



**EU FT-ICR MS**

# **EU\_FT-ICR\_MS**

## **European Network of Fourier-Transform Ion-Cyclotron- Resonance Mass Spectrometry**

### **An INFRA for Starting Communities network**

# The EU\_FT-ICR\_MS network

**11 academic FT-ICR MS  
center from 9 countries**

**2 companies**  
**CAS4CADE**  
**Absiskey**

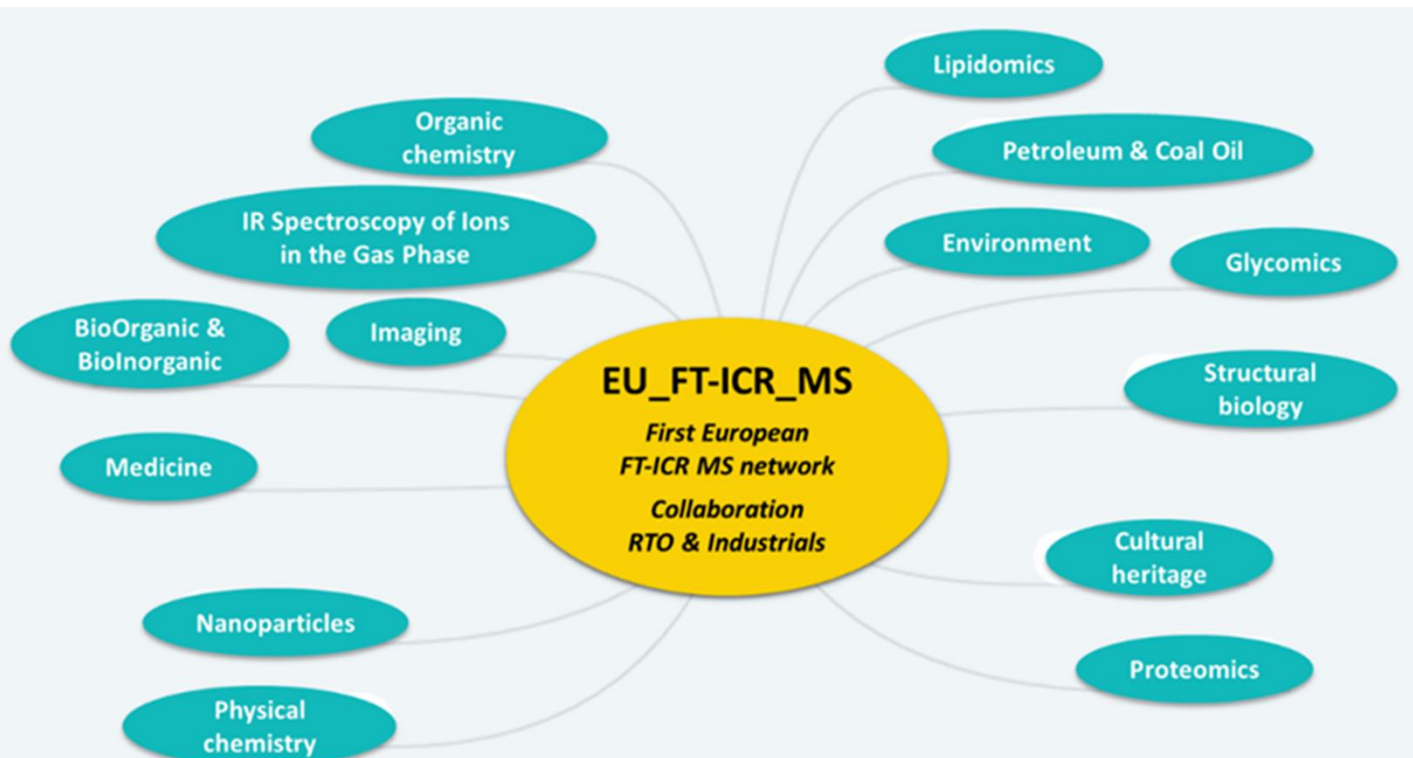
**Bruker Daltonik**

**Started January 1<sup>st</sup>  
2018, 0 hour**





# The workpackages



And the very important WP  
**Open Data & e-Infrastructure**



# Transnational access

- **Free access to the academic centers for EU users (25 days per center and per year), academics & industrials**
- **It must be a center not in your own country**
- **Data are public after an embargo period (18 months)**
- **These 2 rules don't apply to SMEs**
- **Travel and accommodation are also taken in charge by EU**
- **Permanently open application on the EU\_FT-ICR\_MS website**

[www.eu-fticr.eu](http://www.eu-fticr.eu)





**EU FT-ICR MS**

# Formation & Training

Grant Agreement (GA) No: 731077  
IMSC, Florence, EU\_FT-ICR\_MS Workshop

## 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

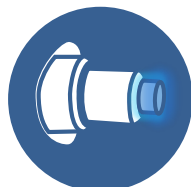


**Tutorial Lectures**  
Basics of FT-ICR MS  
using atmospheric  
pressure ionization



#### **Instrument demos**

**Hands-On Exercises**  
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



You want to learn more about high  
resolution mass spectrometry and  
atmospheric pressure ionisation  
techniques?

#### Registration:

please send an E-Mail using the application  
form to

**[martin.sklorz@uni-rostock.de](mailto:martin.sklorz@uni-rostock.de)**

We will response as fast as possible and  
inform you about acceptance.  
The application form is available as a  
download on our website.

[www.zimmermann.chemie.uni-rostock.de/forschung/advanced-mass-spectrometry/hochaufloesende-massenspektrometrie/eu-ft-icr-ms/](http://www.zimmermann.chemie.uni-rostock.de/forschung/advanced-mass-spectrometry/hochaufloesende-massenspektrometrie/eu-ft-icr-ms/)

#### **NO CONFERENCE FEES !**

Each participant (limited seats) will  
receive support for travelling and  
accommodation.

**REGISTER SOON!**



Universität  
Rostock



Traditio et Innovatio



## EU FT-ICR MS End User School 1

*Want to learn theory, practise and the most prominent applications of Fourier transform ion cyclotron resonance mass spectrometry?*

### When?

20–24 August, 2018

### Where?

University of Eastern Finland  
Department of Chemistry  
Joensuu – Finland  
62° 36' 3.924" N 29° 45' 48.708" E



## Course overview

### *Topics*

- 🌀 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...

### *Content*

- 🌀 Tutorial lectures, short talks, poster session

### *Social activities*

- 🌀 A boat cruise with onboard refreshments/visit to Koli
- 🌀 A midnight smoke sauna and lake swimming experience

*Instructors include world renowned experts in the field of FT-ICR mass spectrometry*

*Organized by EU FT-ICR MS – A European Network funded by EU Horizon 2020 Programme*

**For more information & application to the course:**

[www.eu-fticr-ms.eu/EUS1](http://www.eu-fticr-ms.eu/EUS1)

To navigate to the site, use the QR code below



More information about the venue:  
[www.uef.fi/mass-spectrometry](http://www.uef.fi/mass-spectrometry)

Further enquiries: [janne.janis@uef.fi](mailto:janne.janis@uef.fi)

## **NO PARTICIPATION FEE!**

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.

**APPLY SOON!**





## Second short course of the EU\_FT-ICR\_MS network

### *FT-ICR for gas phase ion spectroscopy and structural characterization*

**November 5 – 7, 2018**

**Université Paris Sud  
Building 201 P2  
Orsay, France**



#### **Location :**

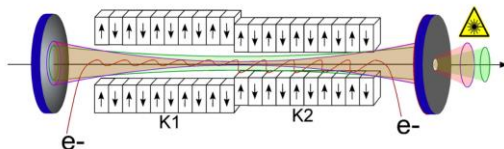
*The Université Paris Sud science campus is located 25 km southwest of Paris. It can be reached by local train from both of Paris major airports as well as from the main line train stations (30 min to 1h30 travel time).*



## Main features of the program

### **Tutorial lectures**

- 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



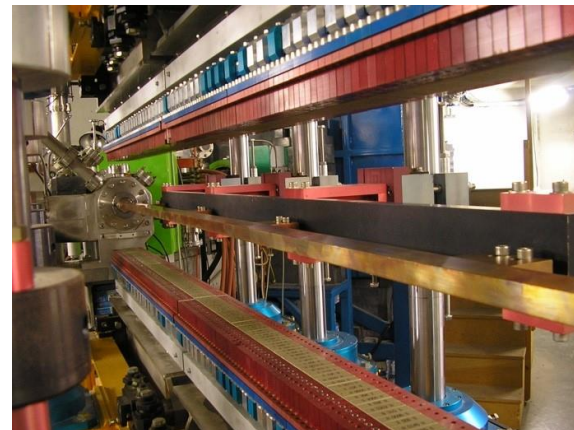
### **Hands on experiments**

- Ion activation with a IR free electron laser
- Ion activation with OPO/OPA table-top laser

### **Data processing and analysis**

- Data processing of action spectra measurements, comparison with simulations.

*Attendants are encouraged to suggest the type of samples for which they would like to have hands on training.*



### **Registration and accomodation:**

The attendance to the short course is free for selected participants!

*The EU\_FT-ICR\_MS will cover accomodation, registration and some travel fees.*

Download the application form on the EU\_FT-ICR\_MS web site ([eu-ft-icr-ms.eu](http://eu-ft-icr-ms.eu))

and send it by email to:

**[guillaume.van-der-rest@u-psud.fr](mailto:guillaume.van-der-rest@u-psud.fr)**

before **September 30th 2018**.

Selected applicants will receive notice of their acceptance to the short course in early October.

Selection will be based on the number of applicants, the scientific project of the attendant, their knowledge in mass spectrometry.



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



## EU FT-ICR MS 1<sup>st</sup> Advanced User School

*Want to master  
Fourier transform ion cyclotron resonance  
mass spectrometry?*

**When?**  
April 2019

### **Where?**

Universidade de Lisboa  
Laboratório de FT-ICR e  
Espectrometria de Massa Estrutural  
Lisboa – Portugal

### **Course preview**

- Advanced FT-ICR MS hardware & instrumentation
- Data acquisition and signal processing beyond FT
- Ion motion in ICR: Pushing the boundaries of resolution
- Extreme resolution and application of isotopic fine structure
- Applications in complex mixtures, protein analysis, forensics, environment

### **Content**

- Tutorial lectures, short talks, poster session
- Advanced instrument tuning
- Computational sessions

### **Social activities**

- Welcome reception and get together in Lisboa
- Half day trip to a breathtaking location in the outskirts of Lisboa
- Free afternoon where your imagination takes you!

**For more information &  
application to the course:**

**<http://ft-icr.rd.ciencias.ulisboa.pt/>**

caac@fc.ul.pt

*Organized by EU FT-ICR MS – A European  
Network funded by  
EU Horizon 2020 Programme*

### **NO PARTICIPATION FEE!**

Accommodation, meals and social  
program are offered!

Up to 50 students  
selected by the scientific committee



**Ciências  
ULisboa**





**EU FT-ICR MS**

# **Open Data & e-Infrastructure**

Grant Agreement (GA) No: 731077  
IMSC, Florence, EU\_FT-ICR\_MS Workshop



# The SME CASC4DE



HOW CAN **BIG DATA** BOOST YOUR **SCIENCE** ?

