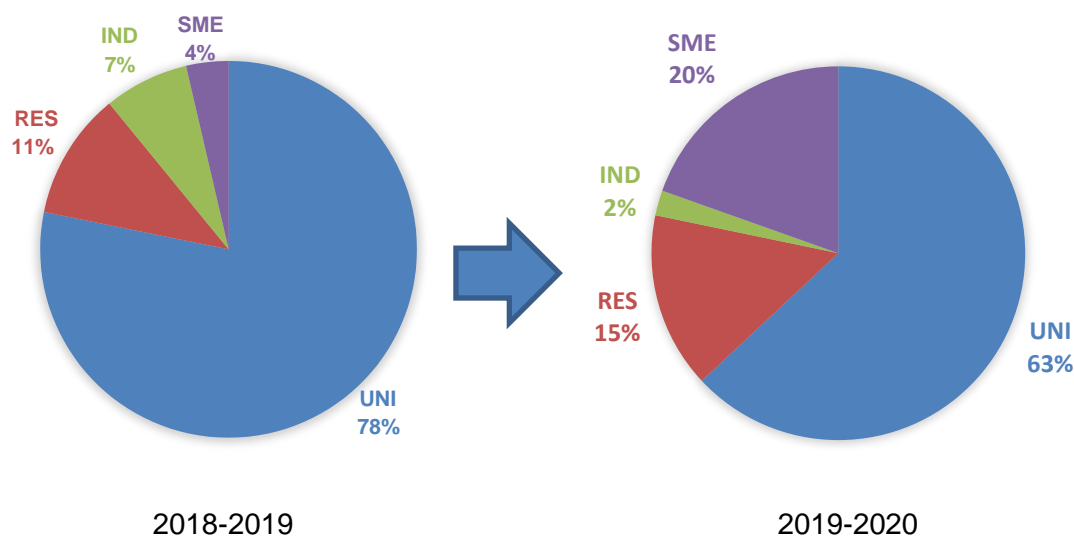


Figure 3: Distribution of TNA projects by Institution type; UNI - University and other higher education organizations, RES - Public research organization (including international and private research organizations controlled by a public authority), IND - Industry, SME - Small and medium-sized enterprises.

Most importantly, the project outreach went beyond Europe, with TNAs being submitted and completed from other continents, most notably Asia as well as North and South Americas,

