

A 12 months' position for a project in structural elucidation is available at LABERCA (Oniris, France) in close cooperation with CEISAM (Nantes University, France). The project will be starting before July 2017.

Proposal title: *Overcoming the challenge of biomarkers structural elucidation*

Acronym: MARKER-ID

Abstract

Food safety has become a major issue worldwide and in particular, detecting the presence of toxins, contaminants or residues of chemical substances constitutes a strong consumers demand. Generally, all these substances and corresponding metabolites of interest are analyzed using efficient targeted methodologies. However, in some cases these targeted approaches do not allow the detection of either those substances or emerging compounds/practices and therefore new approaches and strategies are demanded. Thereby the study of physiological perturbations induced upon exposure to a given chemical substance has emerged as an interesting alternative approach to be applied in chemical food safety. Metabolomics in particular has a growing role in food science and successful applications for food safety purposes are already available. Efficient analytical workflows have thus been developed and implemented to establish descriptive and/or predictive models of food contaminations. If the whole workflow is now well mastered, the only remaining **bottle-neck lies in the structural elucidation of the chemical signals highlighted as candidate biomarkers**. The **identification of metabolites** is however essential to convert analytical data into meaningful biological knowledge, and further validate markers relevance. Such an issue is shared by the whole metabolomics scientific community who recently again reported that confident and unequivocal structure identification requires significant effort and concluded that the most successful strategy is the combination of mass spectrometry (MS) with nuclear magnetic resonance spectroscopy (NMR), to provide additional and complementary information for the identification of metabolites.

Based on previous research works conducted over the last past years, a robust metabolomics model has been achieved to screen for the administration of forbidden growth factors in livestock. Although the model has been validated and is currently under accreditation process, enabling its application in the French national monitoring plans ensuring thus consumers with safe food, it relies on the "blind" monitoring of a number of chemical signals, only characterized with an exact mass and a chromatographic retention time (LC-HRMS technology). Up to now, any attempts to elucidate these markers, using mass spectrometric (MS) strategies only, have failed.

The present project aims at elucidating biomarkers chemical structure by combining the power of MS and NMR, together with advanced fractionation techniques to provide purified and concentrated extracts.

Coordination /Supervision :

Gaud DERVILLY-PINEL ,Dr, HDR (LABERCA)

Gérald REMAUD, Prof (CEISAM)

Qualifications

We are looking for a highly motivated scientist with a PhD degree. The candidate should have experience in structural elucidation.

- Strong chemical background with a PhD in Chemistry, Analytical Chemistry or equivalent
- Strong hands on experience with:
 - Purification and fractionation techniques
 - Structural elucidation using mass spectrometry (tandem and/or high resolution MS) and/or NMR

- Good laboratory skills
- Good collaboration and communication skills (written and oral English)
- Structured and analytical working approach

Salary

The period of employment is 1 year, 2 200 euros net/month.

Further information

For further information please contact the project coordinator, Dr Gaud Dervilly-Pinel (gaud.dervilly@oniris-nantes.fr)

Application

Please submit your application no later than **10th April 2017**.

Applications must be submitted as **one pdf file** containing all materials to be given consideration. The file must include:

- A letter motivating the application (cover letter)
- Curriculum vitae
- 1 or 2 letters of support
- PhD diploma

Candidates may apply prior to obtaining their PhD level, but cannot begin before having received it.

You can read more about LABERCA and CEISAM on www.laberca.org and www.sciences.univ-nantes.fr/CEISAM/

LABERCA's general domain of activity is the chemical food safety, in a global risk assessment perspective: generation and interpretation of exposure and body burden data, study of the transfer and metabolism of investigated chemicals from their sources to the consumers through the food chain. From an analytical point of view, the two main areas of competence of the laboratory are the treatment of complex biological samples for isolating the studied substances present at (ultra-trace)- level, and the hyphenated measurement of these compounds by various mass spectrometric coupling techniques. Besides these targeted approaches, the laboratory has been developing over the last 10 years an expertise in untargeted approaches (metabolomics) to reveal biomarkers of chemical exposure. The analytical platform is considered as one of the most complete at the national and European level (> 15 last generation MS instruments). All these activities (assays and research) are conducted under management quality system combining accreditation (ISO17025) and certification (ISO9001:2008).

CEISAM has a 30-year expertise in the development of NMR methods for applications to analytical chemistry. In particular, the EBSI group has developed innovative approaches in fast 2D NMR for the targeted and untargeted metabolomics of biological samples. EBSI is an internationally recognized leader in its main fields of expertise, ie. NMR isotopomics and ultrafast 2D NMR. The novel NMR methods developed at CEISAM have paved the way towards original applications of quantitative NMR in the fields of metabolism and environment. CEISAM is equipped with a state-of-the art NMR platform (6 spectrometers, including a 700 MHz high-field spectrometer equipped with a cryoprobe and a sample changer dedicated to metabolomics).

LABERCA and CEISAM are highly complementary, since each of these two laboratories is a recognized specialist in a specific technique (MS and NMR, respectively). Both of them are driven by the same leitmotiv of applying their analytical developments to solve applicative issues on samples of metabolomics interest. Their complementary expertise is indispensable to the success of the present project, which is a great opportunity to develop joint efforts in the fields of biomarkers elucidation. Both laboratories are founding members of the CORSAIRE platform (Bretagne-Pays de Loire métabolomique platform) and are members of its steering committee.