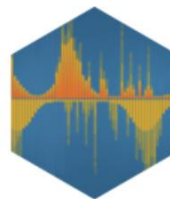


innovating solutions **TO ACCELERATE** your research and **CREATE** new value from your results

# 4 CASC4DE - OUR EXPERTISES



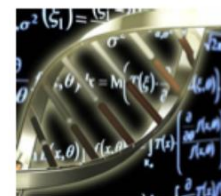
- Mathematics
- Bayesian statistics
- Compressed Sensing
- Massive number crunching



- Signal processing
- Innovative high-speed data processing algorithms and techniques to gain insights from data



- Custom Software Development
- Embeddable software tools



- Biophysic, Sciences
- NMR, Mass spectrometry
- Analyses





## Open data and e-Infrastructure



### Data management plan

To address the issues in intellectual property, confidentiality and scientific policies



### Metadata specification

Metadata and data formats to be used in the common infrastructure data exchanges



### Data storage and data access

To provide access and storage of user data to users from any personal computer



### Virtualization of instrument access

An interface for giving a complete control to the user of its experience on a distant FT-ICR spectrometer



### Data processing and data mining

Development of specific processing, analysis and mining tools



**EU FT-ICR MS**

# **TransNational Access**

Grant Agreement (GA) No: 731077  
IMSC, Florence, EU\_FT-ICR\_MS Workshop





# EU FT-ICR MS Workshop Prague



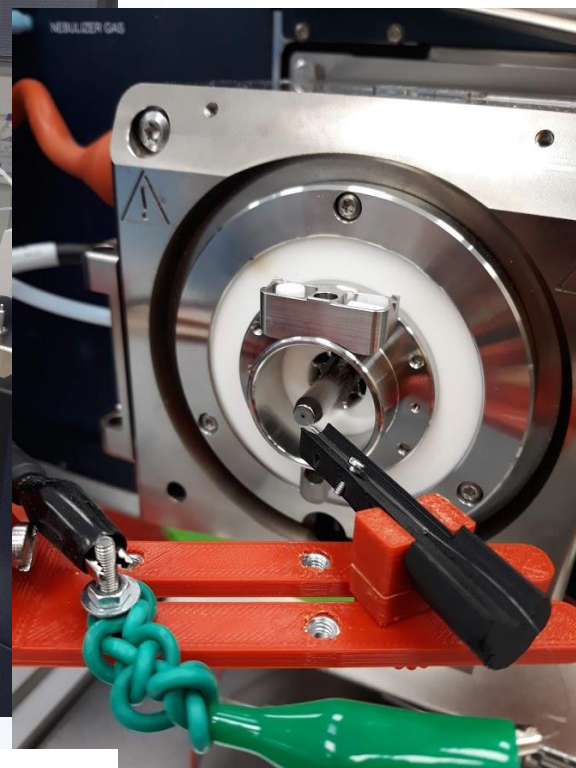
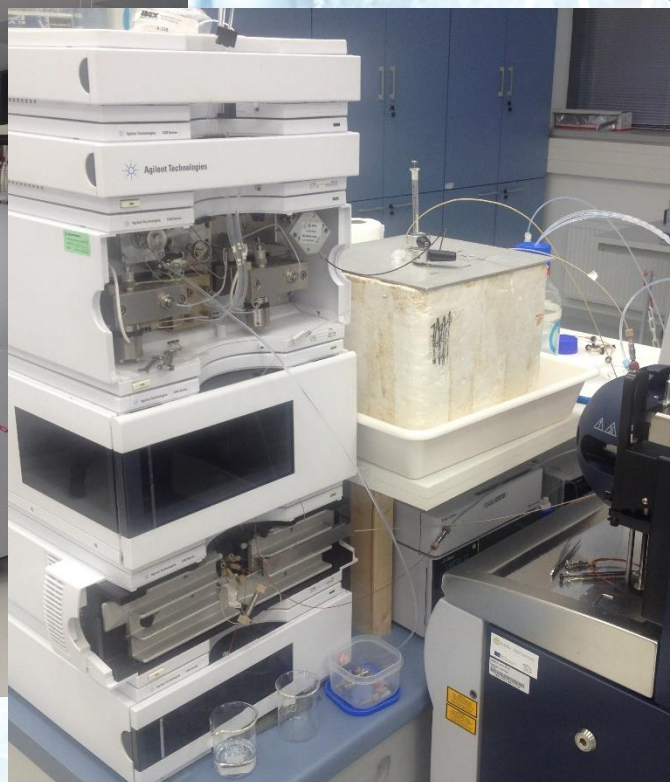
**DAN FABRIS**

28<sup>th</sup> August 2018 | XXII International Mass Spectrometry  
Conference | Florence



## AVAILABLE INSTRUMENTATION

EU FT-ICR MS



**CID, SORI, ETC, ECD and IRMPD dissociation techniques**



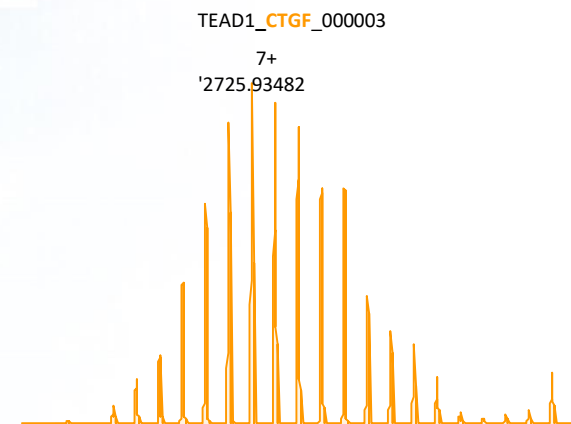


**SERVICES**



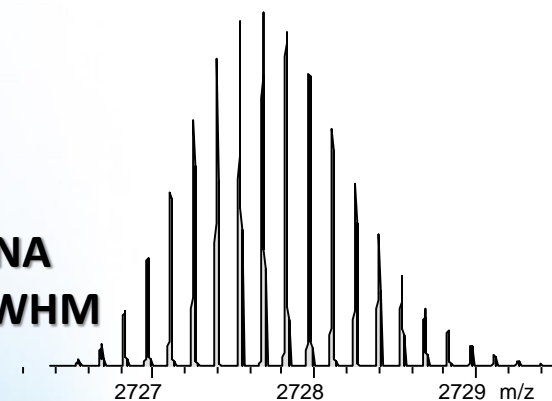
**EU FT-ICR MS**

- Intact protein analysis / TopDown analysis
- Native electrospray
- Hydrogen/deuterium exchange
- Chemical covalent labeling and cross-linking
- Fast photochemical oxidation of proteins
- PTM characterization / oligosaccharide analysis



TEAD1\_CTGF\_C<sub>722</sub>H<sub>1074</sub>N<sub>248</sub>O<sub>306</sub>S<sub>3</sub>P<sub>24</sub>

**15T solarix XR**  
Native TEAD1/dsDNA  
complex @215 000 FWHM







SAPIENZA  
UNIVERSITÀ DI ROMA



Address: Dipartimento di Chimica e Tecnologie  
del Farmaco, Università degli Studi di Roma "La  
Sapienza", P.le A. Moro 5, I-00185, Roma (Italy)

Prof. Maria Elisa Crestoni

Prof. Simonetta Fornarini

Dr. Barbara Chiavarino (research associate)

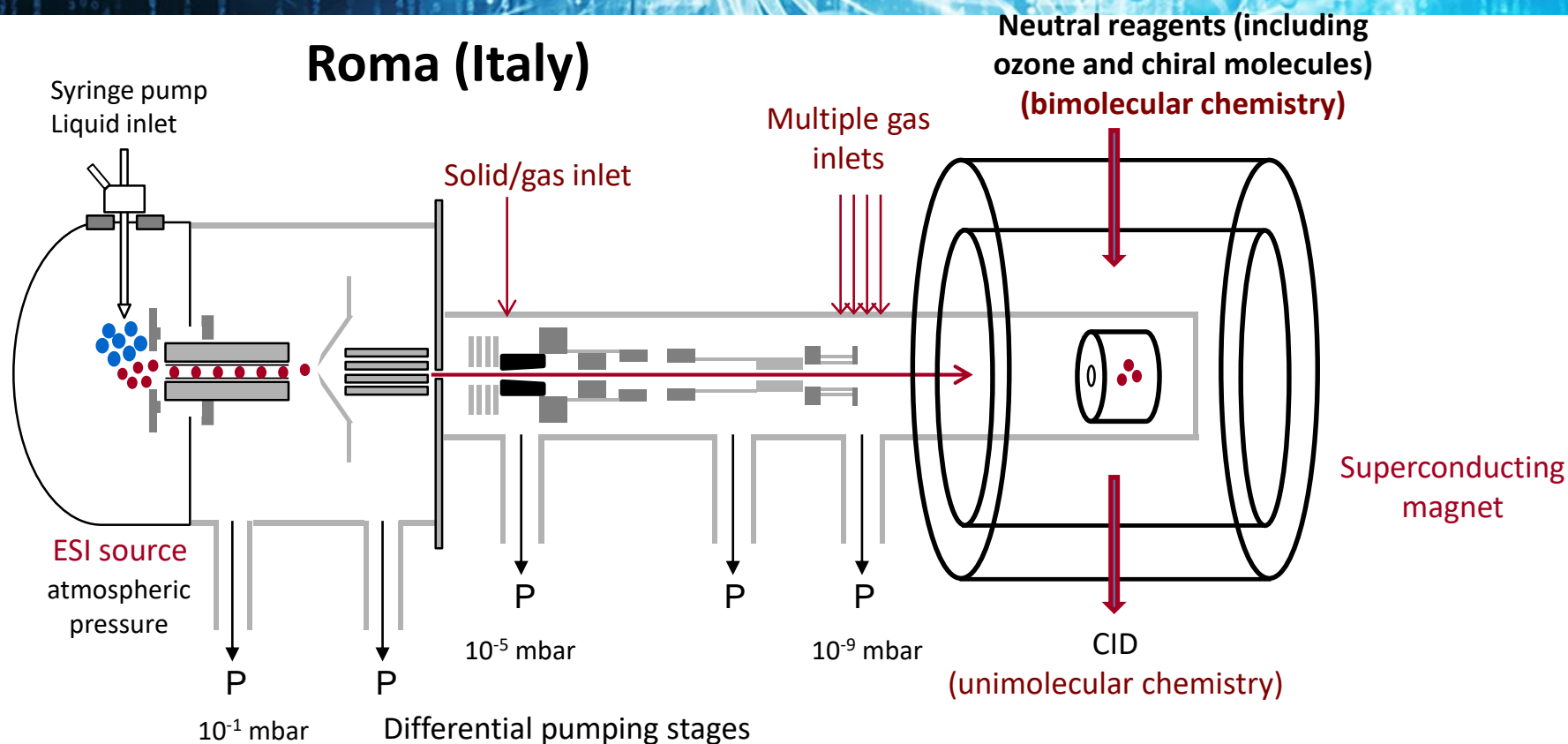
Davide Corinti (PhD student)

Alessandro Maccelli (PhD student)

Annito Di Marzio, Valentina Lilla (technicians)

MSc students

## Roma (Italy)



Other sources: nanoESI, EI/CI

$m/z$  range starting from 14.5 Da

## Expertise in:

- **ion-molecule reactions** : kinetics and thermodynamic data (free energy ladders, linear free energy relationships e.g.  $\log k$  vs.  $\log K$  or IE (calculated and exp.)), use of kinetics as probe of ion structure, and **ion chemistry in general**.

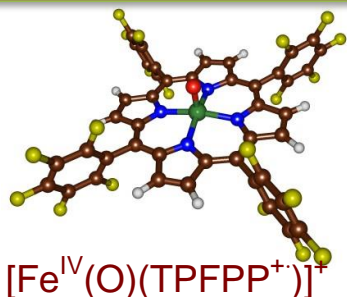
## Research areas include:

- **non-covalent interactions** (electrostatic and hydrogen bonding interactions, cation/anion- $\pi$  and  $\pi$ - $\pi$  interactions);
- **reaction mechanisms and reactive intermediates** in (bio)inorganic / organic chemistry.
- **foodomics**

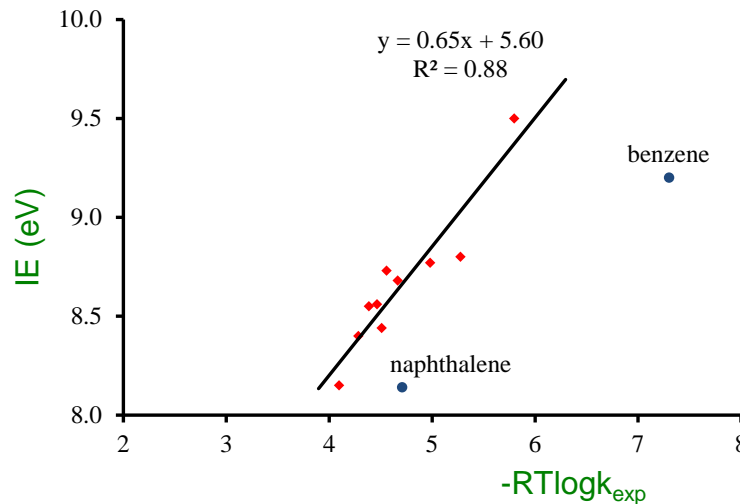
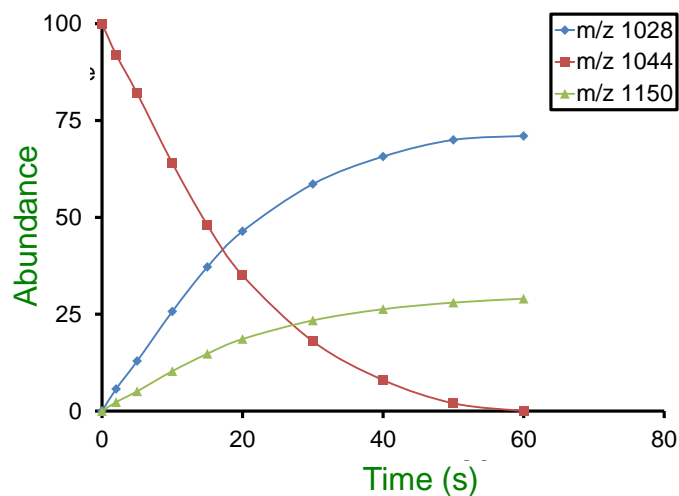
Few examples in the following slides...



