



## OFFRE D'ALLOCATION DE THESE / PhD GRANT

ÉCOLE DOCTORALE SCIENCES EXACTES ET LEURS  
APPLICATIONS - ED 211 / NATURAL SCIENCES DOCTORAL SCHOOL  
Avenue de l'université BP 1155 64 013 PAU Cedex – France

### SUJET DE THESE / PhD SUBJECT

**TITRE:** Impact environnemental non ciblé, évaluation du risque et analyse rétrospective : Application à la qualité des eaux, avec approche génotoxique, mobilité ionique et spectrométrie de masse à haute résolution.

**Project TITLE:** Synergic Experience Theory approaches for the quantitative Assessment of the Structure & Activity Relationship. "SET-ASAR".

**ABSTRACT:**

The global project "SET-ASAR" is led by Dr. Hugues Preud'homme (HDR, LPI) in close relationship with Professor Anna Chrostowska (PI, UPPA), Assistant Professor Clovis Darrigan (UPPA), Assistant Professor Vù Thien Y (TDT University, Ho Chi Minh) and Professor Shih-Yuan Liu (PI, from Boston College, USA), laureate of the International Guest Chair at E2S UPPA and Boron Chemistry Award in 2018.

The first objective will be first of all to summarize the state of the art in analytical chemistry characterization of water. Then we will raise a new synergic approach by merging the multidimensional characterization with High Resolution Trapped Ion Mobility - Mass Spectrometry, collision cross section calculation (CCS), the modelling and the genotoxicity of emerging pollutants and their relatives' byproducts or metabolites in water. We will work closely with academic and industrial partners in Pau Area, Bordeaux, Nantes, Boston, European Network (NORMAN) and Mediterranean Sea with the objective to perform a 2D Non-Target Screening (NTS). We will generate too and work on a global database for a better comprehensive fingerprint of the water quality. We are expecting at the end to be able to propose an Enhanced NTS approach for monitoring and environmental laboratories, with the benefit of Retrospective *In Silico* Analysis for a better risk management.

The GC/UPLC2D-timsTOF (end commissioning in middle 2018) is almost unique in such configuration in Europe. Moreover we will have the opportunity to work on homemade azoborane hybrid compounds for the development of CCS measurement, calculation and modelling.

**Mots clés (Keywords):** Ion Mobility, High Resolution Mass Spectrometry, Non-Target Screening, Chromatography, Genotoxicity, Theoretical calculation, Water quality, Emerging contaminants.

### CONDITIONS D'EXERCICE / WORKING CONDITIONS

**Laboratoires :**

- Institut des Sciences Analytiques et de Physicochimie pour l'Environnement et les Matériaux IPREM - UMR CNRS 5254 ; <http://iprem.univ-pau.fr/live/>
- LaboPL, Atoxigen, Boston College (Boston, USA), TDT University (HCM, Vietnam)

**Directeur de thèse (PhD Director):** Dr. Hugues Preud'homme

**Co-Directeur de thèse (PhD co-Director):** Assistant Prof. Vu Thien Y (TDT University, Ho Chi Minh)

**Lieu (Place) :** IPREM – Pau, France (a few month abroad would be required (Boston, HCM & Bordeaux))

**Date début (start):** October 2019

**Durée (duration):** 3 ans (years)

**Employeur (employer):** Université de Pau et des Pays de l'Adour (UPPA)

**Salaire mensuel brut (monthly salary before taxes):** 1768 €

## SAVOIR-FAIRE DU LABORATOIRE / HOST LABORATORY PROFILE

- The Institute of Analytical Sciences and Physical Chemistry for the Environment and Materials **IPREM** - UMR CNRS 5254 is the concretization of a synergy and a history around research in environment and materials. Its competencies revolve around fundamental disciplines using analytical chemistry, physical chemistry, theoretical chemistry, physics and chemistry of polymers and microbiology. A coupled experience-theory approach guide research within IPREM with in particular comprehension of chemical reactivity, understanding of reaction mechanisms, determination of electronic and opto-electronic properties, chemical-physical and theoretical chemistry.

