



## EU FT-ICR MS 10<sup>th</sup> & 11<sup>th</sup> Short Courses

Liege, Lille, 21 - 27 November 2022

**FTICR Mass Spectrometry Imaging (Liege, Belgium)**

**FTICR MS for Cultural Heritage Science (Lille, France)**

Monday	Tuesday	Wednesday	Thursday	Friday	Saturday
Liege	Liege	Liege	Lille	Lille	Lille
Liege	Liege	Liege- Lille	Lille	Lille	

**Travel, accommodation and meals for European participants are taken in charge by the EU (EU\_FT-ICR\_MS network, Grant Agreement 73107)**

Register before the 14<sup>th</sup> of November by sending an email to Johann FAR (for Liege school) - [johann.far@uliege.be](mailto:johann.far@uliege.be) and/or Christian ROLANDO (for Lille school) - [christian.rolando@univ-lille.fr](mailto:christian.rolando@univ-lille.fr)

## Uliege MSLab contributors for Mass Spectrometry Imaging:

Prof. Edwin DE PAUW (EU FT-ICR MS network supervisor in Liège) and Dr. Johann FAR (site manager)

- Pr. Edwin DE PAUW, Dr. Johann FAR, and Wendy MULLER (matrix assisted laser desorption ionization MALDI, surface enhanced laser desorption ionization SALDI, mass spectrometry hardware used for imaging, mass spectrometry imaging MSI and applications)
- Dr. Virginie BERTRAND, Dr. Johann FAR (histology and tissue section, brain MSI)
- Sophie RAPPE (thin layer chromatography with MSI detection)
- Pierre BURGUET (imaging of interacting bacteria co-culture in agar of metabolites)
- Dr. Kune CHRISTOPHER and Thomas TILMANT (data sciences with Python)

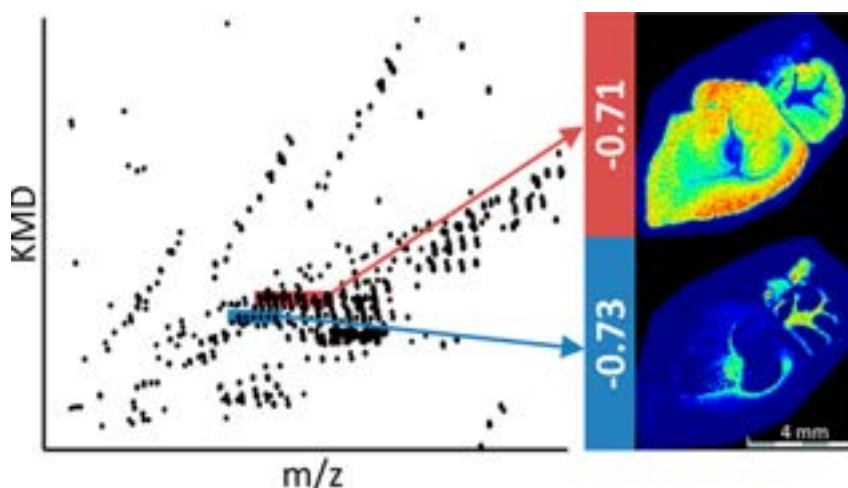
## Uliege MSLab trinind content :

The Mass Spectrometry Imaging (MSI) short course include a few of theoretical aspects of mass spectrometry imaging, especially matrix assisted laser desorption ionization mass spectrometry imaging, MALDI MSI, and a quick overview of other MSI techniques, instrumentation, and applications.

The practical sections of the training include tissue section of mouse brains, preparation of thin layer chromatography (TLC) of lipids, and handling of bacterial co-cultures chemically interacting in agar.

The short course also includes the matrix deposition using an automated sprayer (SunChrom SunCollect), and the MALDI MSI of the various samples using the Bruker dual source ESI/MALDI FT-ICR 9,4T fitted with the paracell, the solarix xR.

Finally, a short introduction about the use of Python for data sciences is scheduled, exploring and extracting some data of interest from mass spectrometry mzML converted data. A short demo will show what could be expected when applying such tools within an in-house software [1], allowing the reconstruction of MSI data using a Kendrick Mass Defect clustering strategy. Additionally, the basic use of SCiLS™ Lab software (Bruker) [2] for processing MSI data will be tackled during the short courses.



A social event is scheduled. A night out in a brasserie (restaurant) will be organized to eat typical food from Liege and drink Belgian beers.

