FRONTIERS IN SPECIATION SCIENCES: THE MARSS CENTER: CENTRE OF MASS SPECTOMETRY FOR REACTIVITY AND SPECIATION SCIENCES

Olivier F.X. Donard[1], Sylvain Bérail[1], David Amouroux[1], E. Tessier[1], Christophe Pécheyran[1], Fanny Claverie[1], Ian Bowen[2], Joanna Szpunar[1], Kashia Bierla[1], Dirk Schaumlöffel[1], Julien Malherbes[1], François Horreard[3], Hervé Martinez[1], Cécile Courrèges[1]

1:Institut des Sciences Analytique et de Physicochimie pour l'Environnement et les Matériaux
MARSS : Center of Mass Spectrometry for reactivity and Speciation Sciences
Université de Pau et des Pays de l'Adour
UMR CNRS 5254
Hélioparc
Pau 64053 (France)

2 : Nu Instruments
Clywedog Rd S, Wrexham LL13 9XS (United Kingdom)

3 : CAMECA
29 Quai des Grésillons
92622 Gennevilliers (France)

Scientific research during the last 20 years has shown that not only simple information on the metals, e.g. their total concentrations in a sample, but rather knowledge on chemical forms of metals and metalloids - their species - is an important issue in order to evaluate their reactivity, transport in the environment or their essentiality and toxicity in organisms. Hyphenated technics using separation techniques to ICP/MS have allowed to promote important knowledge in this domain. However, it is important now to open up further opportunities in this domains to improve our understanding of metals species at environmental traces levels but developing new concepts in sample preparation, detection and integration of detection opportunities by promoting new development in detection in instrumentation.

The originality of this unique platform is to integrate speciation concepts from the isotopic level to 3D imaging in environmental, life, material and industrial applications. The different mass spectrometers of the platform are completely complementary within the concept of advanced speciation analysis: a HR MC ICP-MS serves for high resolution and high sensitive elemental and isotopic measurements and in hyphenation with separation techniques to advanced elemental speciation. Superior molecular identification and structural characterization is assured by a unique Orbitraps FT MS featuring up to 1 000 000 resolution in mass providing unmatched high mass resolution. A NanoSIMS contributes elemental and isotopic imaging at the nanometer scale (50 nm) which is indispensable within this concept for a localization of element species in biological cells or on small surfaces. ToF-SIMS gives elemental and molecular chemical information of the two first layers of atoms and molecules at surfaces with a high sensitivity (ppm/femtomoles), high mass resolution (up to $m/\Delta m$>10 000u) and high spatial resolution (<100nm) for 2D and 3D imaging. Further, this platform is the results of continues new instrumentation development in close collaboration with the instrument manufacturers and other research groups allowing to promote new analytical and detection strategies.

This platform will deliver integrated information between the different instruments. At first, a common effort will be promoted with ultimate quantification and characterization of metals species in environmental matrices. Combining speciation and isotopic signal at the ultra-traces level (ppt) allows to foresee new opportunities to unravel the behavior and fate of metals in all compartment of the environment. Further, the outstanding capabilities in terms of resolution, mass accuracy and sensitivity of the acquired platform will to open new frontiers in elemental speciation

analysis allowing acquisition of molecule-specific information on virtually all species of an element present in biological matrices at different concentration levels. This provides new opportunity for studies in an emerging field of metallomics defined as comprehensive analysis of the entirety of metal and metalloid species (metallome) within a cell or tissue type. Once the new species have been identified it is essential to be locate it at the µ to nano- scale level in 2 or 3 dimensions. Femtosecond laser ablation technologies (3 wavelengths) hyphenated to high sensitivity high resolution multicollector ICP/MS will allow a first level approaches to isotopic imaging at subµm level. 2 D to 3D imaging will be further available with the development of RF plasma oxygen primary ion source for NanoSIMS allowing to address for the first time high resolution and high sensitive elemental and isotopic mapping of medium mass elements such as Ca, Cu, Fe, Se,… at a few tens nanometer spatial resolution. Complementary 2 D and 3 D approaches will be available with a new TOF SIMS featuring also an in-situ Focused Ion Beam, allowing to perform FIB-TOF 3D tomography of materials. . All these instruments are and will be located under clean room conditions under the same building allowing them to be used together to open up and solve key questions in biogeochemistry and life sciences.

The MARSS project is to install a unique Mass Spectrometry Center for Reactivity and Speciation Sciences together with IPREM institute with a top-level (by world standards) instrumental platform of four different high-end mass spectrometers for advanced speciation analysis. This center will be open to research groups. The scientific aims are advancing the frontiers of speciation analysis to: (i) understanding of the role of elements, esp. metals and metalloids, related to their chemical identity or isotopic signature, (ii) understanding of their primary reactivity associated with the chemical identity and transformation kinetics, (iii) identification of chemical species of interest in their surrounding matrices, on surfaces or interfaces leading to their localization by imaging and mapping in 2 or 3 dimensions. There will be five main activities developed on the platform which make it unique: (i) novel speciation research pathways, (ii) new instrumentation developments with the manufacturer's partners of the platform, (iii) academic access to national and international and (iv) an international teaching and training center. The MARSS center is to be opened to other research groups at the national and international level with the aim of being integrated to the national CNRS network and European Research Infrastructure of the ESFRI program.