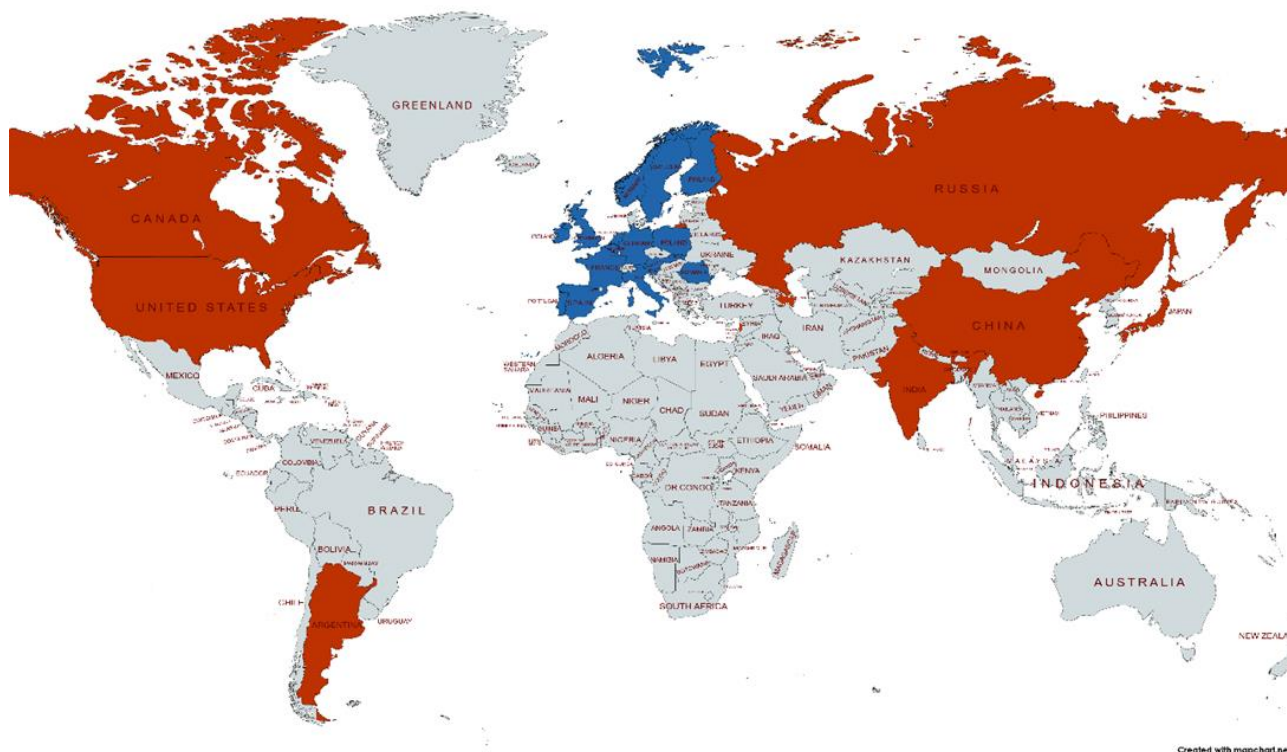


Figure 4: Coloured world map for total TNA accesses (2018-2020); European countries are labelled in blue and non-European in red.

Despite the initial drawbacks concerning smooth portal operation and reviewing process as well as an unforeseen and utterly severe and highly disruptive pandemic, TNA accesses are being successfully completed and there is a high and increasing demand for access, with the actual number of access days exceeding the predicted ones for the project.

The quality of the scientific data generated through the TNA accesses is shown in scientific publications, both articles, poster and oral presentations in international conferences. Since the beginning of the project, 14 papers were jointly published with members of the network and 2 posters or conference proceedings were presented.

During TNA access, knowledge transfer was achieved at individual level. TNA users that visited the EU FT-ICR MS network centers were directly involved in sample preparation, data acquisition and data analysis, gaining training, information and knowledge on FT-ICR-MS. Knowledge was also transferred to users that simply sent the samples, through reports and data analysis guidance. Many researchers that submitted TNA projects also participated (or sent students and team members) to participate in end-users and advanced schools as well as short courses, to increase their training and knowledge on FT-ICR-MS. The demand for these training actions is very high, most courses and schools are fully booked in 24-48 hours upon opening registration. Therefore, it was decided to allow for increased registration numbers on all courses and schools, without compromising training quality. Short courses and advanced schools make ample use of hands on training in the FT-ICR-MS laboratories. Students get hands on training on advanced tuning and instrument operation that are never included in vendor training courses.

The submission of a follow-up project by the same researcher is a highly relevant indicator of satisfaction of the TNA. Several researchers submitted a second (and sometimes a third) project to the same FT-ICR-MS Center, in a total of 20 follow-ups among the 94 TNAs (around 21% of total accesses) during the first 3 years of the project. These researchers clearly expressed an intention to pursue a collaboration with the selected Centers.

3. TRAINING, EDUCATION AND NETWORKING ACTIVITIES

3.1 Staff-exchange

Staff exchange between the different Centers of the network promotes sharing of specific skills and competences. This network activity is particularly valuable for young students and young members of each team. One week of staff exchange per partner per year was predicted.

During the first year of the project, there was one staff exchange, from ROMA to LISB. From this interaction, emerged one poster in an international conference and two joint publications.

In 2019, five staff exchanges were completed: two from LISB to WARW in January, one from MOSC to UHRO in August 2019, one from FC-LISB to LIEG in December 2019, and one between UHRO and UEF also in December 2019.

During 2020, there was one staff exchange from PRAG to LISB in February, but the other envisaged one, from PRAG to FC-LISB was postponed due to the pandemic situation. Another one was planned to occur in September 2020, from WARW to PRAG, but was also postponed due to COVID-19.

For 2021, five staff exchanges are foreseen: ROMA to UEF (started); WARW to PRAGUE; PRAGUE to LISB; UHRO to UEF (autumn); and UEF to PRAGUE (autumn). Uncertainties concerning the pandemic evolution as well as state and EU policies concerning travelling dictate caution on planning staff exchange events. Nevertheless, as successful vaccination programs are underway all over Europe, covering all staff and students, we foresee a strong enhancement in staff exchange starting in late 2021 (October onwards) and hopefully throughout 2022.

