

CAPT Day

Jeudi 24 novembre 2022, 9h00 - Amphi

Le 23 novembre 2022



Voici le programme des présentations de la journée, vous êtes tous les bienvenus dans l'amphithéâtre de l'IPREM et participer à nos discussions.

CAPT Seminar – The program

IPREM : AMPHITHEATRE

Session 1

Chairman: Panos Karamanis

9h00-9h30

Sandra Mounicou & Panos Karamanis

Introduction

9h30-9h50

Luisa Ronga

Mass spectrometry investigation of peptide and protein metalation: recent advances in the field of metallodrugs and heavy metals reactivity

9h50-10h10

Matthieu Wolff

Introduction to SnookRMol, a new python framework for fast probing of molecular reactivity

10h10-10h30

Flash presentations

Falk Richter: *Computational Modelling for tricky molecular IR Spectra*

Camilla Kafino: *Strontium Isotopes Applied as provenance Proxy for Brazilian Woods*

Corine Parat: *Study of the conformational change of an aptamer in the presence of its target, glyphosate*



10h30 - 11h00

Coffee break and posters

Chairman: Germain Salvato Vallverdú

Session 2

11h00-11h20

Laurie Labeyrie

Quantitative bioimaging of selenium and mercury in rainbow trout by LA-ICP MS

11h20-11h40

Mohammed Lemaalem

Microscopic insight in PVDF-based Solid Polymer Electrolyte using MD simulation: From molecular design to promising applications

11h40-12h

Christophe Peycheran

A trip to laser ablation land - From femtoseconds to hundreds of thousands years

12h-12h20

Fanny Claverie & Gaëlle Barbotin

Visite virtuelle de la halle IPREM2

12H30 - 14H00

Lunch and posters

Chairman: Luisa Rongga

Session 3

14H00-14h20

Carlos Celis Cornejo

A python-based framework for mass spectrometry data treatment and time-resolved mass spectrometry applications

14h20-14h40

Estelle Ricard

Development of sensors and biosensors for on-situ measurement of emergent contaminant in water

14h40-15h

Kasia Bierla

Methodological developments for seleno and sulfometabolite speciation in animal tissues

15h-15h20

Flash presentations

Alejandro Gutierrez Quintanilla – *The PACMAN project*

Valentin De Carsalade Du Pont – *Project U-MON*

15H20 - 16H

Coffee break and posters

Session 4

Chairman: Sandra Mounicou

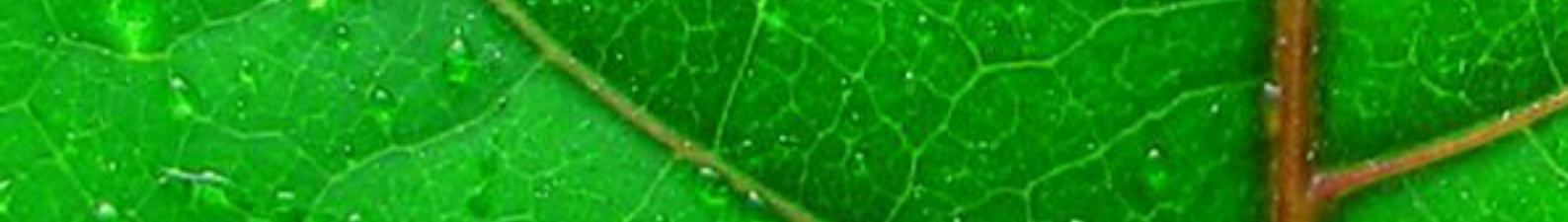
16h-16h20

Florence Pannier

Presentation of the doctoral school SFRI GREEN

16h20-16h40

Chen Zhang & Danilo Hatych



Experimental and Theoretical studies of BN-doped Arenes.

16h40-17h

Maria Angles Subirana

NanoSIMS trace element and isotopic imaging

17h-17h20

Panagiotis Karamanis

Molecules and 2D materials in strong electric fields

17h30

Conclusion

Posters' titles

Alba Rodriguez Otero • *Application of nano-silica particles generated from pyrolyzed rice husk for cadmium elimination from aqueous media.*

Yuping Dai • *Mechanism Insights into Pd(B,N)-Catalyzed Hydroalkylation of 1,3-Enynes with Ketones. A Synergy between Experiments and Theory*

Asmodée Galy • *Ultra-trace isotope imaging by fsLA SF-ICP-MS: a new approach for U-series dating of archaeological biominerals*

Joseph Come • *Analytical developments for metallodrugs monitoring in drinking water resources*

Walid Lamine • *A Syn Outer-Sphere Oxidative Addition: The Reaction Mechanism in Pd/Senphos-Catalyzed Carboboration of 1,3-Enynes*

Mikel Bernabeu De Maria • *Structural insights into the interactions of gold metallodrugs with proteins by mass spectrometry: the case of gold(I) complexes binding Thioredoxin*

Yaidel Toledo González • *Molecular design for catalytic activities of helical chiral oligoureas*

Alex goupil • *Analytical Development in order to understand the mobilisation and absorption of toxic metals by plants*

Carine Arnauguilhem • *Study of the impact of iodinated contrast agents on two aquatic organism (project ACTIONS)*

Antonia Toska • *Quantification post-synthèse par Sp-ICPMS de nanoparticules de magnétite encapsulées dans un nanocomposite hybride coeur-coquille*

Matthieu Boccas • *Couplage d'un LIBS-portable avec un module de récupération des particules induites par ablation laser comme méthode de micro-échantillonnage de terrain : application à l'étude de pigments de cinabre et à la datation de carbonates secondaires par les séries de l'uranium*

Aleksandra Izdebska • *Analytical approaches to study metabolism of different arsenic forms in *Tilia cordata* Mill*