- Dr. Hugues Preud'homme (HDR) is expert in High Resolution Mass Spectrometry and was leading the granted project Aquitraces (890k€ HT, 2013-2018) for challenging new frontiers in analytical sciences within IPREM-UMR5254 Institute. He is (Research) CNRS Engineer since 2004. Hugues Preud'homme was also a former senior scientist (2014-2016), head of core facilities and team Lead in QEERI (Qatar Foundation, HBK University, Doha – Qatar). He was and he is an international expert in analytical chemistry and environmental sciences for government institution and industry. He is also author of 4 international patents.

## MISSION - ACTIVITES PRINCIPALES / MISSION – PRINCIPAL ACTIVITIES

### **I. Le contexte scientifique / *Scientific Context***

The major challenge of the 21<sup>st</sup> century will inevitably be related to our ability to provide an efficient and cost-effective complete fingerprint of our environment and water in order to address the future challenge of preservation, treatment, reuse, accessibility and water quality. Standards are most of the time, just dealing with hundred contaminants without considering the 80,000 existing chemicals which would be even more if we have to consider their byproducts and metabolites (> 1,000,000 traces to monitor). Up today, there is any universal technique which will be able to describe and to provide a global fingerprint of water. The recent development of trapped ion mobility working in synergy with high resolution mass spectrometry give us for the first time the skill to characterize in real time conformers (different structure with same exact mass) and also to be able to proceed to in silico retrospective analysis. Here we are in the edge of a new area where we will be able to generate Non-Target Screening Big Data for a more comprehensive water quality description and moreover with an enhanced risk management on long term.

The hot topic and last update research related to water are mainly focused on a few sets of microplastic, organic molecules, or on heteroelements containing contaminants. But there is any synergic approach which is mixing high end resolution mass spectrometry and ion mobility. Our objective here, « having a nonspecific monitoring » is almost unique.

The Challenge is real and it is offering a tremendous field of opportunities and new frontiers to discover.

Thus, this project is in line with our (internal and external) expertise and with our high-end analytical facilities as showed before.

### **II. Les objectifs / *Objectives***

The goal of this proposal is to explore a new approach for water quality non-targeted and high resolution fingerprint. A comprehensive understanding of molecular structure – property relationships in parallel of genotoxicity studies will held for creating unique database for a better and more comprehensive risk management and environmental monitoring.

### **III. Plan de travail / *Work plan***

After a short state of the art of water contaminants characterization; first sampling and high-resolution targeted analysis and broadband CID HRMSMS would start shortly (first 6 months). First NTS and Tims (ion

mobility) analysis (by GC and UHPLC2D) will be done under the supervision of Hugues Preud'homme by end of the first year. Enhancement and automation of extraction, sample preparation and concentration with diverse approach with help of dispersive solid phase, functionalized nanomaterials and MEPS would be evaluated, optimized to reach a ppt sensitivity level (LOD) as an objective for water analysis (included in NTS).

In parallel, DFT calculations will be obtained using Gaussian software and CCS by Collidoscope. The analysis will yield key information on structures, conformation and exact mass on new/emerging contaminants, their relative metabolites, their fate and transport, and with particular interest on planar aromatic compounds (included the BN containing).

At the University of Pau, research will be supervised by Dr. Hugues Preud'homme (HDR) during his stay at IPREM, and under the joint direction of Ass. Prof. Vu Thien Y / Clovis Darrigan.

