

## Concours de l'Ecole Doctorale de Chimie de Lyon - 2023

### Two-dimensional LC x SFC-HRMS for the characterization of lignin depolymerization

*Chromatographie bidimensionnelle impliquant la chromatographie liquide et la chromatographie en fluide supercritique pour la caractérisation de la dépolymérisation de la lignine*

#### Context

The depolymerization of lignin provides a source of oligomers enriched in OH (phenolic) functions which can be used for the formulation of biosourced polyhydroxyurethane polymers. The catalysis conditions of this depolymerization lead to extremely complex mixtures of monomers and oligomers which should be operated finely for any chemical functionalization. Characterization of such a complex sample is an analytical challenge that can be transposed to any biowaste used as petroleum alternative (algae, coffee ground, agriwaste). Comprehensive two-dimensional chromatography provides such a large peak capacity that it is foreseen as the most efficient separative tool for the analysis of complex samples, especially when coupled to mass spectrometry detection.

While the lignin monomers can be characterized by GC x GC-MS, the most common technique for the separation of oligomers via 2DLC relies on the combination of GPC and RPLC. But the orthogonality is limited in this combination because the hydrophobicity of the oligomer is related to its size, leading to correlated 2D information. Neutral molecules, such as the oligomers we concentrate on, are quite difficult to separate in conventional LC x LC. Supercritical fluid chromatography (SFC) is a separation technique using a non-polar CO<sub>2</sub> - based mobile phase. Comprehensive mode separation involving a combination of LC and SFC appears promising [Burlet-Parendel, Trends in Analytical Chemistry 144 (2021) 116422]. This two-dimensional approach describes a large separation space that increases peak capacity and allows the creation of a sample map represented as a 2D plot. The combination of LC and SFC is currently the main axis of research of the chromatography team of the Institute of Analytical Sciences and will therefore be the main axis of development in this project.

The PhD fellow will be in charge of the optimization of the LC x SFC method, its coupling with mass spectrometry and the comparison of performances with an RPLC x RPLC approach. It will also be necessary to develop the methods of multidimensional data processing (commercial or custom software) and their use, in order to lead to relevant comparisons with the other methods. Developing classification of the relevant information to improve identification will be part of the project, with strategies such as molecular networks.

#### Key tasks

- Development of chromatographic methods for untargeted analysis
- Multidimensional data processing, molecular networks
- Propose, when necessary, instrumental developments
- Present the research work through the publication of scientific and communication articles at national and international congresses.

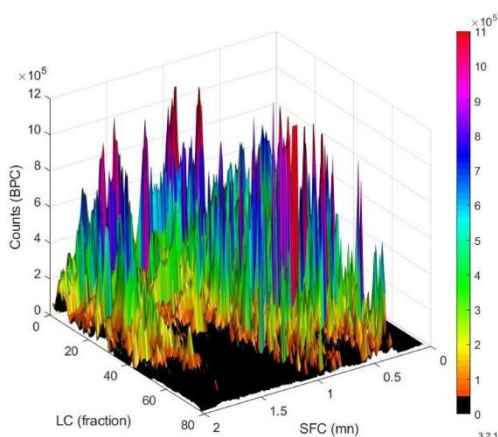
### Candidate profile

The candidate must:

- have a first experience in LC-MS
- know how to communicate orally and in writing in scientific English,
- demonstrate autonomy and be proactive
- have good working skills in a collaboration (contributions to a collective project, meetings and missions outside the laboratory)

The Institute of Analytical Sciences (ISA) is a laboratory dedicated to the development of new analytical techniques applied to complex mixtures. The team "Chromatography and Hyphenated Techniques" has a strong expertise on the optimization of chromatographic methods and has been working for several years on LCxLC for fundamental understanding and for different application areas in collaboration with different industrial partners.

By joining the Chromatography and Coupled Techniques team, the PhD student will have access to a state-of-the-art instrumental platform, including two-dimensional liquid chromatography instruments from various manufacturers, supercritical fluid chromatography, ion mobility and high resolution mass spectrometry instruments (QToF).



### Deadlines

Contact thesis director before 1<sup>st</sup> May 2023, with cover letter, CV and academic record.

Application to Ecole Doctorale Chimie Lyon

Selection on academic record

Audition: beginning of June 2023

Beginning of contract: 1<sup>st</sup> October 2023

ANR BIOPOLIOL: <https://anr.fr/Projet-ANR-21-CE43-0026>

1-M. Burllet-Parendel, K. Faure Trends in Analytical Chemistry 144 (2021) 116422

2- M. Iguiniz, E. Corbel, N. Roques, S. Heinisch, J Pharm. Biomed. Analysis, 159 (2018) 237-244

3- M. Sarrut, A. Corgier, G. Crétier, A Le Masle, S. Dubant, S. Heinisch, J Chromatogr. A 1402 (2015) 124-133

4- M. Batteau, K. Faure, Journal of Chromatography A, 1673 (2022) 463056