# Kinetics and linear free energy relationships: Cytochrome P450 model compound I



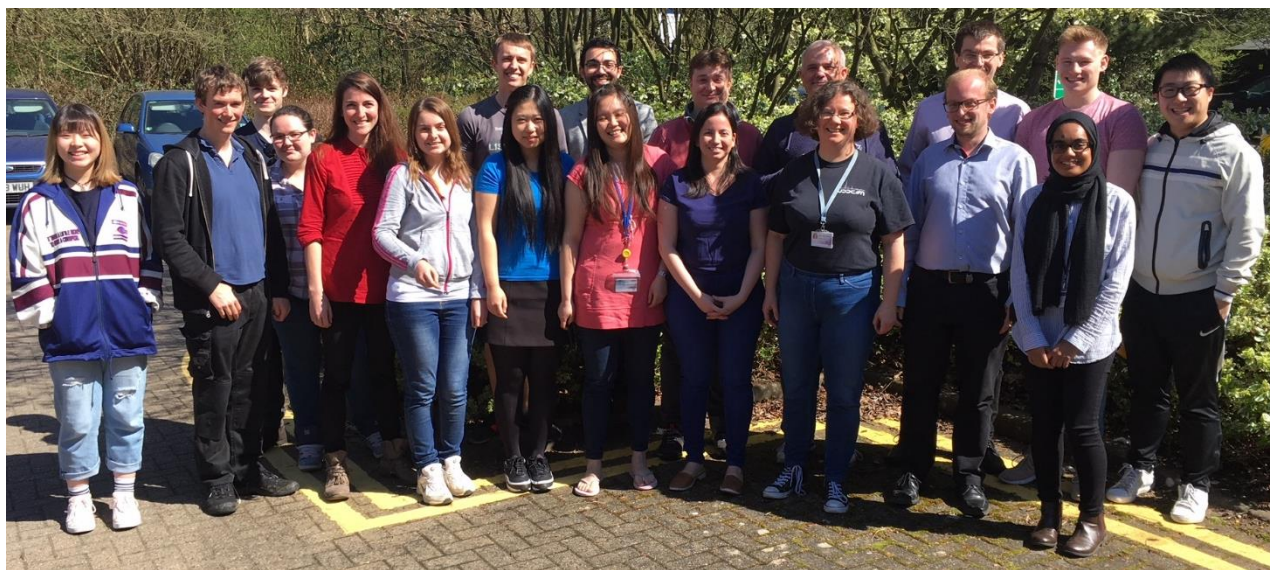
Structure of SubO determined by ion-molecule reaction kinetics



Oxidation mechanism determined by linear log<sub>k<sub>exp</sub></sub> vs. IE relationship

# Who are we?

## The joint research groups of Peter O'Connor and Mark Barrow





## 12 T Solarix FTICR mass spectrometer

### Capabilities:

500k RP routinely, >3M RP with effort

<0.3 ppm typically

IRMPD, ECD, EID, EDD, CAD

UVPD (213 nm / 193 nm) soon...

2D mass spectrometry routinely with IRMPD, ECD, EID, EDD





Finding covalent and non-covalent binding sites in protein.

Finding amyloid aggregation points

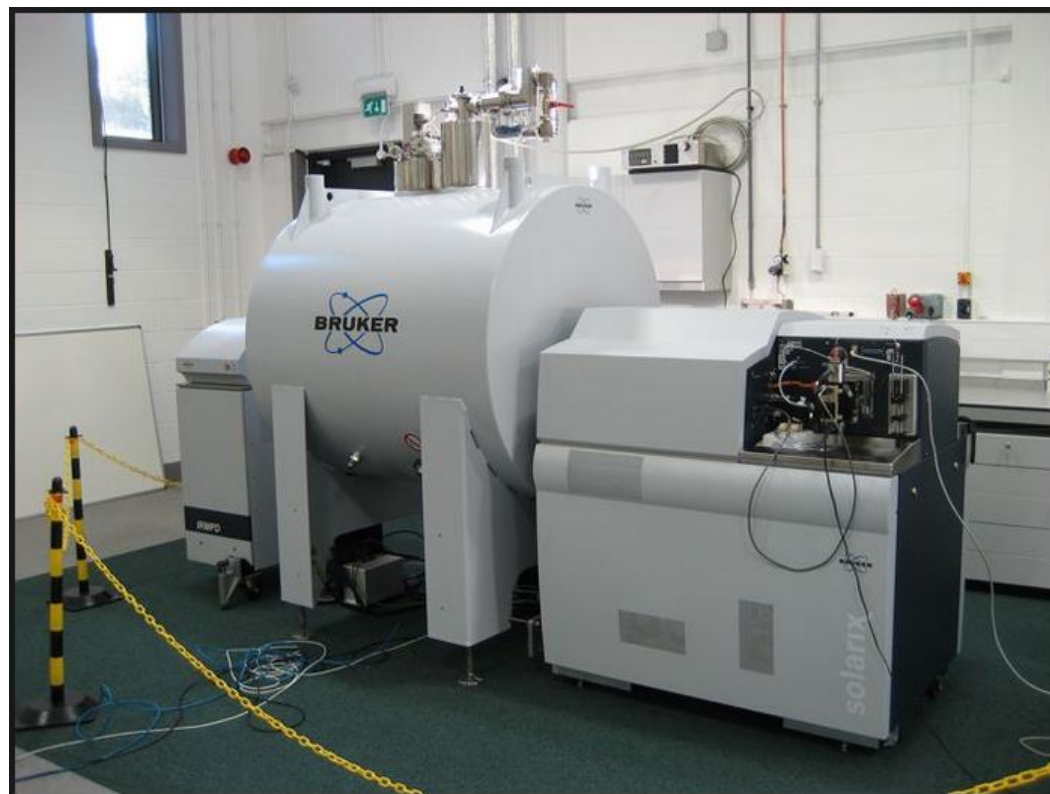
Top-down de-novo protein sequencing.

Polymer tandem mass spectrometry

Small molecule tandem mass spec using many fragmentation techniques

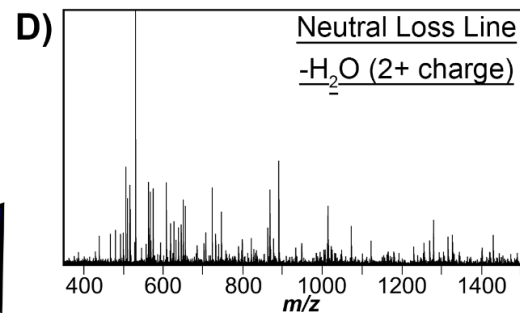
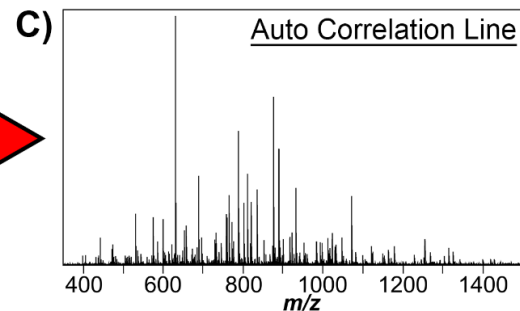
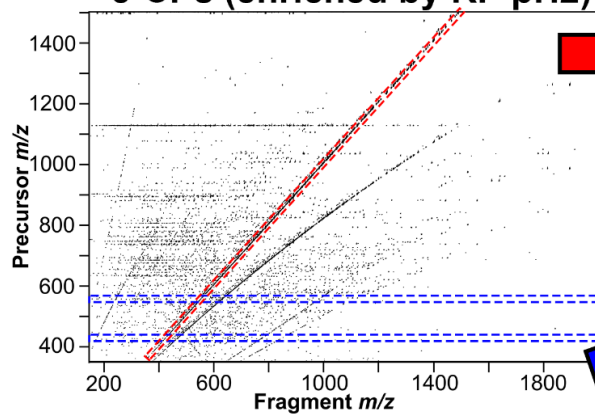
Glycomics, PTM-omics, genomics, ...

2DMS of anything...

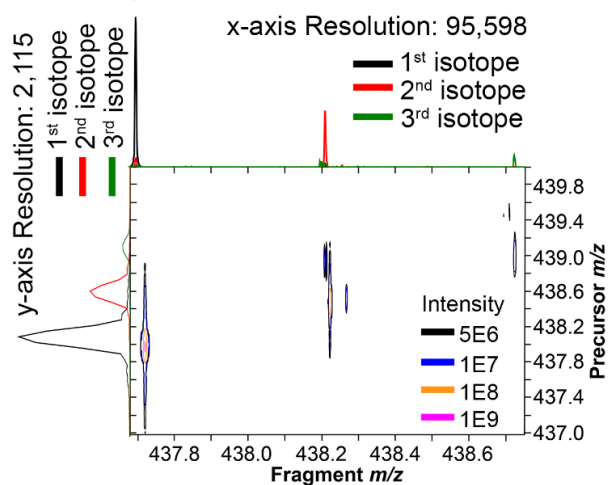


With Mark Barrow: Petroleomics, environmental analysis, biofuels, and statistically defined automated data analysis.

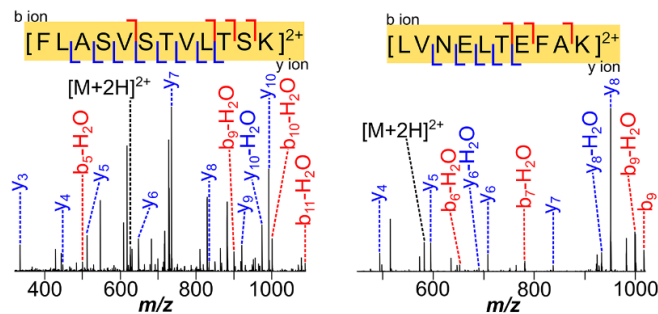
**A) 2D-MS (1 MW \* 8 K) of digested 5-CPs (enriched by RP pH2)**



**B) Zoom in  $m/z$  437.8**



**E) Peptides identified by 2D-MS only**



## Instrument :

- Bruker Solarix XR (harmonized cell ) FT-ICR 9.4 T
- CID, ECD, ETD IRMPD dissociation
- Hyphenated with nanoLC

## Specificity :

- Cultural heritage samples (proteins, lipids and carbohydrates)
- Bidimensionnal (2D FT-ICR) at precursor high resolution

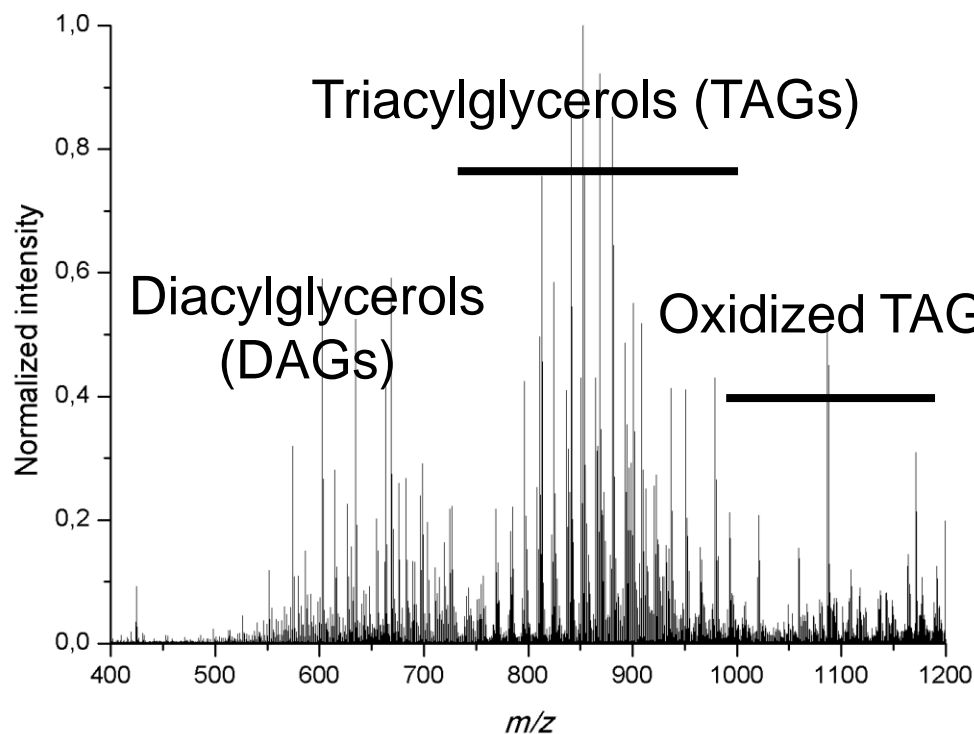
## Staff :

- Technical staff : Dr Fabrice BRAY
- Associated staff : Pr Caroline TOKARSKI
- Scientific PI : Christian ROLANDO