3.2 Courses and schools




During the first year of the project, two short courses and one end-user school were organized. One of the organized short courses took place in Rostock, from 5-7 March 2018 and was focused on atmospheric pressure ionization techniques for high resolution mass spectrometry of complex samples (Figure 2). The other one was organized in Orsay, from 5-7 November 2018 and covered FT-ICR for gas phase ion spectroscopy and structural characterization (Figure 5). The 1st End-User School (EUS) was organized in from 20-24 August 2018 in Joensuu (Figure 6).

**FIRST SHORT COURSE OF
THE EU FT-ICR MS
NETWORK**




**ATMOSPHERIC PRESSURE
IONIZATION TECHNIQUES FOR HIGH
RESOLUTION MASS SPECTROMETRY
OF COMPLEX SAMPLES**

When?
5-7 March 2018

Where?
University of Rostock
Research building LL&M
Albert-Einstein-Strasse 25
18059 Rostock

Overview of the program

-  **Tutorial Lectures**
Basics of FT-ICR MS
using atmospheric
pressure ionization
-  **Instrument demos**
Electrospray
ionization (ESI) and
Atmospheric
pressure chemical
ionization (APCI)
-  **Data analysis**
Comparison of
ionization features
of ESI, APCI and
GC- APCI/
Atmospheric
pressure photo
ionization (APPI)
samples;
In parallel: running
GC – APCI/APPI
measurements

Schedule for the first short course

**Atmospheric pressure ionization
techniques for high resolution mass
spectrometry of complex samples**

Tuesday 6.3. 9:00 – 11:00	Welcome and start with tutorial lecture (basics of FT-ICR MS using atmospheric pressure ionization)
11:00 – 12:00	Lab tour (2 groups)
12:00 – 13:00	Lunch
13:00 – 15:00	Hands on – Electrospray ionization (direct infusion)
15:30 – 17:00	Hands on – Atmospheric pressure chemical ionization
18:30 – 22:00	Social event (guided tour downtown Rostock) and dinner
Wednesday 7.3. 9:00 – 12:00	Data analysis of ESI, APCI and GC- APCI/APPI samples – comparison of ionization features In parallel: running GC – APCI/APPI measurements
12:00 – 13:00	Lunch
13:00 – 14:00	Closing meeting and wrap up




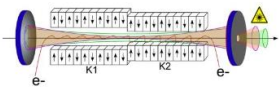


 <p>Second short course of the EU_FT-ICR_MS network</p> <p><i>FT-ICR for gas phase ion spectroscopy and structural characterization</i></p> <p>November 5 – 7, 2018</p> <p>Université Paris Sud Building 201 P2 Orsay, France</p>  <p>Location : The Université Paris Sud science campus is located 25 km southwest of Paris. It can be reached by local train from both of Paris major airports as well as from the main line train stations (30 min to 1h30 travel time).</p> 	<p>Main features of the program</p> <p>Tutorial lectures</p> <ul style="list-style-type: none"> Principles of action spectroscopy for ion structures in FT-ICR instruments Applications for the structural characterization of ions Selecting conformers or isomers through ion mobility  <p>Hands on experiments</p> <ul style="list-style-type: none"> Ion activation with a IR free electron laser Ion activation with OPO/OPA table-top laser <p>Data processing and analysis</p> <ul style="list-style-type: none"> Data processing of action spectra measurements, comparison with simulations. <p><i>Attendants are encouraged to suggest the type of samples for which they would like to have hands on training.</i></p>	 <p>Registration and accomodation: The attendance to the short course is free for selected participants! The EU_FT-ICR_MS will cover accomodation, registration and most travel fees.</p> <p>Download the application form on the EU_FT-ICR_MS web site (eu-fticr-ms.eu) and send it by email to: guillaume.van-der-rest@u-psud.fr</p> <p>Extended deadline for application starting on October 8th, on the basis of a first come first served. Application is open until the course is fully registered!</p>  <p><small>This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 731077 .</small></p>
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Figure 5: Flyers of the two short courses organized during 2018, in Rostock and in Orsay.

