











**Prague, 26 - 30 September 2021** 



#### WHEN:

September 26 - 30, 2021

#### WHERE:

BIOCEV Center, Průmyslová 595, 252 50 Vestec <a href="https://www.biocev.eu/en">https://www.biocev.eu/en</a> and Institute of Microbiology of the Czech Academy of Sciences, Vídeňská 1083, 142 20 Prague 4, (<a href="https://mbucas.cz/en/">https://mbucas.cz/en/</a>), Czech Republic

#### **ACCOMMODATION:**

HOTEL REZIDENCE EMMY \*\*\*\*, K Zelené louce 2a, 148 00 Prague 4 - Kunratice (Czechia), <a href="https://www.rezidenceemmy.com">https://www.rezidenceemmy.com</a>. The accommodation is already booked for all participants of the course.

#### **ORGANIZATION:**

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

#### **VIRTUAL ROOM FOR ONLINE PARTICIPANTS:**

https://cesnet.zoom.us/j/94769182565?pwd=c3lKYlRjc2lUZ1dURFFuaHFqblZjQT09

Meeting ID: 947 6918 2565

Passcode: 253160

To download ZOOM: https://zoom.us/download

#### **MATERIALS FOR DOWNLOAD**

2<sup>nd</sup> Advanced user school material available at https://peterslab.org/2ndAUS









### Prague, 26 - 30 September 2021

### **Program**

### 26<sup>th</sup> September, Sunday

12:00 – 17:30	Registration @ IMIC – hotel EMMY, Prague – see details below
17:30 – 22:00	Orienteering in Kunratice forest and Welcome reception @ Restaurant "On the green meadow/Na tý louce zelený",
	Prague (https://www.natyloucezeleny.cz/)

### 27<sup>th</sup> September, Monday

WHERE: BIOCEV Center, Průmyslová 595, 252 50 Vestec,

Transfer by private bus from hotel EMMY to BIOCEV – departure at 8:30 am from EMMY

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" (on-line)
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"









## Prague, 26 - 30 September 2021

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" (on-line)
17:40 – 18:30	Short presentations of participants I
18:30 – 21:00	Dinner and poster session

Transfer by private bus from BIOCEV to EMMY – departure at 21:00

### 28<sup>th</sup> September, Tuesday

WHERE: BIOCEV Center, Průmyslová 595, 252 50 Vestec

Transfer by private bus from hotel EMMY to BIOCEV – departure at 8:30 am from EMMY

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 at BIOCEV (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"







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13:00 – 14:00	Lunch
14:00 – 17:30	Sightseeing tour "Karlštejn castle" – transfer by private bus
19:00 – 23:00	<b>Boat trip and course dinner -</b> transfer by private bus from castle to the boat. Transfer from the boat back to the hotel EMMY by municipal transport

### 29th September, Wednesday

WHERE: BIOCEV Center, Průmyslová 595, 252 50 Vestec,

Transfer by private bus from hotel EMMY to BIOCEV – departure at 8:30 am from EMMY

9:00 – 10:20	Peter O'Connor "Current capabilities in 2DMS on FTICR mass spectrometers" (on-line)
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
13:30 – 14:50	Maria Andrea van Agthoven "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"







# EU\_FT-ICR\_MS 2<sup>nd</sup> Advanced Users School Prague, 26 - 30 September 2021



16:30 – 17:30	Short	presentations	of	participants III	1
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17:30 – 20:00 Dinner and poster session

Transport to hotel EMMY by private bus from BIOCEV – departure at 20:00

### 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









### Prague, 26 - 30 September 2021

### 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"

### **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"** 

### **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"









### Prague, 26 - 30 September 2021

Rutuja Patil "Freeing Aspergillus fumigatus of Polymycovirus 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"

#### **Posters**

Alpesh Thakker "An improved semi targeted mass spectrometry approach to provide broader coverage of oxidised lipidome in inflammatory disease model"

Kas J.Houthuijs "Towards IR ion spectroscopy on a trapped ion mobility enabled API/MALDI dual source FT-ICR MS platform"

Josef Dvořák "Identification of procalcitonin in septic patients by affinity chips and mass spectrometry"

Marek Polák "Combination of fast photochemical oxidation of protein and topdown mass spectrometry enables structural characterization of protein/DNA complex"

Maxime Sueur "Characterization of organic aerosol using DIP-APCI FT-ICR MS"

Charlotte Mase "Molecular characterization of a mixed plastic pyrolysis oil from municipal wastes by direct infusion FTICR mass spectrometry"









### Prague, 26 - 30 September 2021

Limei Han "FT-ICR MS hyphenated with liquid chromatography enables advanced characterization of DOM and DBPs"

Filip Dyčka "Studying of hexameric viral helicase by hydrogen-deuterium exchange mass spectrometry"

Zuzana Kalaninová "Detection of Botulinum Neurotoxin Type BoNT/A1 Using Modified MALDI Surfaces"

### **Useful information:**

#### 1/ Contact persons:

Petr Novák – e-mail: <a href="mailto:pnovak@biomed.cas.cz">pnovak@biomed.cas.cz</a>, phone: +420 607 856 809

Pavla Kramlová – e-mail: <a href="mailto:pavla.kramlova@biomed.cas.cz">pavla.kramlova@biomed.cas.cz</a>, phone: +420 773 031 220

2/ Prague transport: <a href="https://www.dpp.cz/en">https://www.dpp.cz/en</a>

3/ How to get to the accommodation in hotel "Rezidence EMMY"  $\,$ 

From Václav Havel Airport:

**Bus nr. 119** from Terminal 1 or 2 to bus stop: **Nádraží Veleslavín,** transfer to the **underground/metro** – green line A to station **Muzeum.** Transfer to red line C to the station **Kačerov** (direction Háje). Transfer to the **bus nr. 138** (direction Ústavy Akademie věd) to the bus stop: **IKEM** (the bus stop is directly in front of the hotel).

From Central Railway Station in Prague, Wilsonova 300/8, Praha 2:

**Underground/metro** red line C – from station **Hlavní nádraží** (direction Háje) to the station **Kačerov**. Transfer to the **bus nr. 138** (direction Ústavy Akademie věd) to the bus stop: **IKEM** (the bus stop is directly in front of the hotel).

Payment for the Prague transport – after your arrival to Prague (airport, Central Station) buy the ticket for 40 CZK / 90 minutes (you can pay cash in CZK or by card in a vending machine). Exchange rate: 1 EUR = 25,80 CZK.

Due to COVID pandemic situation, please check the link: <a href="https://koronavirus.mzcr.cz/en/list-of-countries-according-to-the-level-of-risk/">https://koronavirus.mzcr.cz/en/list-of-countries-according-to-the-level-of-risk/</a> - the restriction on entering the Czech Republic from your country.



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### Prague, 26 - 30 September 2021

If you are vaccinated in the EU (and you hold the EU digital COVID certificate or confirmation about the vaccination approved by EMA) or if you had COVID-19 during last 180 days (again with EU digital COVID certificate), you have the exception from testing. Even if you are from the country with a high or very high risk – see att.

Please print your EU digital COVID certificate on paper, we will need a copy of it and you should also show this certificate at the hotel!

Please, DO NOT FORGET TO CARRY YOUR FFP2 RESPIRATOR during the travel, it is mandatory at public transportation.