## Cultural Heritage and Archaeological Samples

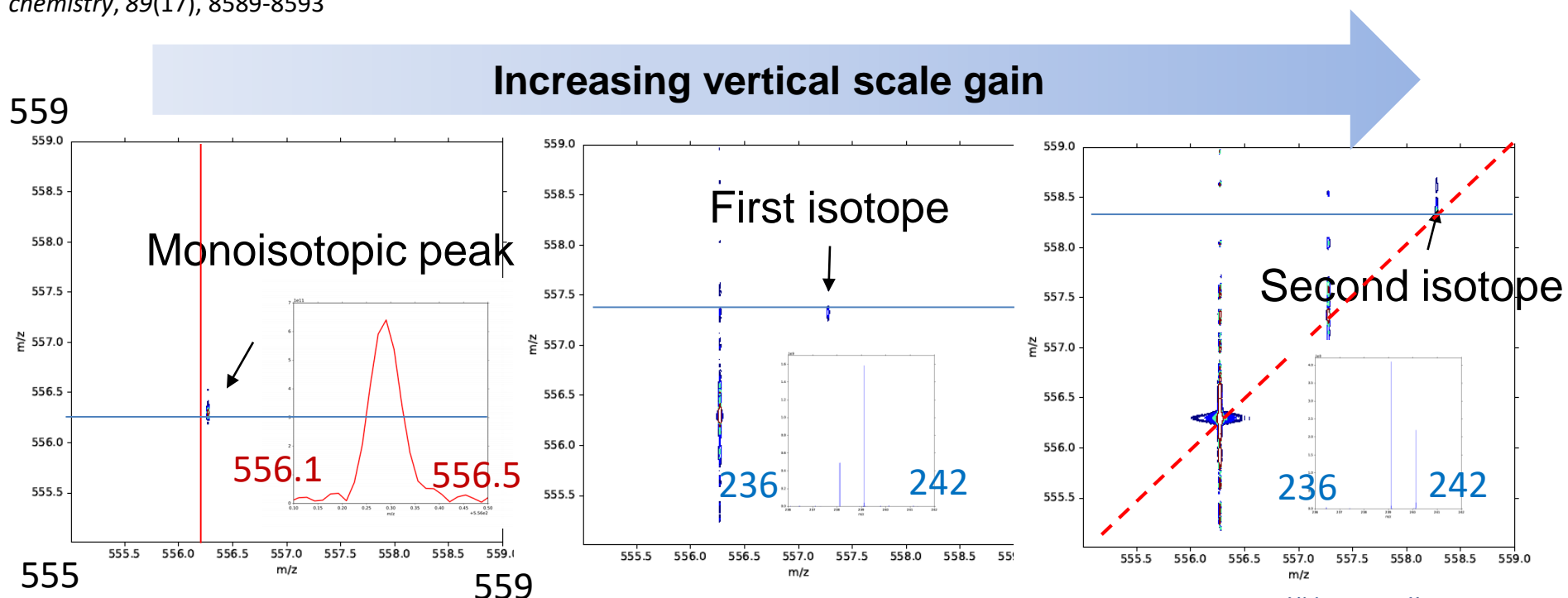
**See :** Caroline TOKARSKI, FOr.03 - Cultural heritage and archaeology, Art and cultural heritage natural polymers by bottom up and top down approaches



**Ceramic aryballos** from Tenedo necropolis (Bad Zurzach), Switzerland, 41 - 54 AD

# Bidimensionnel (2D FT-ICR) at precursor high resolution

Bray, F., Bouclon, J., Chiron, L., Witt, M., Delsuc, M. A., & Rolando, C. (2017). Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions. *Analytical chemistry*, 89(17), 8589-8593



Precursor resolution > 10 000 @  $m/z$  400

Universität  
Rostock



Traditio et Innovatio

HelmholtzZentrum münchen

Deutsches Forschungszentrum für Gesundheit und Umwelt

## JOINT MASS SPECTROMETRY CENTRE



EU FT-ICR MS

Chair for  
Analytical  
Chemistry

Universität  
Rostock



Traditio et Innovatio

Thermal Analysis /  
Photonization MS



Thorsten Streibel

Aerosol and Laser-  
MS



Johannes Passig

Ultra-high Resolution  
MS



Martin Sklorz

Aerosol  
Chemistry



Jürgen Schnelle-Kreis

Aerosol  
Toxicology



Sebastian Öder

Aerosol  
Physics



Thomas Adam

Bio-  
monitoring



(Jutta Lintemann)

Comprehensive  
Separation



Thomas Gröger

München /  
Munich

**CMA**  
Cooperation Group  
Comprehensive  
Molecular Analytics

der Bundeswehr  
Universität **München**

Chair for Chemistry,  
Environmental- & Energy  
process technology

**photonion**

Spin-off Company  
Photoionization mass  
spectrometry and online  
process analytics

HelmholtzZentrum münchen

German Research Center for Environmental Health



**Ralf Zimmermann**  
University Rostock  
Chair for Analytical  
Chemistry and Head of  
the Cooperation Group  
Complex Molecular  
Analysis



Aerosol & Health

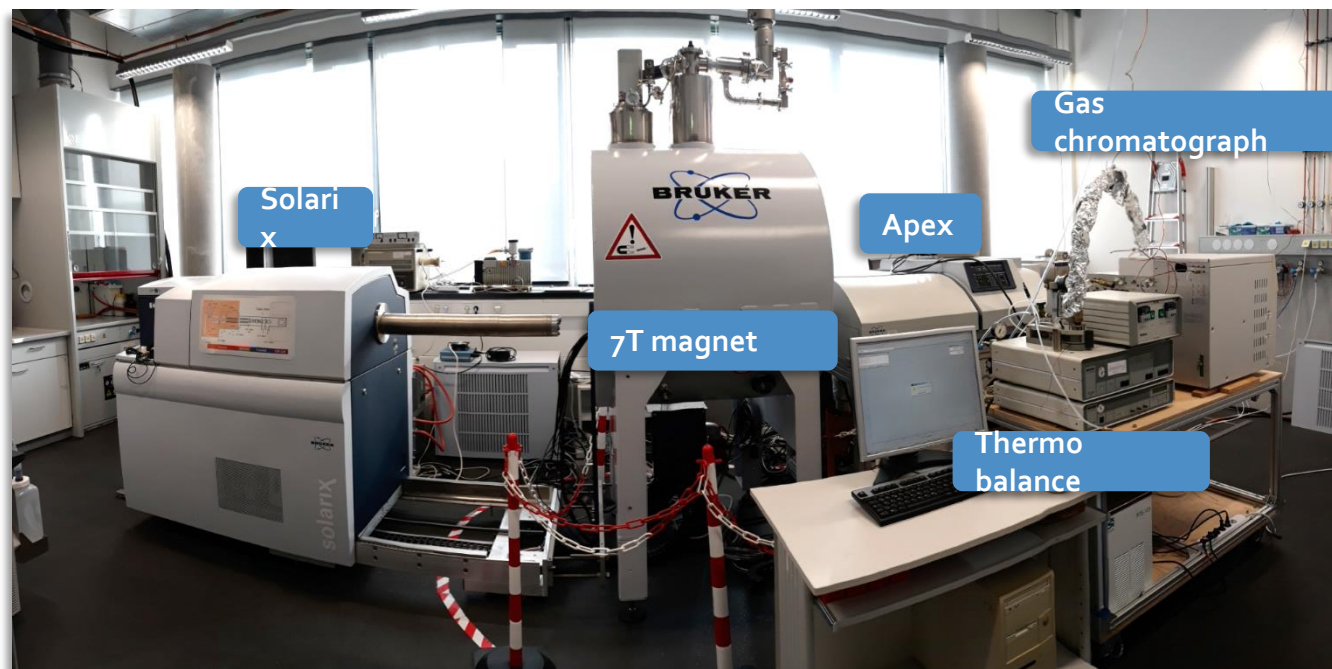
Enabling  
Technologies

(Staff: about 40 people)





## View at Rostock FTICR -MS laboratory



FTMS laboratory at the interdisciplinary faculty of the University of Rostock

### Ion Sources available

@Solarix (direct liquid infusion)

- ESI
- APCI
- APPI (Krypton and Xenon lamp)

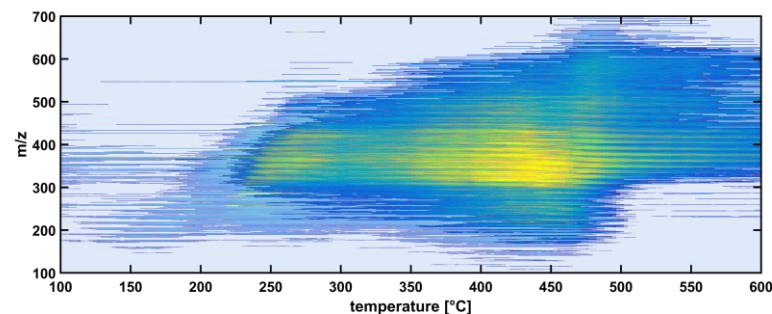
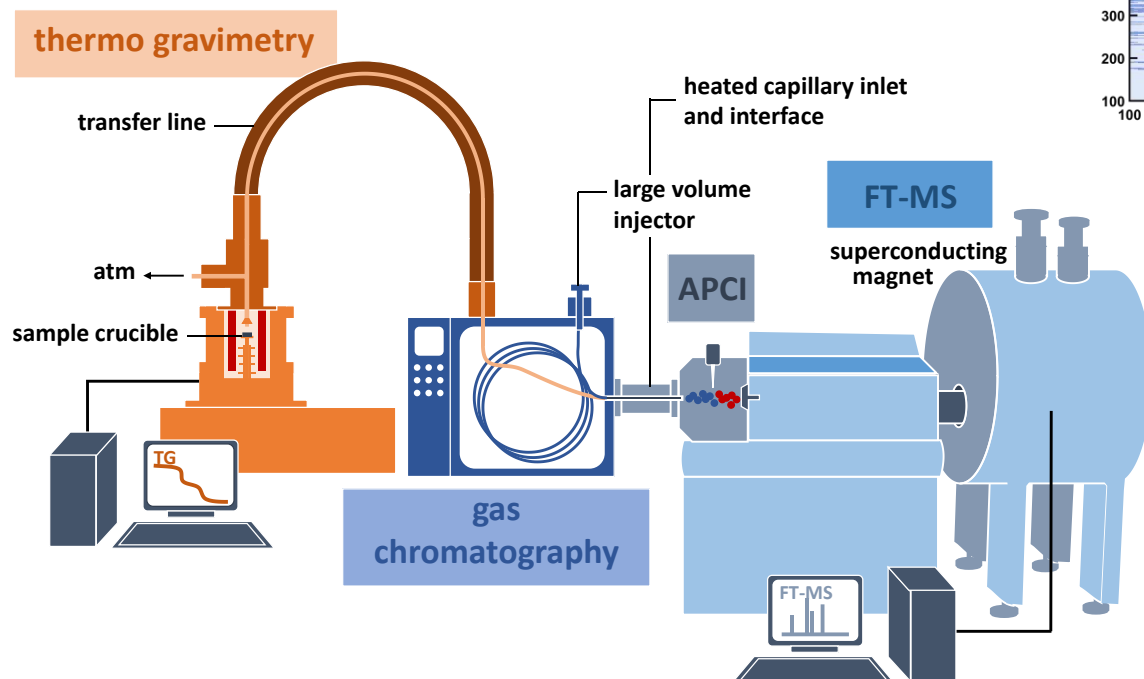
@Solarix

- MALDI

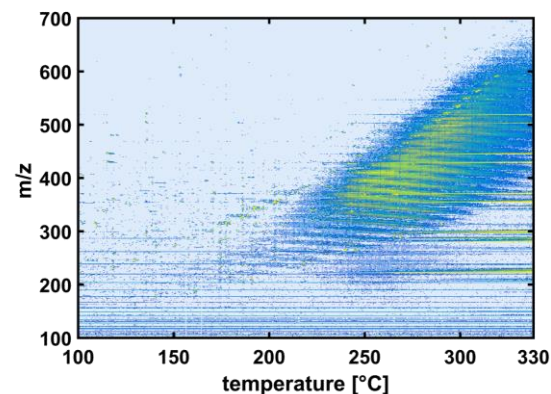
@APEX (coupled to TG or GC)

- APCI
- APPI (Krypton and Xenon lamp)
- APLI (266nm NdYag)

# Gaschromatography and evolved gas analysis (APCI)

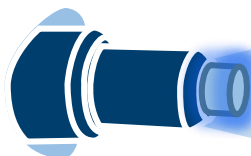


evolved gas analysis / pyrolysis of bitumen



gas chromatography of bitumen

# Special ionisation techniques



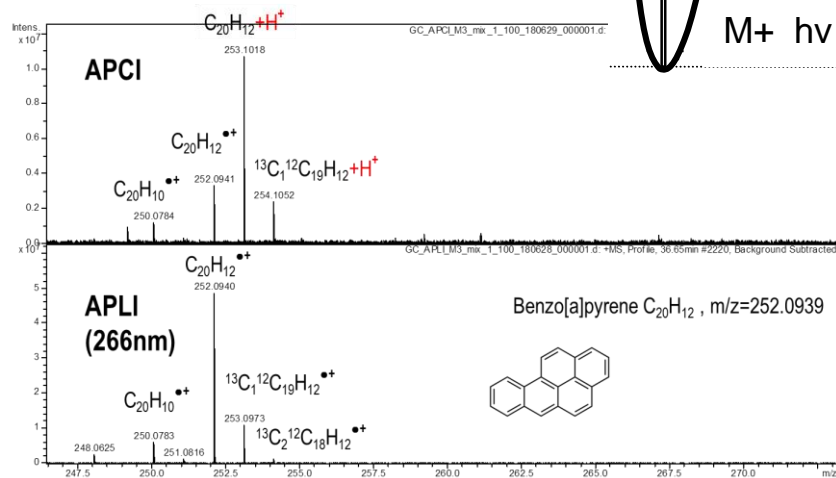
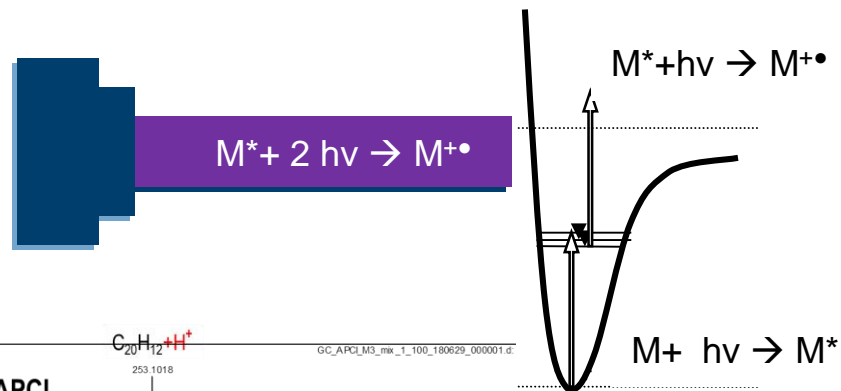
## Single photon ionization (APPI)