<p>EU FT-ICR MS End User School 1</p> <p><i>Want to learn theory, practise and the most prominent applications of Fourier transform ion cyclotron resonance mass spectrometry?</i></p> <p>When? 20–24 August, 2018</p> <p>Where? University of Eastern Finland Department of Chemistry Joensuu – Finland 62° 36' 3.924" N 29° 45' 48.708" E</p>  	<p>Course overview</p> <p>Topics</p> <ul style="list-style-type: none"> Fundamentals of FT-ICR MS FT-ICR hardware & instrumentation Basic data acquisition and signal processing Data post-processing and quality evaluation Applications of FT-ICR MS in proteomics, metabolomics, petroleomics, structural biology and many more... <p>Content</p> <ul style="list-style-type: none"> Tutorial lectures, short talks, poster session <p>Social activities</p> <ul style="list-style-type: none"> A boat cruise with onboard refreshments A midnight smoke sauna and lake swimming experience <p><i>Instructors include world renowned experts in the field of FT-ICR mass spectrometry</i></p> <p><i>Organized by EU FT-ICR MS – A European Network funded by EU Horizon 2020 Programme</i></p>	<p>For more information & application to the course:</p> <p>www.eu-fticr-ms.eu</p> <p>To navigate to the site, use the QR code below</p>  <p>More information about the venue: www.uef.fi</p> <p>Further enquiries: janne.janis@uef.fi</p> <p>NO PARTICIPATION FEE!</p> <p>Also, complimentary accommodation, meals and social program are offered! Up to 50 attendees will be selected to the course by the scientific committee on the basis of applications.</p> <p>THE DEADLINE FOR APPLICATIONS IS JULY 1ST</p> 
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Figure 6: Flyer of the 1st End-User School (EUS) organized in Joensuu.



During the second year of the project, three short courses and one advanced-user school were organized. The first short course took place in Rome, from 25 - 27 June 2019 and was focused on fundamental and analytical aspects of ion-molecule reactions (Figure 7). The second one was organized in Warwick, from 21 - 23 August 2019 and covered high-resolution tandem mass spectrometry of biomolecules, with tutorial lectures, instrument demos, hands-on exercises and data analysis (Figure 7). The third course took place in Moscow, from 10 - 12 October 2019 and focused on the basics of FT-ICR: dynamic harmonization and computer simulation (Figure 7). The 1st Advanced-User School (AUS) was organized in Lisbon from 14 - 18 April 2019 (Figure 8).



Third short course of the EU_FT-ICR_MS network

"Ion-molecule reactions: fundamental and analytical aspects"



Facoltà di Farmacia e Medicina
Dipartimento di Chimica e
Tecnologie del Farmaco

25-27 June 2019



Program

Tutorial lectures

- Principles of ion-molecule reactions in FT-ICR mass spectrometry
- Applications for identification of functional groups, structural features, physicochemical properties, counting active Hs, chiral differentiation, atom transfer reactions



Time →

Hands on experiments

- Kinetics of bimolecular reactions: single and multiple steps
- Equilibria: examples of ligand association/exchange reactions

Data processing and analysis

- Data processing of kinetics and equilibrium measurements

Registration



Attendance to the short course is free for all participants !

The EU_FT-ICR_MS network will cover accommodation, registration and most of travel expenses.

Please download the application form on the EU_FT-ICR_MS web site:
eu-fticr-ms.eu
and send it by email to:
mariaelisa.crestoni@uniroma1.it
before May 15th, 2019.

Applications will be open till the course is fully registered and acceptance will be notified before May 20th, 2019.



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 731077.


5th Short Course of the EU FT-ICR MS Network

Basics of FT-ICR: dynamic harmonization and computer simulation

Venue and dates

10th-12th October 2019

Mass Spectrometry Lab, CDISE CREI, Skolkovo Institute of Science and Technology
Nobelya 3 str., Moscow, 121205, Russia



Contacts


Prof. Evgeny Nikolaev
e.nikolaev@skoltech.ru
Dr. Alexander Zhrebker
a.zhrebker@skoltech.ru

Course Overview

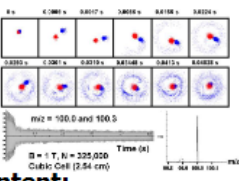
Topics:

- ✓ Fundamentals of FT-ICR MS
- ✓ Dynamic harmonization
- ✓ Simulation of ion motion
- ✓ Advanced electronics for FT-ICR
- ✓ Application of PIC-code

The dynamically harmonized ICR cell



X-Y projection of ion clouds and corresponding FT-ICR data processing



Content:

- ✓ Tutorial lectures, Instrument demos, Hands-on exercises, Computer lab, Data analysis

Application Details

For more information and application to the course, please visit:


