



## 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

## PhD SUBJECT

**TITLE: Untargeted dissolved organic matter analysis by FT ICR MS and ICP MS hyphenated to LC techniques**

### **ABSTRACT:**

Dissolved organic matter (DOM) is a major organic component of natural waters coming from the partial decomposition of, or exudation from, living organisms, including microorganisms, plants and animals. Its composition is highly variable, although a general consensus is to consider DOM as a mixture of a small proportion of low-molecular weight compounds, such as carbohydrate and amino acids, and a larger proportion of higher-molecular weight compounds called humic substances. These organic compounds are also known to bind inorganic compounds, forming a complex matrix not fully understood. DOM plays important roles in the functioning of aquatic ecosystems through its acid buffering capacity, light absorbance, and/or binding of metals [1,2]. The current global changes impact the concentration and quality of DOM, which in turn, is expected to affect metal speciation [3].

The present PhD project will be part of larger projects initiated at IPREM with the research partnership chairs e2s-UPPA-Total held by Dr. Rodgers and e2s-UPPA-Total-Rio Tinto held by Dr. Le Faucheur. These chairs address the challenge of elucidating how the current global climate changes affect the DOM concentration/composition of rivers and how that modification impacts metal speciation in natural waters. Such an understanding will be achieved through the development of better analytical methods for molecular characterization. Thus, the objective of this PhD is to use inorganic mass spectrometry (ICP MS) and molecular mass spectrometry (FT-ICR MS) for advanced characterization of DOM, similar to existing methods used in petroleomic studies. ICP MS will be a useful technique for the mass balance study of the sample preparation / preconcentration step and subsequent liquid chromatography hyphenated to both inorganic- and molecular-MS can be used for “molecular fingerprints” of all samples. Ultimately, the untargeted analysis will be applied to the characterization of natural river waters sampled under different environmental conditions (site and seasonal variations).

This PhD will be mainly focused on the analytical method development and implementation. Thus, a student with a Master in analytical chemistry (with a solid background in mass spectrometry) will be welcome. Environmental chemistry experience will be also a good additional knowledge. English is mandatory.

The student will take place in different locations, UPPA (IPREM - France), TOTAL (PERL Lab, experimental rivers - France), Florida State University (USA) and at the different iC2MC Lab facilities.

[1] Wetzel, R.G. (2001) Limnology – Lake and river ecosystems, Academic Press

[2] Aiken G.R., Hsu-Kim H. and Ryan J.N. Influence of dissolved organic matter on the environmental fate of metals, nanoparticles, and colloids. *Environmental Science and Technology* (2011) 45: 3196-3201

[3] Lipczynska-Kochany E. Effect of climate change on humic substances and associated impacts on the quality of surface water and groundwater: a review. *Science of the Total Environment* (2018) 640-641:1548-1565

**Mots clés (Keywords):** DOM, FT ICR MS, ICP MS, Speciation

## WORKING CONDITIONS

Laboratoire : IPREM (UPPA) / NHMF Lab (FSU) / PERL (TOTAL Lacq) (iC2MC Lab facilities)

Site web : <https://iprem.univ-pau.fr/fr/index.html>

<https://c2mclab.wordpress.com/>

PhD Director: Ryan RODGERS

PhD co-Director: Brice BOUYSSIERE

In Collaboration with Séverine Le Faucher

Place: IPREM (Pau, France), NHMF Lab (FSU, Floride, US), PERL (Lacq, France)

start: 10/2020

Duration: 3 years

Employer: Université de Pau et des Pays de l'Adour (UPPA)

Monthly salary before taxes: 1878 €

## HOST LABORATORY PROFILE

C2MC is a joint laboratory created in 2014 on the basis of two analytical groups from the universities of Pau and Rouen and a part of the analytical department from the research direction of TOTAL Refining and Chemical.