→ universal

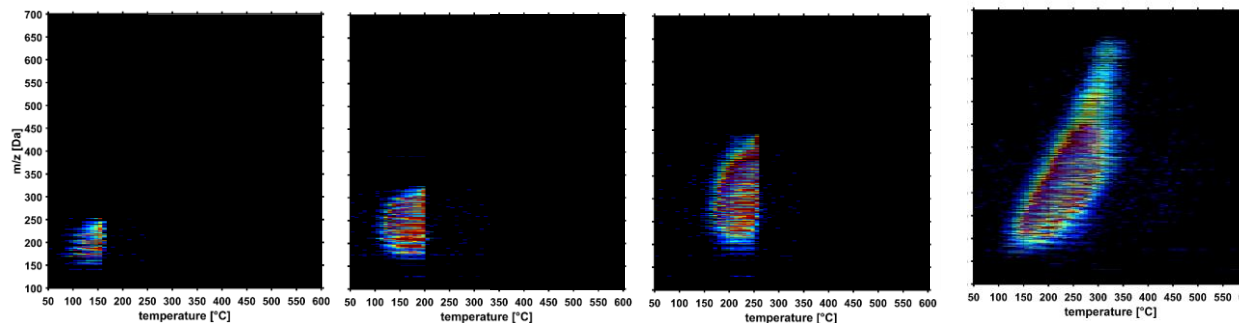
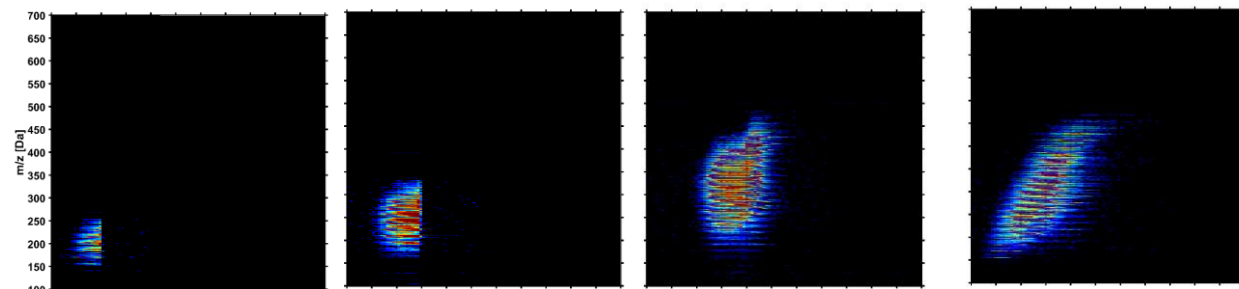
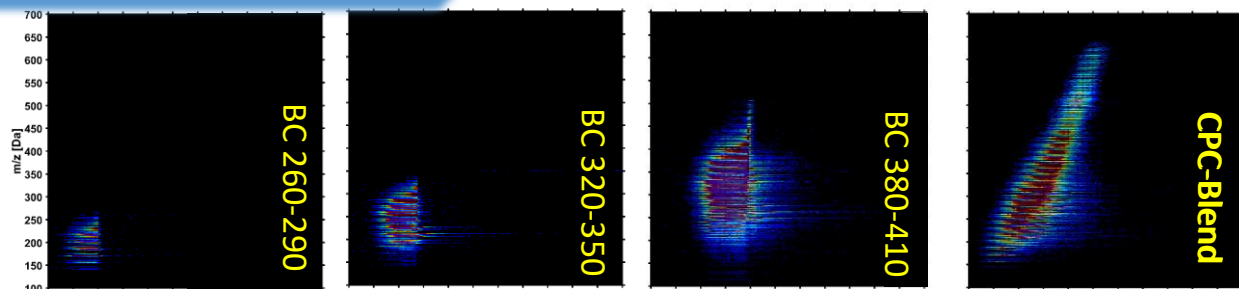
	type of UV lamp and photon energies	Compounds	Ionisation energy [eV]
INERT		N <sub>2</sub>	15,6
		H <sub>2</sub> O	12,6
		Acetonitril	12,2
		O <sub>2</sub>	12,1
IONISATION	Argon (11.2 eV)		
		Methanol	10,8
		Isopropanol	10,2
		Hexan	10,1
	Krypton (10.0 and 10.6 eV)		
		Heptan	9,9
		Aceton	9,7
		Pyridin	9,3
		Benzol	9,2
		Toluol	8,8
	Xenon (8.4 and 9.6 eV)		
		Naphthalin	8,1
		Anthracen	7,4

## Multiphoton ionization (APLI)

→ high selective and sensitive for aromatic compounds









 **UNIVERSITÉ  
DE ROUEN**

30,000 Students



Normandie Université

70,000 Students







## Instrument

- 12 T Solarix XR
- Highly Complex mixtures
  - Petroleum
  - Polymers
  - Environmental samples
  - Metabolomics
- Ionization
  - API (ESI, APCI/APPI, DIP)
  - MALDI/LDI
- Glove Box coupling
  - Air sensitive compounds analysis



RÉGION  
NORMANDIE



ERDF



TOTAL

## Staff

- Group leader: Carlos Afonso (Prof.)
- Scientific officer: Helene Lavanant (Ass. Prof.)
- Organic/inorganic clusters, peptide structure...
- Reception Manager: Isabelle Schmitz (Res. Ing.)
- Natural substances, metabolomics
- Corinne Loutelier (Ass. Prof.)
- Glycans, Lipids, Polymers...
- Marie Hubert (Res. Ing.)
- Polymers, Petroleomics...



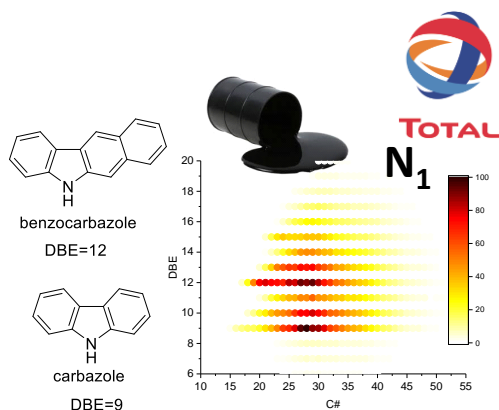
**C2MC**

Complex Matrices  
Molecular Characterization



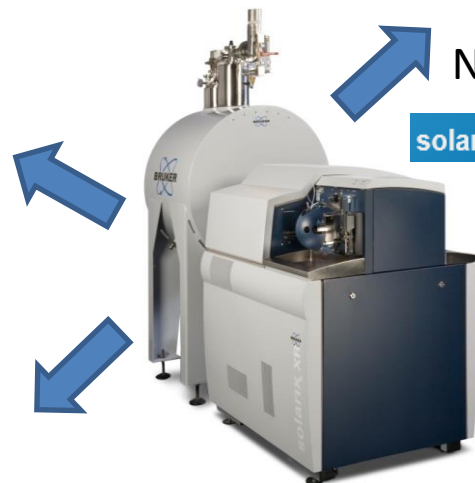
## Complex mixtures analysis

Titan atmosphere particles



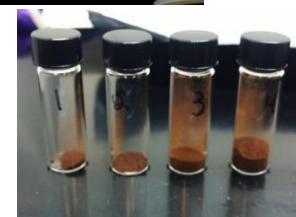
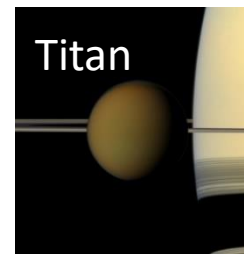
**Petroleomics**

**Environment**



**LATMOS**  
Nathalie Carasco

**solarix XR** 95 % N<sub>2</sub>  
5 % CH<sub>4</sub>



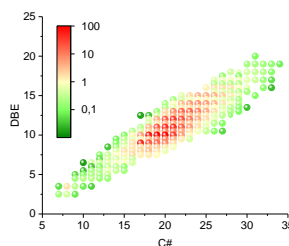
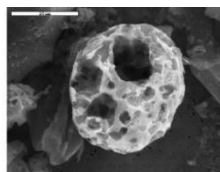
**Tholinomics**

UMR 6614  
**coRia**  
COMPLEXE DE RECHERCHE  
INTERPROFESSIONNEL EN AÉROTHERMOCIMIE

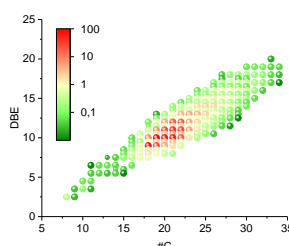
particulate matter analysis



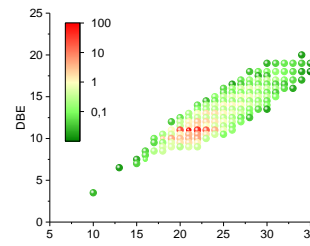
biomass combustion



O5



O6

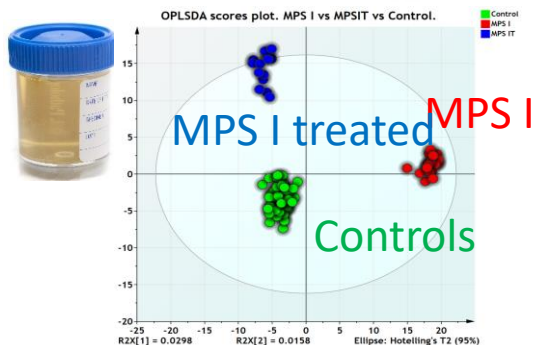


O7

## Biomedical applications

Soumeiya Bekri

### Metabolomics



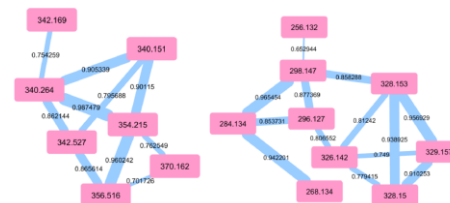
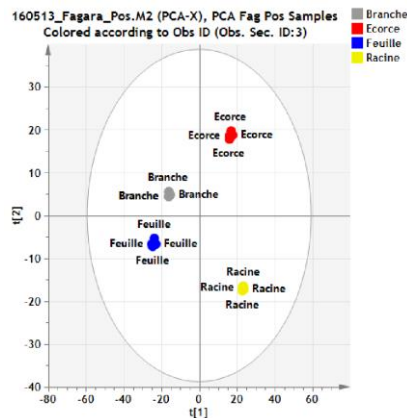
type I mucopolysaccharidose

### Plantomics

Hakim Elomri



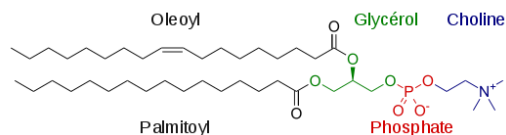
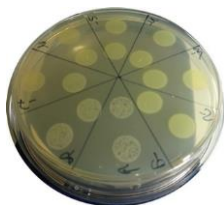
*Fagara heitzii*



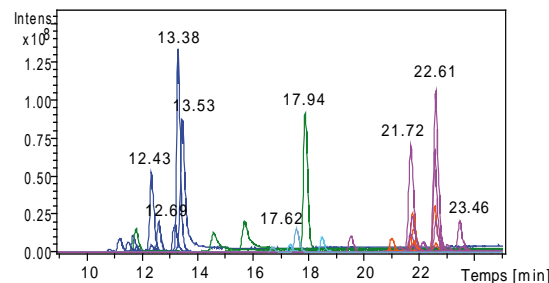
Molecular network

### Lipidomics

Stéphane Alexandre



### LC-FTICR





## Orsay (France) site summary

### Instrument :

- Bruker APEX Qh FT-ICR 7 T (installed 2006)
- Three IR laser sources coupled with the FT-ICR mass spectrometer:
  - Table-top OPO/OPA ( $2300\text{ cm}^{-1}$  –  $4000\text{ cm}^{-1}$ ) laser (Laser Vision).
  - CLIO Free Electron Laser facility ( $400\text{--}2000\text{ cm}^{-1}$  )
  - $\text{CO}_2$  fixed wavelength laser

### Specificity :

- Using specific activation through wavelength tuned IR action spectroscopy
- Characterization and quantitation of isomers and structural characterization
- Current developments on coupling ion mobility with IR spectroscopy (DIMS).

