

Master internship: Semi-quantitative analyses of bio-oils by High Resolution Mass Spectrometry (4-6 months)

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Keywords	Mass spectrometry, pyrolysis, bio-oils, structural analysis, instrumentation.
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Scientific environment	Mass spectrometry platform of the LCP–A2MC Laboratory Réseau National de Spectrométrie de Masse FT-ICR à Haut Champ – FR3624 CNRS

Context

In the context of the increase of the energy demand and the environmental issues relative to the use of fossil energies, more sustainable resources have to be developed. Among the existing renewable routes, the lignocellulosic biomass is very promising. This biomass resource is mainly based on by-products from the wood industries and therefore, it does not impact the foodstuff for both human and livestock neither the crops surfaces. Its conversion by fast-pyrolysis may lead to biofuel or chemicals for the industries. However different steps of the process such as the use of catalysts have to be considered. To assist the optimization of such process, analytical chemistry is a key point. In regards to the complexity of bio-oils, high resolution mass spectrometry is able to provide their exhaustive description. Nevertheless, the structural identification of their different components remains an important analytical challenge. To obtain more structural insights for a deeper bio-oil description, the semi-directed analysis of the biomass pyrolysis products has been recently introduced by the Mass Spectrometry team of the LCP-A2MC laboratory. This approach allows to identify compounds with a given chemical function by a selective derivatization process, which take place during the ionization event by ESI.

The first investigations were focused on carbonyl compounds (aldehyde and ketone). The main objectives of this Master internship are to optimize the specific detection of carbonyl compounds and to define the most appropriate reagent able to identify the compounds which present other chemical functions by a fast and specific reaction during the ionization step. Such derivatization agent may be commercial products and/or compounds specifically designed and synthetized by the LCP-A2MC organic chemistry group.

Detailed scientific environment

This work will be involved in a more global collaborative project between the LCP–A2MC and the LRGP (Nancy-CNRS) and will benefit from the expertise of both laboratories in the fields of mass spectrometry (Metz) and biomass pyrolysis (Nancy).

The master internship may be the first step of a doctoral research program. Indeed, the project will be opened for a PhD MESR position.

Profile

In the last year of her (his) master degree or engineering school, the candidate should have a combination of strong analytical and organization skills, excellent communications abilities and an extensive knowledge in mass spectrometry.

Accommodations and How to applied

The internship is contracted and rewarded, it will begin between mid-January and mid-March 2019 for a period of 4-6 months (a 6 month-period will be preferred). The laboratory is accessible by public transport (15 minutes from Metz city center and TGV station), please send your application (CV and cover letter) to the following address: <u>frederic.aubriet@univ-lorraine.fr</u>

Papers of the group linked to this proposal

Selectivity of bio-oils catalytic hydrotreatment assessed by petroleomic and GC* GC/MS-FID analysis Roberto Olcese, Vincent Carré, Frédéric Aubriet, Anthony Dufour Energy & Fuels 27 (4), 2135-2145 (2013)

Aromatic Chemicals by Iron-Catalyzed Hydrotreatment of Lignin Pyrolysis Vapor Roberto Nicolas Olcese, George Lardier, Mohammed Bettahar, Jaafar Ghanbaja, Sébastien Fontana, Vincent Carré, Frédéric Aubriet, Dominique Petitjean, Anthony Dufour ChemSusChem 6 (8), 1490-1499 (2013)

Toward controlled ionization conditions for ESI-FT-ICR-MS analysis of bio-oils from lignocellulosic material Jasmine Hertzog, Vincent Carré, Yann Le Brech, Anthony Dufour, Frédéric Aubriet Energy & Fuels 30 (7), 5729-5739 (2016)

Combination of electrospray ionization, atmospheric pressure photoionization and laser desorption ionization Fourier transform ion cyclotronic resonance mass spectrometry for ... Jasmine Hertzog, Vincent Carré, Yann Le Brech, Colin Logan Mackay, Anthony Dufour, Ondřej Mašek, Frédéric Aubriet Analytica chimica acta 969, 26-34 (2018)

A Multitechnique Characterization of Lignin Softening and Pyrolysis Binod Shrestha, Yann Le Brech, Thierry Ghislain, Sébastien Leclerc, Vincent Carré, Frédéric Aubriet, Sandrine Hoppe, Philippe Marchal, Steve Pontvianne, Nicolas Brosse, Anthony Dufour ACS Sustainable Chemistry & Engineering 5 (8), 6940-6949 (2017)

Catalytic Fast Pyrolysis of Biomass over Microporous and Hierarchical Zeolites: Characterization of Heavy Products J Hertzog, V Carré, L Jia, CL Mackay, L Pinard, A Dufour, O Mašek, F. Aubriet ACS Sustainable Chemistry & Engineering 6 (4), 4717-4728 (2018)

Semi-Targeted Analysis of Complex Matrices by ESI FT-ICR MS or How an Experimental Bias may be Used as an Analytical Tool

J Hertzog, V Carré, A Dufour, F Aubriet

Journal of The American Society for Mass Spectrometry 29 (3), 543-557 (2018)

Characterization of biomass and biochar by LDI-FTICRMS–Effect of the laser wavelength and biomass material F Aubriet, T Ghislain, J Hertzog, A Sonnette, A Dufour, G Mauviel, V Carré Journal of The American Society for Mass Spectrometry 29 (10), 1951-1962 (2018)