[1] *Anal. Chem.* 2019, 91, 20, 13112–13118 ; <https://doi.org/10.1021/acs.analchem.9b03333>

[2] <https://www.bruker.com/en/products-and-solutions/mass-spectrometry/ms-software/scils-lab.html>

## ULille TopOmics contributors for Mass Spectrometry for Cultural Heritage Science:

Dr Christian ROLANDO, CNRS Senior scientist (EU FT-ICR MS network supervisor for Lille and global coordinator of the network) and Dr. Fabrice BRAY (site manager)

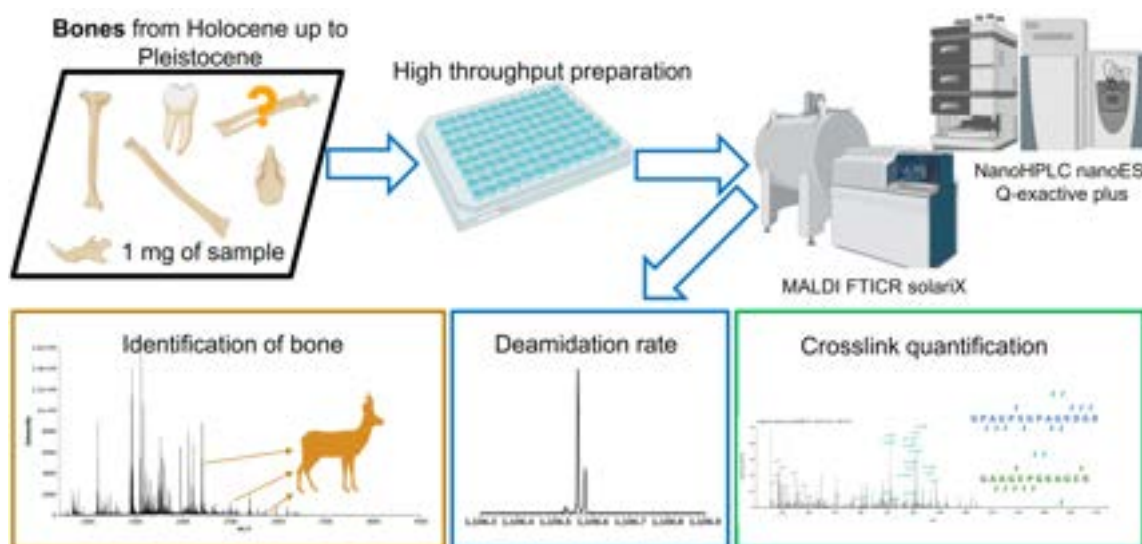
- Dr. Fabrice BRAY (Species identification for paleolithic and archeological bones by proteomics [1]; analysis of lipids in bones and sherds [2])
- Stéphanie FLAMENT (identification of proteins in sherds and tempera painting [3])
- Dr Marie YAMMINE (analysis of watercolor and gouache [4])
- Dr. Christian ROLANDO (analysis of oil or alkyd artist paint)

## ULille TopOmics training content:

The Mass Spectrometry Short course for Cultural Heritage is focused on the identification of natural products preserved over the centuries which are very often polymeric. The short course will begin with brief theoretical courses covering an overview of Mass Spectrometry applied to Cultural Heritage, the principle of Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS), the concept of fine isotopic structure as well as the basis of proteomics, glycomics and lipidomics.

The practical sections of the training comprise examples from these various topics. Firstly, demonstration of sample preparation will be held: (i) collagen extraction and digestion with minimal induction of posttranslational modifications, quantification of deamidation; (ii) digestion of model gums, watercolor or gouache modern paint and (iii) and depolymerization of alkyd artist paint. Subsequently, the prepared samples will be analyzed with high resolution MALDI FT-ICR and nanoLC Orbitrap results. The obtained spectra will be further compared to their corresponding ones acquired through lower resolution instruments such as MALDI TOF MS. And finally, for proteomics, a comparison related to data treatment will show different outcomes from the same spectra depending on the database sources, with publicly available and in-house established data bases.

The short course will be carried out using our Bruker solariX xR ESI/MALDI FT-ICR 9.4 Tesla fitted with a harmonized cell, our Q-Exactive+ Orbitrap fitted with a nanoLC U3000 RSLC and on our server running commercial and homemade software.



!!!! You may bring your own samples if they are not too precious (100 mg of bones, 1 g of sherds, 100 µg of paints (watercolor or oil). It's a hundred times the minimum amount required for precious sample analysis. !!!!

A social event is scheduled. A competitive night out in a brasserie (restaurant) is arranged to compare Flemish specialties in Lille to their counterparts in Liège.

[1] *Archaeometry* (2022). <https://doi.org/10.1111/arcm.12800>; [2] *Int. J. Mass Spectrom.* 284.1-3 (2009): 47-56. <https://doi.org/10.1016/j.ijms.2009.03.003>; [3] *Anal. Chem.* 83.24 (2011): 9431-9437. <https://doi.org/10.1021/ac201978j>; [4] *Scientific reports* 7.1 (2017): 1-15. <https://doi.org/10.1038/srep44538>.