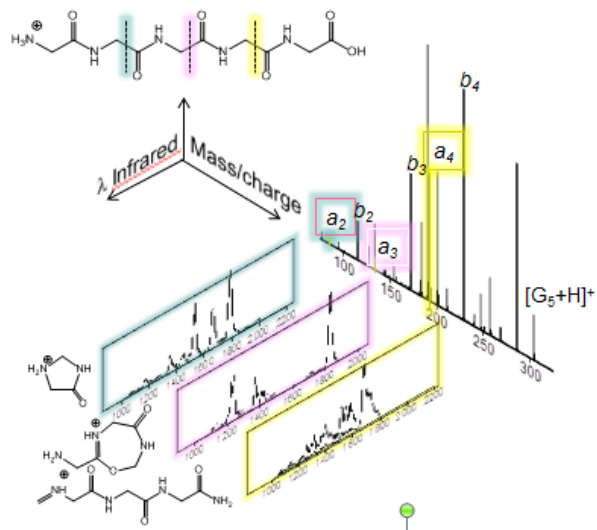
### Staff :

- Scientific PI : P. Maître
- Technical staff : E. Loire
- Associated staff : F. Halgand, D. Scuderi, G. van der Rest



## Infra-red activation combined with mass spectrometry

### Bruker Apex IV Hybrid FT-ICR



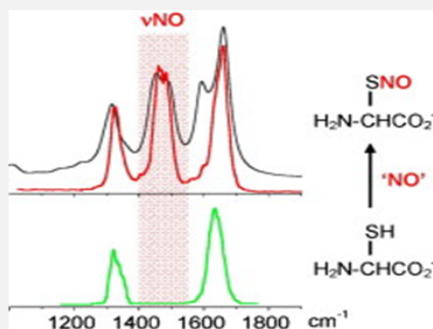
- Simple implementation, based on commercial instrumentation and software.
- Ambient temperature ions, collisionnally thermalized.
- IR activation can be used for all ion types, including those **strongly bonded**.
- IR spectroscopy can be integrated to MS<sup>n</sup> sequences:  
IR spectra of fragment ions (CID+IR, ECD+IR) and ion molecule reaction products.

## An example: characterization of post translational modifications

- Phosphorylation:
  - IR signature of pTyr, pSer, and pThr
  - IR characterization of phosphate containing peptides
- Nitrosylation
  - IR signature of S-nitrosylation

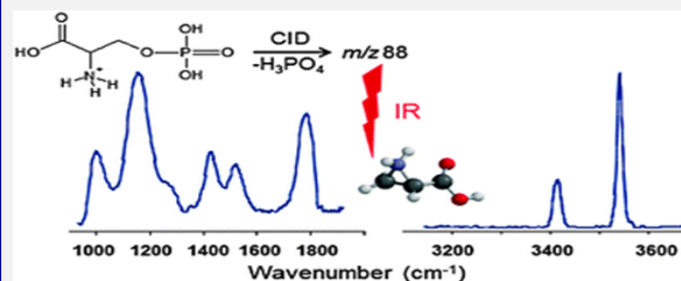
Parent<sup>+</sup>  $\longrightarrow$  Fragment<sup>+</sup>  
Only if IR on resonance with a vibrational mode of parent

### S-Nitrosylation evidenced by IRMPD



*Int. J. Mass Spectrom.* **330-332** 160-167 (2012).

### IR characterization of CID fragment of phosphate containing peptides

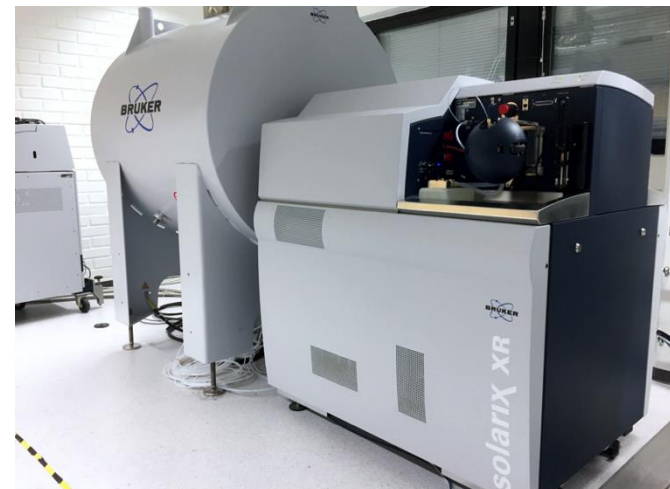


*Chem. Commun.* **50** 3845-3848 (2014)

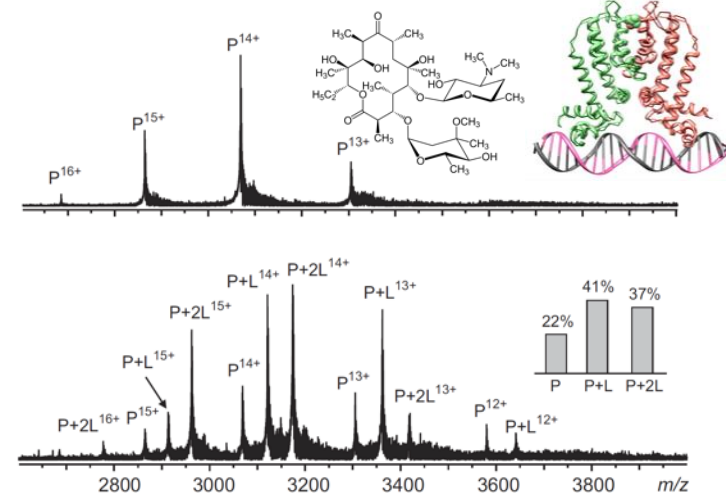
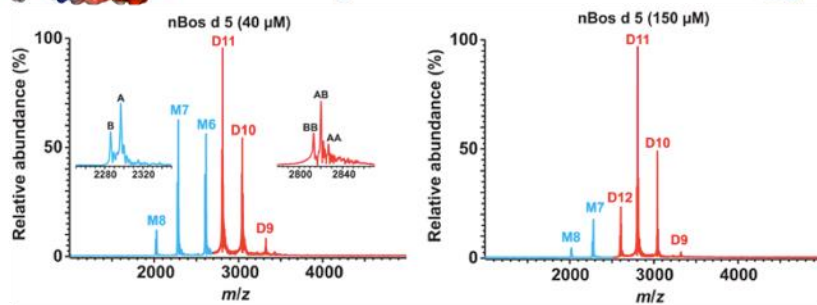
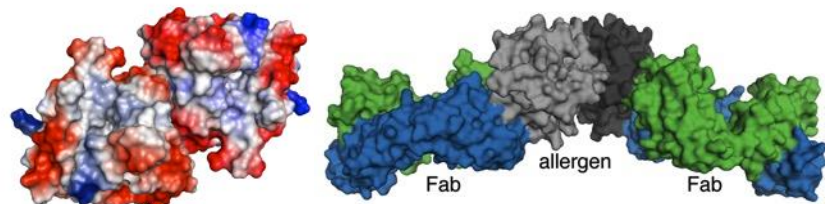
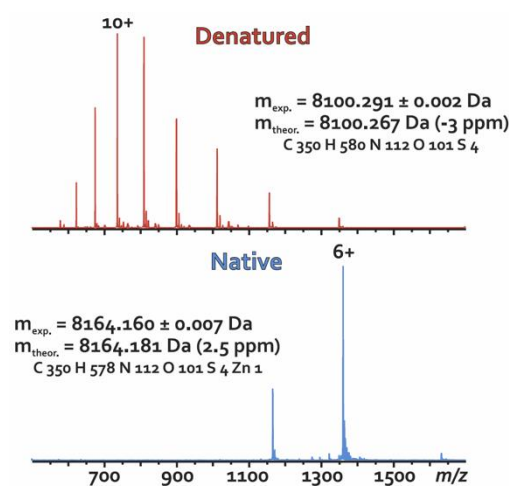
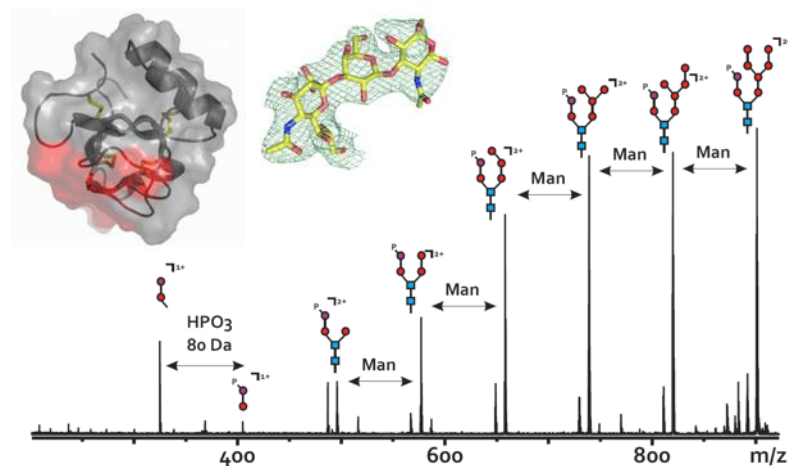


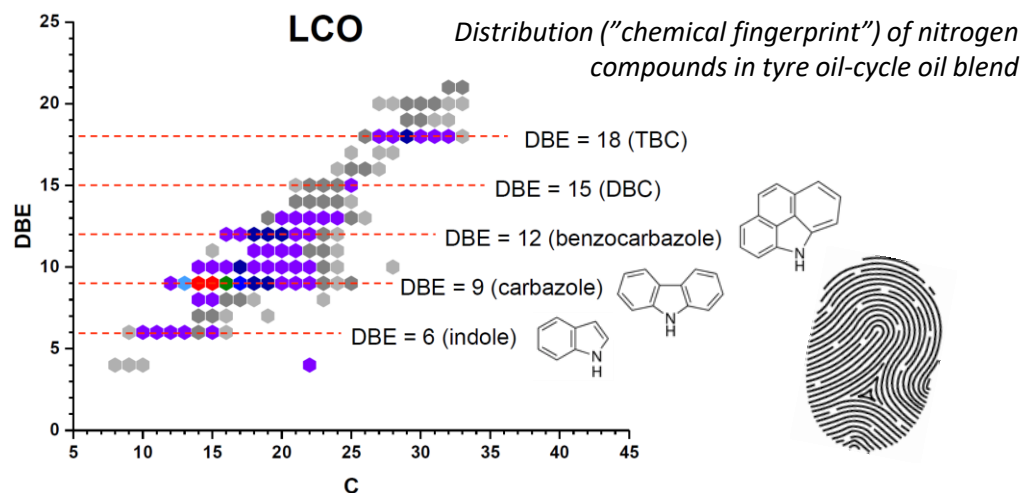
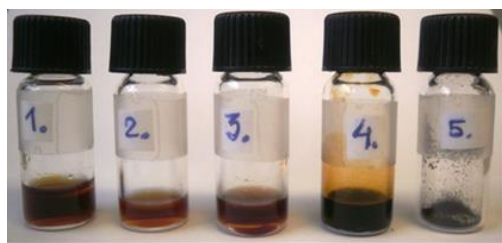
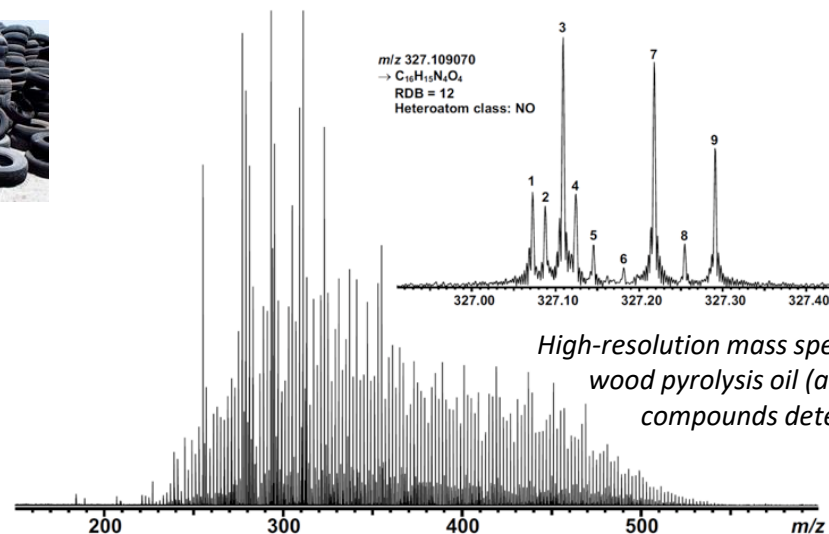
## 12-T Bruker Solarix XR FT-ICR MS

- Mass range:  $m/z$  70–15.000
- Resolution:
  - Up to 7 million @  $m/z$  500 with narrowband detection
  - > 1 million @  $m/z$  500 with broadband detection ( $m/z$  150-3000)
- Mass error (RMS)
  - < 1 ppm (external calibration)
  - < 0.1 ppm (internal calibration)
- Sensitivity
  - nM-level with direct infusion
  - aM-level with LC (a few ng's injected into column)