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

No PARTICIPATION FEE!
Accommodation, travel, meals, and social program included

Up to 10 applicants will be selected by the scientific committee

Deadline for Applications:
August 31st 2019

Link to the Prof. Nikolaev Lab:
<https://www.skoltech.ru/masssp-eclab/>



This project has received funding from the EU Horizon 2020 research and Innovation program under grant agreement No 731077




4th Short Course of the EU FT-ICR MS Network

High Resolution Tandem Mass Spectrometry of Biomolecules

When & Where


21st - 23rd August 2019

Ion Cyclotron Resonance Laboratory
Millburn House, University of Warwick
Coventry CV4 7HS
United Kingdom



Local Organisation

Prof. Peter O'Connor
Contact: p.oconnor@warwick.ac.uk

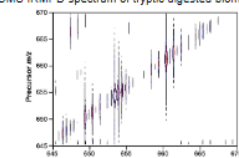


Course Overview

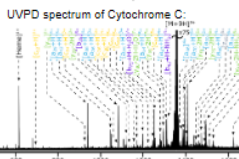
Topics:

- Fundamentals of FT-ICR MS
- Fundamentals of tandem MS (CAD, IRMPD, UVPD, ExD)
- Data Analysis of tandem MS
- Applications of tandem MS

2DMS IRMPD spectrum of tryptic digested biomolecule:



UVPD spectrum of Cytochrome C:



Content:

- Tutorial lectures, Instrument demos, Hands-on exercises, and Data analysis

Speakers:

P. B. O'Connor
E. N. Nikolaev
M. P. Barrow
C. A. Wootton

Application


For more information and application to the course, please visit:
<https://eu-fticr-ms.eu/>

No PARTICIPATION FEE!
Accommodation, meals, and social program included

Up to 10 applicants will be selected by the scientific committee on the basis of applications

Deadline for Applications: July 22nd 2019

More information about Prof. O'Connor research group:
<https://warwick.ac.uk/fac/sci/chemistry/research/oconnor/oconnorgroup>



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 731077

Figure 7: Flyers of the three short courses organized during 2019, in Rome, Warwick and Moscow.


EU FT-ICR MS 1st Advanced User School

Want to master Fourier transform ion cyclotron resonance MS and its cutting edge applications? Join us!

Where and when

LISBOA, 14 - 18 April 2019


Faculdade de Ciências
Universidade de Lisboa, Portugal
ciencias.ulisboa.pt



Local organization:

Carlos Cordeiro
Marta Sousa Silva
Marisa Maia

Contact: cacordeiro@fc.ul.pt



Extreme FT-ICR MS

- 2D FT-ICR
- Phasing
- Isotopic fine structure
- Advanced Fourier transform

C Rolando
C Afonso
MA Delsuc
ME Crestoni
P Maître
M Sklorz
E Nikolaev

Small is beautiful

- Metabolomics
- Imaging
- Petroleomics
- Visualizing complex mixtures

C Cordeiro
E de Pauw
P O'Connor
J Jānis
P Novák
M Witt

Gas phase wonders

- Gas-phase chemistry
- Structural spectroscopy
- Atmospheric pressure ionization

Proteins, the core of life

- Native MS
- Top-down proteomics
- Post-translational modifications


NO PARTICIPATION FEE!
Accommodation, meals and social program included

Up to 50 applicants will be selected by the Scientific Committee

DEADLINE FOR APPLICATIONS MARCH 10th

Application: eu-fticr-ms.eu

Tutorial lectures by world leading experts in FT-ICR MS
Live demo on modern FT-ICR
Student poster sessions and short talks



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 732077

Figure 8: Flyer of first Advanced-Users School organized during 2019, in Lisbon.

During the third year of the project (2020), two short courses were envisioned to be organized, one in Lisbon (in March) and the other on Prague (in August). The first one was postponed to 2021 due to the pandemic situation in Portugal in that time of the year. The second one was organized in Prague, from 16 - 19 August 2020 and was focused on structural proteomics (Figure 9).