#### IV. Références bibliographiques (*Literature References*)

- [1] Schymanski, E.L., Singer, H.P., Slobodnik, J., Ipolyi, I.M., Oswald, P., Krauss, M., Schulze, T., Haglund, P., Letzel, T., Grosse, S., Thomaidis, N.S., Bletsou, A., Zwiener, C., Ibáñez, M., Portolés, T., De Boer, R., Reid, M.J., Onghena, M., Kunkel, U., Schulz, W., Guillon, A., Noyon, N., Leroy, G., Bados, P., Bogialli, S., Stipanich, D., Rostkowski, P., Hollender, J.; Non-target screening with high-resolution mass spectrometry: Critical review using a collaborative trial on water analysis (2015) *Analytical and Bioanalytical Chemistry*, 407 (21), pp. 6237-6255.
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- [3] Park, M.A.; TimsTOF MS for Life Science Problem Solving: A New High-Performance, Yet Flexible, Method for Life Science Applications (2016) *Genetic Engineering and Biotechnology News*, 36 (19), .
- [4] Brumovský, M., Bečanová, J., Kohoutek, J., Borghini, M., Nizzetto, L. Contaminants of emerging concern in the open sea waters of the Western Mediterranean (2017) *Environmental Pollution*, 229, pp. 976-983.
- [5] Llorca, M., Farré, M., Eljarrat, E., Díaz-Cruz, S., Rodríguez-Mozaz, S., Wunderlin, D., Barcelo, D. Review of emerging contaminants in aquatic biota from Latin America: 2002–2016 (2017) *Environmental Toxicology and Chemistry*, 36 (7), pp. 1716-1727.
- [6] Stephan, S., Hippler, J., Köhler, T., Deeb, A.A., Schmidt, T.C., Schmitz, O.J.; Contaminant screening of wastewater with HPLC-IM-qTOF-MS and LC+LC-IM-qTOF-MS using a CCS database (2016) *Analytical and Bioanalytical Chemistry*, 408 (24), pp. 6545-6555.
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- [10] Bijlsma, L., Bade, R., Celma, A., Mullin, L., Cleland, G., Stead, S., Hernandez, F., Sancho, J.V.; Prediction of Collision Cross-Section Values for Small Molecules: Application to Pesticide Residue Analysis (2017) *Analytical Chemistry*, 89 (12), pp. 6583-6589.
- [11] Zühlke, M., Riebe, D., Beitz, T., Löhmannsröben, H.-G., Andreotti, S., Reinert, K., Zenichowski, K., Diener, M.; High-performance liquid chromatography with electrospray ionization ion mobility spectrometry: Characterization, data management, and applications (2016) *Journal of Separation Science*, 39 (24), pp. 4756-4764.
- [12] Vautz, W., Hariharan, C., Weigend, M.; Smell the change: On the potential of gas-chromatographic ion mobility spectrometry in ecosystem monitoring (2018) *Ecology and Evolution*, 8 (9), pp. 4370-4377.

## COMPÉTENCES REQUISES / REQUIRED COMPETENCES

The skills required for such a subject are necessarily multiple. A sound knowledge and background in chemistry, water chemistry, sample preparation, chromatography, data mining and mass spectrometry is required. Thus, competencies in use of experimental techniques for are essential (UHPLC, GC, HRMS, Ion Mobility & ICPMS...) and knowledge in theoretical chemistry calculation (Gaussian) and Genotoxicity would be considered as a key additional skill. Her/his ability to work in a team, in an interdisciplinary scientific context, and in an international and collaborative environment will be appreciated. Good English will be necessary to follow efficiently this project.

## CRITÈRES D'ÉVALUATION DE LA CANDIDATURE / CRITERIA USED TO SELECT CANDIDATE

Processus de sélection (Selection process steps):

- Constitution d'un Jury de sélection. (Establishment of the selection committee.)
- Sélection des candidats sur dossier de candidature. (evaluation of the applicants cv's)
- Audition des candidats et classement. (Interview with the selected candidates and ranking.)

Critères d'évaluation de la candidature (Criteria used in selection of the candidate):

- La motivation, la maturité scientifique et la curiosité du candidat. (The candidate's motivation, scientific maturity and curiosity.)
- Ses connaissances en chimie analytique et chimie-physique. (candidate's knowledge in analytical and physical chemistry.)
- Ses notes et son classement en M1 et en M2. (candidate's marks and rankings in M1 and M2.)
- Maîtrise de l'anglais. (English proficiency)

## CONSTITUTION DU DOSSIER DE CANDIDATURE / REQUIRED DOSSIER,

Envoyer par email un dossier de candidature comprenant (send an e-mail with your candidature containing):

- CV (CV)
- lettre de motivation (cover letter detailing candidate's motivations)
- relevé de notes et classements en Master (candidate's MSc marks and ranking)
- lettres de recommandation (any letters of recommendation)
- coordonnées de personnes du milieu professionnel (minimum two) à contacter (contact details for 2 referees)

**DATE LIMITE DE DEPOT DU DOSSIER (limiting date):**

**September 6th, 2019**

## CONTACTS

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