## Contacts and further information

- General enquiries, structural biology & biological chemistry
  - Prof. Janne Jänis ([janne.janis@uef.fi](mailto:janne.janis@uef.fi))
  - Prof. Juha Rouvinen ([juha.rouvinen@uef.fi](mailto:juha.rouvinen@uef.fi))
- General enquiries, petroleomics & biofuels, complex mixtures
  - Prof. Janne Jänis ([janne.janis@uef.fi](mailto:janne.janis@uef.fi))
- Instruments, sample delivery
  - Dr. Mikko Laitaoja ([mikko.laitaoja@uef.fi](mailto:mikko.laitaoja@uef.fi))
  - Dr. Marko Mäkinen ([marko.makinen@uef.fi](mailto:marko.makinen@uef.fi))





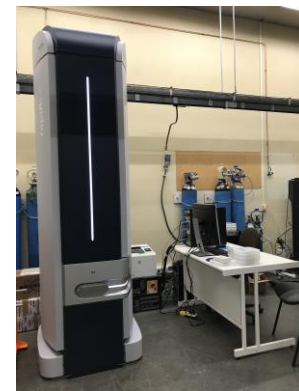
# Mass Spectrometry Laboratory



University of Liege

# Instruments and facilities

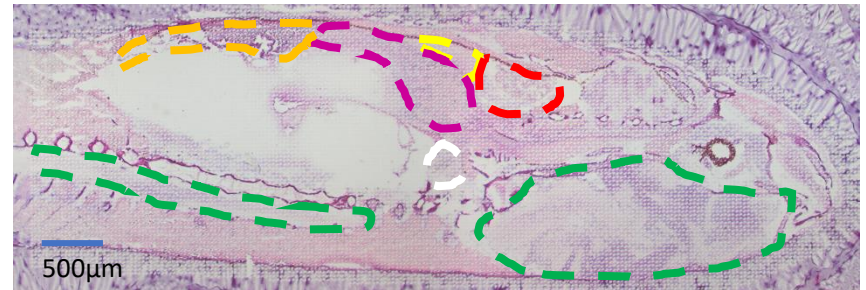
- 9.4T Bruker Solarix instrument
- 7T Thermo LTQFT coupled wit CE
- Accompanying instruments
  - TIMS TOF
  - Rapiflex
  - Synapt
  - Q exactives
  - Triple Quadrupoles
- Full proteomics facility including wet lab and dedicated orbitraps
- Microscopy and laser microdissection
- FTIR and Raman microscopy



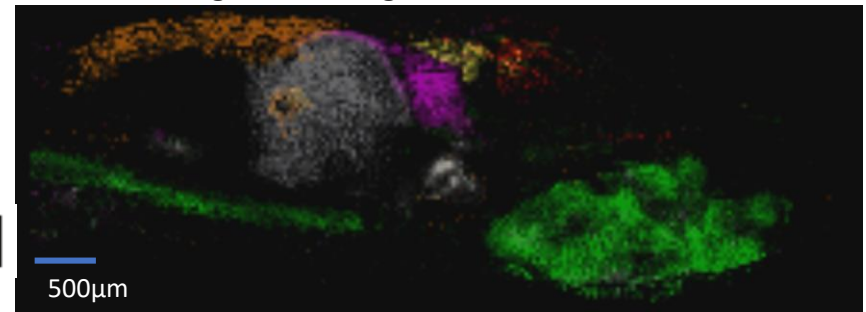
# Examples of collaborative projects

- **Eurlipids**

Building on the Euregio's knowledge and expertise in the field of lipid-technologies, the project aims at establishing an excellence platform for lipid-based research and technological solutions ("Lipid Valley").



histological staining of the slice used for MSI.



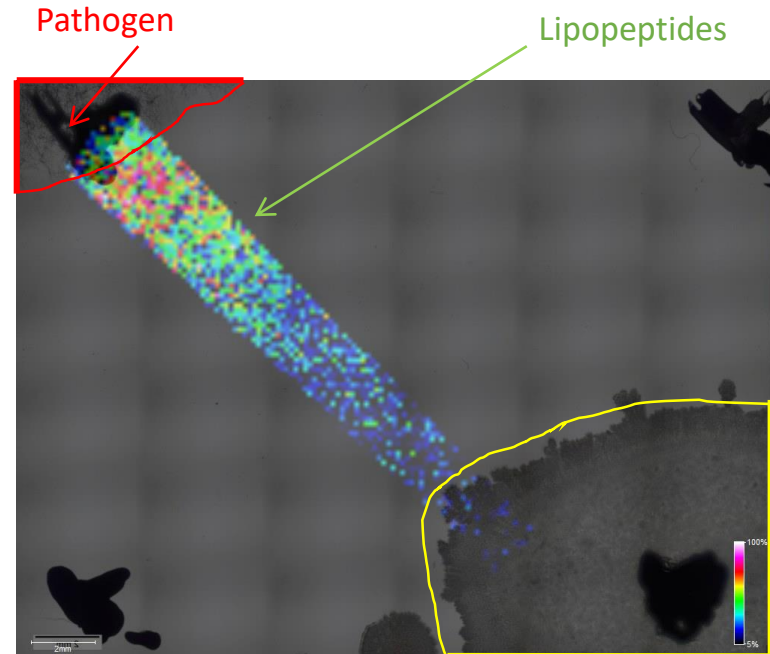
organ-specific *m/z* localizations selected with a 0.001% mass range. 549.2546 (gall bladder - uncertain); 571.4811 (intestine); 587.562 (kidney); 601.0739 (liver); 732.9773 (heart); 789.40617; 880.4465 (intestinal bulb).



# Examples of collaborative projects

## Rhizoclip

Ecological roles of cyclic lipopeptides from plant-beneficiary rhizobacteria: A chemical-biology approach to decipher primary functions of secondary metabolites.



Sample directly grown on agar support

### FTICR MS Instruments :

- Dual source Bruker APEX FTMS 7 T with harmonized cell (ParaCell™)
- Thermo LTQ FT 7T with ESI source and HPLC system
- Bruker Solarix XR (expecting by the end of the year)

### Staff :

- Scientific PI : E. Nikolaev
- Associated staff : A. Zhrebker, O. Kharybin
- And all our team to assist

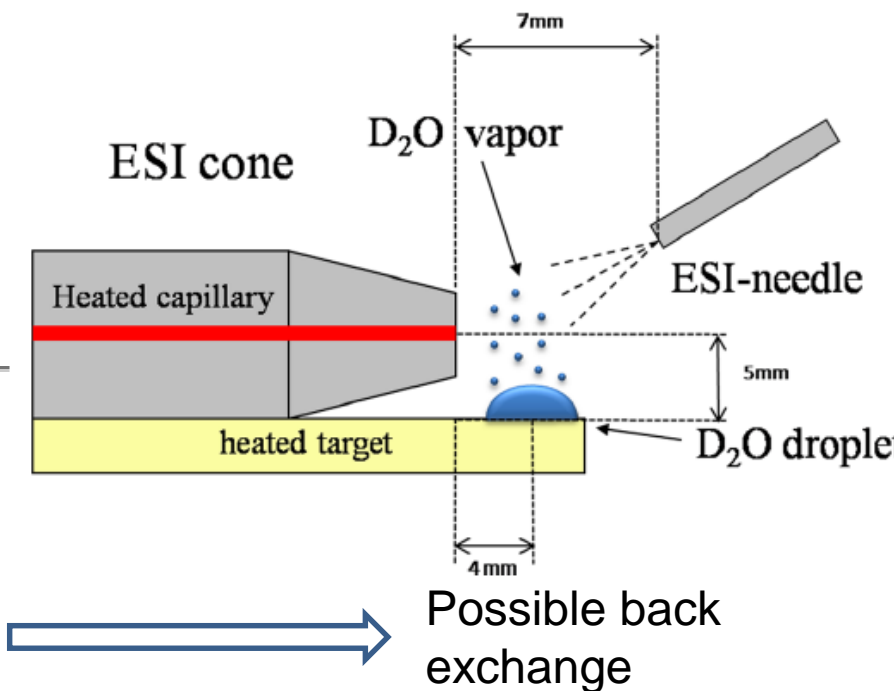
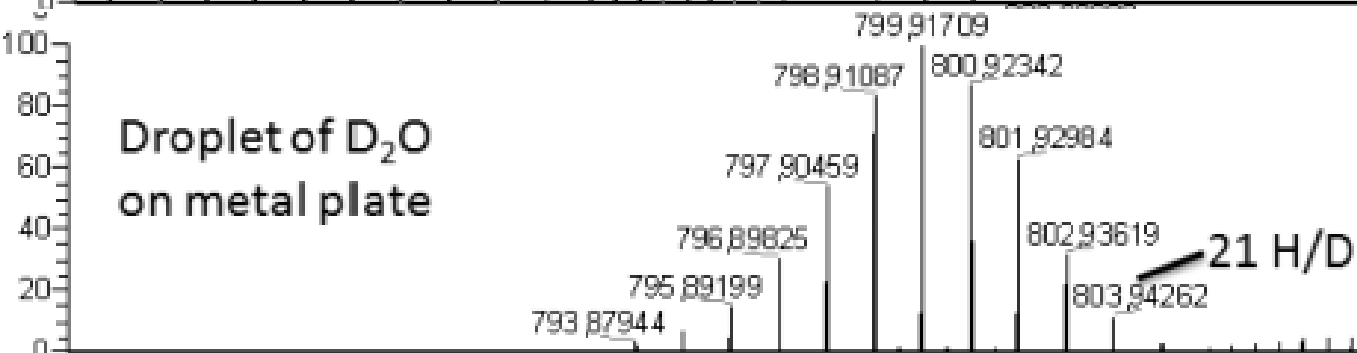
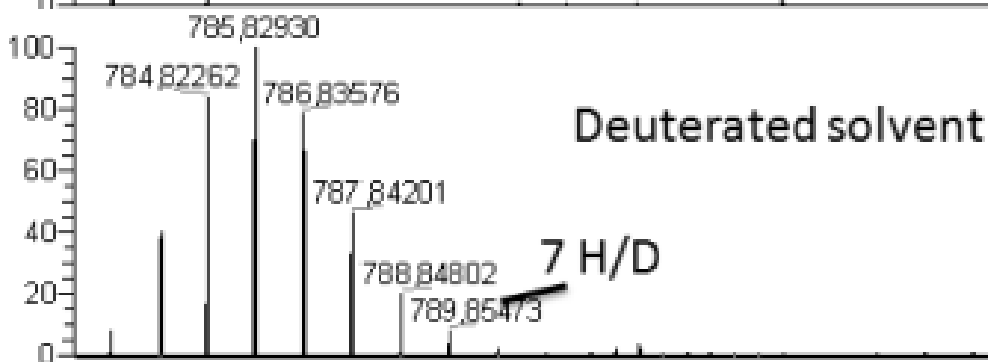
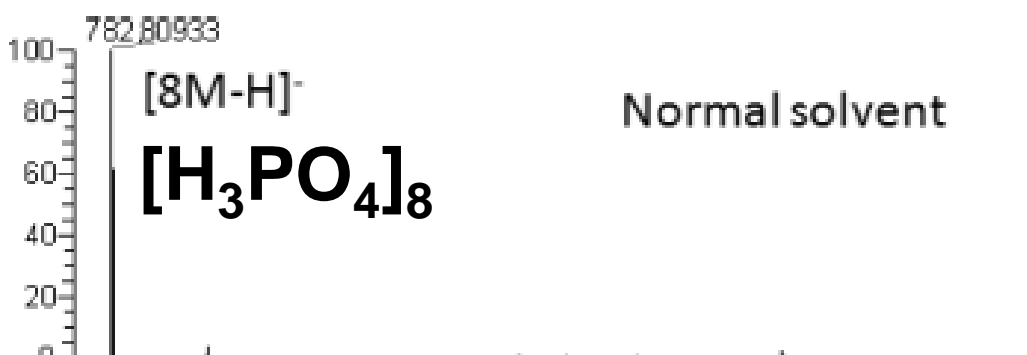
## Capabilities:

- 500k RP in broadband mode (routinely)
- >2M RP in narrowband mode
- typically 0.1-0.4 ppm error

## Research:

- Proteomics, metabolomics including dry blood spot (DBS)
- Isotopic fine structure of unknown compounds (e.g. new antibiotics)
- Petroleum and oils
- Natural organic matter (soil, coal, aquatic, permafrost etc...)
- Isotopic labeling including
  - H/D exchange (solution and in-source)
  - $^{18}\text{O}/^{16}\text{O}$  exchange
  - Selective chemical modification (deuteromethylation, deuteration etc...)