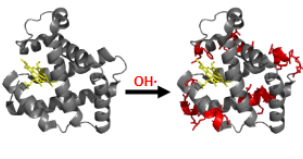



<p>EU FT-ICR_MS 7th Short Course</p> <p>Structural Proteomics: Analysis of protein surface accessibility by Top Down mass spectrometry</p> <p>PRAGUE, 16 - 19 August 2020</p> <p>Institute of Microbiology The Czech Academy of Sciences https://mbucas.cz/en/</p>	<p>Course overview</p> <p>This course will cover the analysis and mapping of protein landscape using FT-ICR mass spectrometry</p>  <p>Specific topics include:</p> <ul style="list-style-type: none"> Sample preparation Ionization Protein covalent labeling Data analysis 	<p>Tutorial lectures Instrument demos Hands-on exercises Computational data analysis</p>  <p>Faculty</p> <ul style="list-style-type: none"> Petr NOVAK Peter O'CONNOR Petr MAN
<p>Centrum BIOCEV Vestec, Prumyslova 595, Czech Republic</p> 	<p>NO PARTICIPATION FEE! Travel, accommodation, meals and social program included</p> <p>Up to 10 applicants will be selected by the Scientific Committee</p>	<p>Application: www.eu-fticr-ms.eu</p> <p>DEADLINE FOR APPLICATIONS: July 13th 2020</p>  <p><small>This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 731077</small></p>

Figure 9: Flyer of the short course organized during 2020, in Prague.

3.3 The proposal for the organization of the European Fourier Transform Mass Spectrometry Conference in 2020

An important contribution for networking is the organization of high-profile international conferences in the field, targeting the European FT-ICR users' community. One highly relevant conference is the European Fourier Transform Mass Spectrometry conference (EFTMS), already organized or co-organized in the past by members of this Consortium (E. Nikolaev: Moscow, 2008; P. O'Connor: Warwick, 2012; G. van der Rest: Paris, 2014).

The proposal for the organization of the 14th EFTMS conference, placed during the 13th EFTMS in Freising by FC-LISB (on behalf of the EU FT-ICR MS Consortium), was successful. Lisbon will organize the 14th EFTMS in 2020, with the confirmed participation of Alan Marshall, Alexander Makarov, Jonathan Amster, Neil Kelleher, Philippe Schmitt-Kopplin, Julia Chamot-Rooke and Roman Zubarev as well as others among the world leading developers of FTMS

This task is crucial for the visibility of the EU FT-ICR MS network among the FT-ICR MS community. Despite its title, the European FTMS conference is also attended by non-European Union scientists (mainly European scientists from outside the European Union, scientists from Canada and the United States) and will lead to a broader diffusion of the EU FT-ICR MS network concept and of its results worldwide. It will be an outstanding opportunity to engineers, PhD students and post-docs to present their work in collaboration with the end-users of the EU FT-ICR MS Centers.

Due to the pandemic situation, the 14th EFTMS conference was postponed to 2022 and will take place in Lisbon, from 26 to 29 April 2022..

4. JOINT RESEARCH ACTIONS

4.1 The first round-robin test

The first Round-robin test performed within the EU_FT-ICR_MS network aimed to provide information on the different equipment performance among the network centers, as well as the consistency of data including mass accuracy, sensitivity and MSMS performance. This test was performed in August / September 2018 and the chosen sample was the peptide Leucine-enkephalin (Sigma), shipped from FC-LISB to all EU FT-ICR MS Centers. The minimum requirements for the analysis were the determination of the exact mass of the molecular ion in positive and negative ionization modes, the measurement of the relative intensities of the molecular ion and the two first isotopes in positive and negative ionization modes, and the measurement of the exact mass of the MS/MS spectra also in positive and negative ion modes.

4.2 The second round-robin test

The second Round-robin test performed within the EU_FT-ICR_MS network was performed in June / July 2021 and the chosen sample was the peptide glutathione. Its aims to test dynamic range and resolving power to achieve the highest possible accuracy in isotopologue assignment, a unique feature of FT-ICR-MS and the most accurate way to establish molecular formulas ab initio. Moreover, spectral data processing from each center will be performed, for the first time using consortium developed software (CASC4DE).

5. CONCLUSION AND PERSPECTIVES

The first 3 years of the project were extremely well successful concerning dissemination and training activities. All courses and schools had more applicants than available seats, showing the high interest that the project is generating in the European Scientific community, laying the foundation for new generations of FT-ICR-MS scientists and experts. Staff exchanging has increased, taking advantage of all different skills and instrumentation available in all centers. Concerning TNA, the number of access days were above the expected in the project for this period. During TNA access, knowledge transfer was achieved at individual level, either by TNA users that visited the EU FT-ICR MS network centers, more directly involved in sample analysis, data acquisition and data analysis, but also by users that sent the samples, through reports and data analysis guidance lines.