The addition of skills and synergies arising from these three groups is already generating a creative ambiance in cutting-edge research into the molecular characterization of complex matrices such as petroleum and polymers.

In 2019 C2MC is becoming international with the participation of the analytical group of Ryan Rodgers (Maglab, Tallahassee). As a consequence, the new name of the joint lab is iC2MC.

## MISSION - ACTIVITÉS PRINCIPALES / MISSION – PRINCIPAL ACTIVITIES

### I. Scientific Context

Dissolved organic matter (DOM) is a major organic component of natural waters coming from the partial decomposition of, or exudation from, living organisms, including microorganisms, plants and animals. Its composition is highly variable, although a general consensus is to consider DOM as a mixture of a small proportion of low-molecular weight compounds, such as carbohydrate and amino acids, and a larger proportion of higher-molecular weight compounds called humic substances. These organic compounds are also known to bind inorganic compounds, forming a complex matrix not fully understood yet. DOM plays important roles in the functioning of aquatic ecosystems through its acid buffering capacity, light absorbance, and/or binding of metals [1,2]. The current global changes impact the concentration and quality of DOM, which in turn, is expected to affect metal speciation [3].

### II. Objectives

The objective of this PhD is to use inorganic mass spectrometry (ICP MS) and molecular mass spectrometry (FT-ICR MS) for advanced characterization of DOM, similar to existing methods used in petroleomic studies. ICP MS will be a useful technique for the mass balance study of the sample preparation / preconcentration step and subsequent liquid chromatography hyphenated to both inorganic- and molecular-MS can be used for “molecular fingerprints” of all

samples. Ultimately, the untargeted analysis will be applied to the characterization of natural river waters sampled under different environmental conditions (site and seasonal variations).

This PhD will be mainly focused on the analytical method development and implementation. Thus, a student with a Master in analytical chemistry (with a solid background in mass spectrometry) will be welcome. Environmental chemistry experience will be also a good additional knowledge. English is mandatory.

### III. Work plan

The work plan will be done depending of the PhD candidate background but it can be divided in 4 parts:

- Bibliography revue (mainly focused on DOM analysis/ sample prep and the link of between metals and DOM).
- Comparison of DOM preconcentration methods
- Implementation of FT ICR MS and ICP MS
- Real Sample analysis

### IV. Literature References

[1] Wetzel, R.G. (2001) *Limnology – Lake and river ecosystems*, Academic Press

[2] Aiken G.R., Hsu-Kim H. and Ryan J.N. Influence of dissolved organic matter on the environmental fate of metals, nanoparticles, and colloids. *Environmental Science and Technology* (2011) 45: 3196-3201

[3] Lipczynska-Kochany E. Effect of climate change on humic substances and associated impacts on the quality of surface water and groundwater: a review. *Science of the Total Environment* (2018) 640-641:1548-1565

## COMPÉTENCES REQUISES / REQUIRED COMPETENCES

This PhD will be mainly focused on the analytical method development and implementation. Thus, a student with a Master in analytical chemistry (with a solid background in mass spectrometry) will be welcome. Environmental chemistry experience will be also a good additional knowledge. English is mandatory.

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

Selection process steps:

- Establishment of the selection committee.
- Evaluation of the applicants CV's
- Interview with the selected candidates and ranking.

Criteria used in selection of the candidate:

- The candidate's motivation, scientific maturity and curiosity.
- Candidate's marks and rankings in M1 and M2.
- English proficiency

## CONSTITUTION DU DOSSIER DE CANDIDATURE / REQUIRED DOSSIER,

Send an e-mail with your candidature containing:

- CV
- Cover letter detailing candidate's motivations

- Copy of the diploma
- Candidate's MSc or equivalent: marks and ranking
- Any letters of recommendation)
- Contact details for 2 referees

**Limiting date : 15/06/2020**

**CONTACTS** e-mail : [brice.bouysiere@univ-pau.fr](mailto:brice.bouysiere@univ-pau.fr)