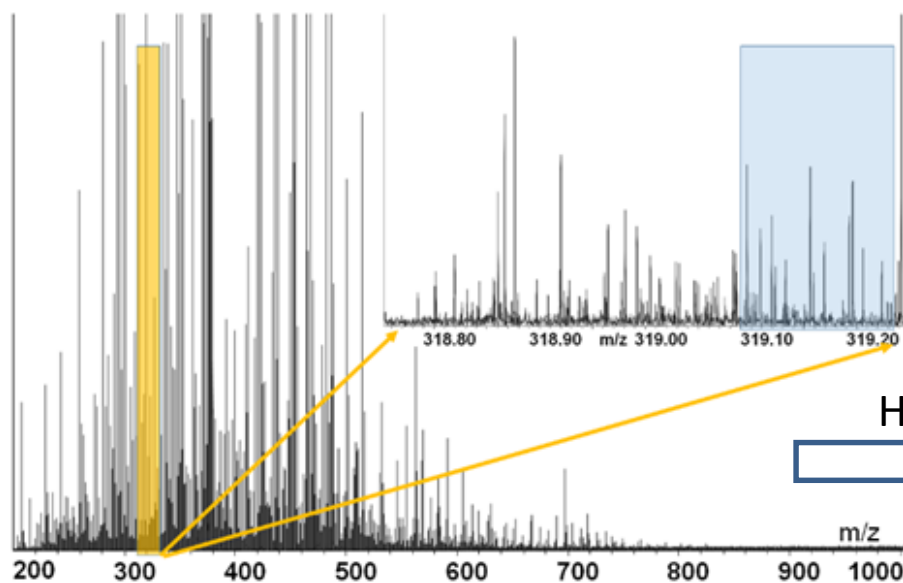
Kostyukevich et al.,  
Anal Chem., 2013



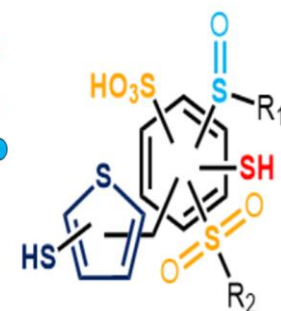
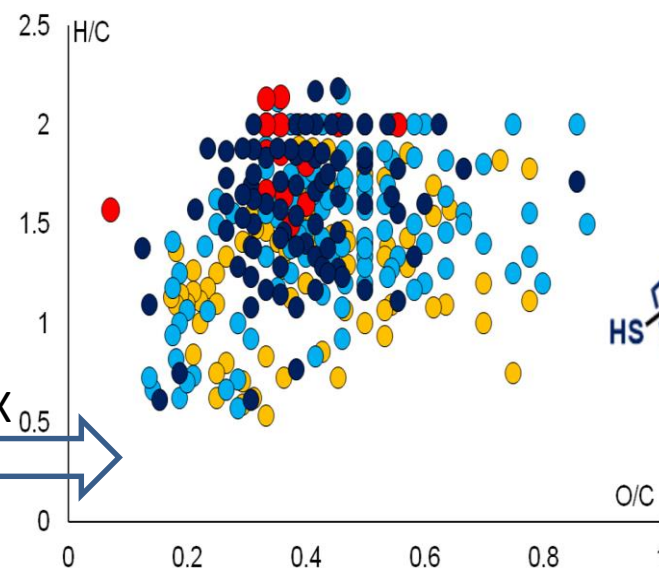
Extraction



Murchison OM



HDX



Speciation of heteroatoms chemistry



### Instruments :

- Bruker Solarix XR FT-ICR 7 T (upgrade from Apex 2018)
- High mass Qtof (Micromass – MSVision modified 2014)

### Specificity :

- Chemical profiling of complex samples
- Top Down and Middle Down protein analysis
- Native mass spectrometry

### Staff :

- Scientific PI : Carlos Cordeiro
- Associated staff : Marta Sousa Silva
- Technician : Ana Marques





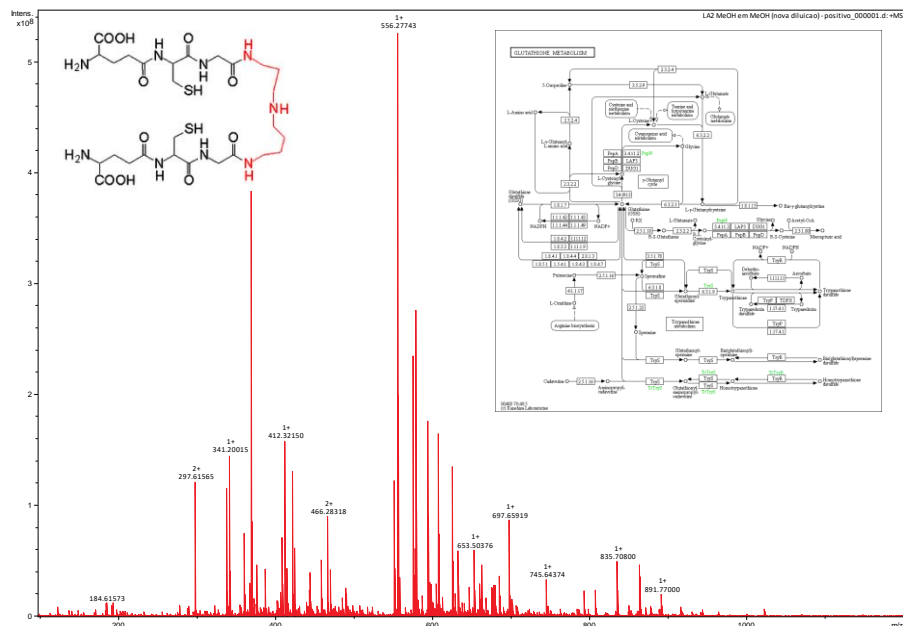
Ciências  
ULisboa

## FT-ICR and Structural Mass Spectrometry Laboratory

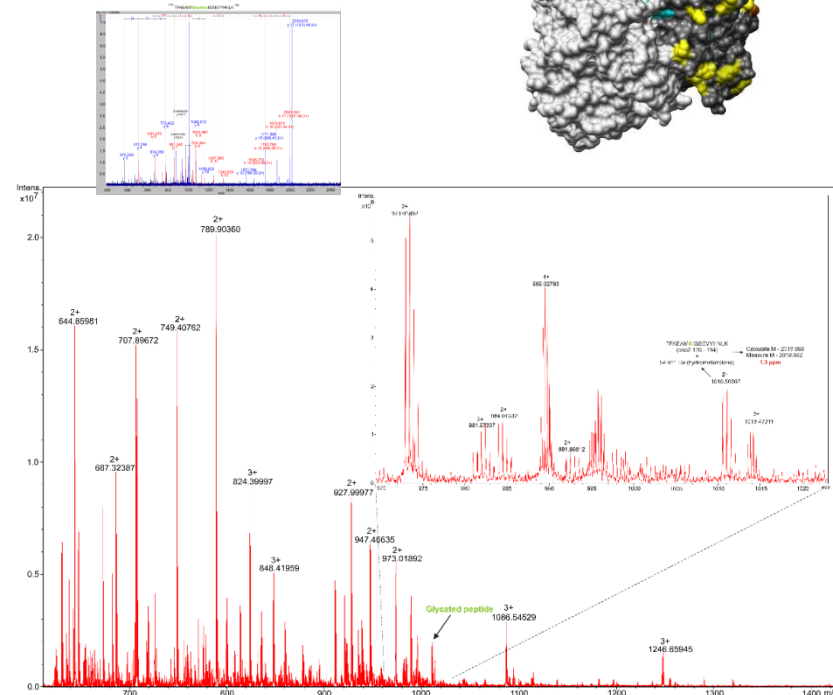


- Sample preparation (protein production, mutagenesis, native MS)
- Forensics (explosives, drugs, fingerprints, other samples...)
- Structural protein characterization (PTMs, native MS, CD)

## Trypanosomatid metabolomics



## Protein glycation







**EU FT-ICR MS**

# **EFTMS 2020**

## **Lisbon**

Grant Agreement (GA) No: 731077  
IMSC, Florence, EU\_FT-ICR\_MS Workshop



# EFTMS 2020 Lisboa





# 14<sup>th</sup> EFTMS

## *Proposed scientific program*

### 14<sup>th</sup> EFTMS Workshop

- **Topics:**

- Fundamentals of FTMS
- FT-ICR-MS
- Orbitrap
- 2D FT-ICR
- Proteomics
- Native MS
- Metabolomics

- **Confirmed speakers:**

- Alan Marshal
- Christian Rolando
- Eugeny Nikolaev
- Peter O'Connor
- Roman Zubarev
- Alexander Makarov
- Jonathan Amster
- Philippe Schmitt-Kopplin





**EU FT-ICR MS**

# How to apply?





**EU\_FT-ICR\_MS**

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



## THE UPPCON2018 MEETING

The Uppcon2018 meeting is being held in Leeds on 16-18 July. It is a tandem mass spectrometry conference focused on advanced tandem mass spectrometry techniques such as ExD and UVPD.

for more informations, please check the website : <https://kuhmassy.wixsite.com/uppcon18/programme>

## DOCUMENTS

### Submission documents

Submission Procedures

 [download](#)

Charter of Access for TransNational Access to the EU\_FT-ICR\_MS Research Infrastructure

 [download](#)

Submission form

 [download](#)

### 01 EU\_FT-ICR\_MS - 1st Short Course - 5-7 March 2018 - Rostock

Rostock\_March2018\_FundamentalsFTICR

 [download](#)





EU\_FT-ICR\_MS

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

## EU\_FTICR\_MS Project submission template

*Text in red italics is an indication of the expected content. This can be deleted from the final form submission. Mandatory sections (1-3) are indicated with a red star. The mandatory section is expected to fit within one page.*

Project PI	
Project Acronym	

### 1. Scientific context of the project\*

*Indicate the scientific context in which this work is to be carried out: What is the general background? What are the main current issues with the project? Why is FT-ICR mass spectrometry needed? If previous experiments were performed by mass spectrometry and show the need for FT-ICR measurement, please include these results in the "5. Previous results" section.*

### 2. Samples and experiments\*

*Describe the experimental methodology to be carried out and the samples that are intended to be used for the experimental session. What are the samples? How many samples? Which experiments will be carried out? Are there specific needs for scientific / technical expertise? How will the data processing be performed (on site / at user's site)? This should justify the requested experimental and processing times. If specific additional equipment is needed, specify here the nature of these equipment and indicate if they are (a) to be provided by the hosting site and listed on the website as "peripheral equipment" or (b) to be provided by the User.*

*Specific sample handling and ethical issues with the samples should be mentioned in section "6. Sample handling" and section "7. Ethical issues".*

### 3. Expected impact of the results\*

*Once the experiments are done, how will they be used in the context of the project described in section 1.*

### 4. References

*Include a list of references either to outside literature or to proposer's work. If needed, a pre-print or submitted manuscript can also be attached to the submission as an additional file, but please mention it in this section.*

### 5. Previous results

*Include previous results if available. If mass spectrometry experiments were already performed on the same samples (or similar ones), please include here all the experimental details (ionization source, solvents, source conditions, chromatographic separation) as well as some (or all) of the data. If previous experiments were obtained in the course of TNA, please include an experimental report of the previous TNA access session here. This section can be included as an additional document in the submission system, but please mention the file name in this section "Data submitted in file XXXXXX submitted with the current proposal."*

### 6. Sample information

*Include all information that can be needed by the site: sample safety issues, sample handling procedure, samples storing and disposal procedures, sample transportation requirements... By default, if not indicated at this stage, the sites will not be able to provide any assistance in handling / storing / disposing of the samples.*

*Also include solvents / chromatography conditions that the site will be expected to provide to the user. If specific consumables are needed, please list them here also and indicate if the user intends to provide them upon his visits.*

*See Charter of Access for TranNational Access Sections 6.f. and 6.g. of the for details concerning samples and consumables and Sections 7.a. and 7.b. for sample safety issues.*

### 7. Ethical issues

*Are there any ethical issues associated with this work (use of animal/human tissues or extracts, ...) as required in Charter of Access for TranNational Access Sections 7.c.*

### 8. Data embargo period and intellectual property

*By default these are set by the Charter of Access for TranNational Access Sections 6.e. (which defaults to an 18 months embargo period) and the consortium Data Management Plan. If a derogatory regime is foreseen please mention here the motivations and changes from the general regime.*

### 9. Possible conflicts of interest

*If a conflict of interest is possible with members of the evaluation panel, please indicate the names of the members you do not want to be evaluated by.*





## Submit project

[Previous section](#)
[Next section](#)

[Previous section](#)
[Next section](#)

## General project information

Please fill each section, click on the 'Next section' button to go to the next page, and validate after 3rd section is filled by clicking the 'Submit' button. All \* fields are required.

**Submission documents:**

- Submission procedures
- Charter of Access for TransNational Access to the EU\_FT-ICR\_MS Research Infrastructure
- Submission form

### Project title

Project acronym (15 char. max.)

**Project abstract (500 char. max.)**

The screenshot shows the top toolbar of the LibreOffice Writer application. The toolbar is organized into several groups of icons. The first group includes icons for undo, redo, and document management (save, print, export). The second group contains icons for text formatting (bold, italic, underline, strikethrough, subscript, superscript, text color, background color). The third group includes icons for text alignment (left, center, right, justified), bulleted list, numbered list, and quote. The fourth group has dropdown menus for 'Styles' and 'Format', and an information icon. The background of the toolbar is light gray with a subtle gradient.



Project abstract (500 char. max.)

Project PI information

Title

Mrs ▼

First name

Middle name or initials

Last name

Gender

Female ▼

Status of the project PI

Permanent staff ▼

E-mail address

Confirm E-mail address