

INRAE UR1268 BIA – BIBS

✉ Rue de la Géraudière
F-44316 Nantes France
<https://www.bibs.inrae.fr>

Postdoctoral researcher position in high-resolution ion mobility mass spectrometry applied to carbohydrate analyses

Keywords: Mass spectrometry, ion mobility, carbohydrates, structural analyses, isomerism

A fully funded postdoctoral position in the field of ion mobility mass spectrometry (IMS-MS) is available in the group of Dr. David Ropartz at the BIA-BIBS mass spectrometry lab, embedded in the INRAE institute in Nantes, France.

JOB DESCRIPTION

The inherent complexity of carbohydrates remains a challenge for analytical sciences. No single method is currently able to fully resolving the various isomerisms present within the subunits and in glycosidic bonds, although these are determining structural features of carbohydrates. Mass spectrometry (MS) alone is blind to many cases of isomerism, and thus gives incomplete information for carbohydrates. Over the last ten years, the coupling of MS with ion mobility (IMS)—which is sensitive to gas-phase conformations of molecules and thus, to (stereo)isomerisms—has kept gaining momentum.

A recent PhD work in our group has explored the potential of high-resolution IMS approaches for structural glycosciences, by using a state-of-the-art SELECT SERIES Cyclic IMS (cIMS) instrument (Waters Corp.™). The work has demonstrated, through a series of case studies, that cIMS could resolve the various cases of isomerism found in carbohydrates. The work then aimed at developing a sequencing strategy based on the high-resolution IMS signature of oligosaccharides building blocks.

Although this work has clearly established the potential of high-resolution IMS as a pivotal method in structural glycoscience, we have encountered difficulties in setting up the direct sequencing approach. These difficulties stem in part from the confusing information generated on the fragments by low-energy CID fragmentation. However, our group has a long experience in high-energy fragmentation of carbohydrates (such as those involving ion-ion, ion-photon or ion-electron interactions) that highlighted a highly efficient fragmentation and less confusing information by employing these methods. We have therefore recently implemented an ExD cell on the cIMS instrument, which will allow access to high-energy fragmentation upstream of highly resolved ion mobility.

You will have the ambitious goal of exploring and optimising this IMS/MS set-up, with the aim to achieve a high-throughput direct sequencing strategy of complex carbohydrates. The application subject will concern plant polysaccharides used for the design of biomaterials with innovative functional features. It falls within the framework of a PEPR-type programme funded by the French ANR agency (Diademe program, Amethyst sub-project). Your contribution to the project will be to assist in the intelligent design of hydrogels thanks to an efficient structural characterization of candidate polysaccharides by the IMS/MS sequencing approach that will be implemented.

You will present your findings at leading international conferences in mass spectrometry and/or glycosciences, and will publish in peer review journals.

Your work will be supervised by Dr. David Ropartz and co-supervised by Dr. Helene Rogniaux. The anticipated start date is Nov. 1, 2023, but reasonable accommodations can be made for the right candidate.

Related publications of the group:

Cyclic IMS

- Ollivier, S.; Legentil, L.; Yeni, O.; David, L.-P.; Ferrières, V.; Compagnon, I.; Rogniaux, H.; Ropartz, D. Gas-Phase Behavior of Galactofuranosides upon Collisional Fragmentation: A Multistage High-Resolution Ion Mobility Study. *J. Am. Soc. Mass Spectrom.* 2023, 34 (4) 627–639. <https://doi.org/10.1021/jasms.2c00333>.
- Ollivier, S.; Tarquis, L.; Fanuel, M.; Li, A.; Durand, J.; Laville, E.; Potocki-Veronese, G.; Ropartz, D.; Rogniaux, H. Anomeric Retention of Carbohydrates in Multistage Cyclic Ion Mobility (IMS_n): De Novo Structural Elucidation of Enzymatically Produced Mannosides. *Anal. Chem.* 2021, 93 (15), 6254–6261. <https://doi.org/10.1021/acs.analchem.1c00673>.
- Ollivier, S.; Fanuel, M.; Rogniaux, H.; Ropartz, D. Molecular Networking of High-Resolution Tandem Ion Mobility Spectra: A Structurally Relevant Way of Organizing Data in Glycomics? *Anal. Chem.* 2021, 93 (31), 10871–10878. <https://doi.org/10.1021/acs.analchem.1c01244>.
- Ujma, J.; Ropartz, D.; Giles, K.; Richardson, K.; Langridge, D.; Wildgoose, J.; Green, M.; Pringle, S. Cyclic Ion Mobility Mass Spectrometry Distinguishes Anomers and Open-Ring Forms of Pentasaccharides. *J. Am. Soc. Mass Spectrom.* 2019, 30 (6), 1028–1037. <https://doi.org/10.1007/s13361-019-02168-9>.
- Ropartz, D.; Fanuel, M.; Ujma, J.; Palmer, M.; Giles, K.; Rogniaux, H. Structure Determination of Large Isomeric Oligosaccharides of Natural Origin through Multipass and Multistage Cyclic Traveling-Wave Ion Mobility Mass Spectrometry. *Anal. Chem.* 2019, 91 (18), 12030–12037. <https://doi.org/10.1021/acs.analchem.9b03036>.

High-energy fragmentation through ion-ion or ion-photon interaction mechanisms

6. Ropartz, D.; Li, P.; Jackson, G. P.; Rogniaux, H. Negative Polarity Helium Charge Transfer Dissociation Tandem Mass Spectrometry: Radical-Initiated Fragmentation of Complex Polysulfated Anions. *Anal. Chem.* 2017, 89 (7), 3824–3828. <https://doi.org/10.1021/acs.analchem.7b00473>
7. Ropartz, D.; Li, P.; Fanuel, M.; Giuliani, A.; Rogniaux, H.; Jackson, G. P. Charge Transfer Dissociation of Complex Oligosaccharides: Comparison with Collision-Induced Dissociation and Extreme Ultraviolet Dissociative Photoionization. *J. Am. Soc. Mass Spectrom.* 2016, 27 (10), 1614–1619. <https://doi.org/10.1021/jasms.8b05150>.
8. Ropartz, D.; Giuliani, A.; Fanuel, M.; Hervé, C.; Czjzek, M.; Rogniaux, H. Online Coupling of High-Resolution Chromatography with Extreme UV Photon Activation Tandem Mass Spectrometry: Application to the Structural Investigation of Complex Glycans by Dissociative Photoionization. *Anal. Chim. Acta* 2016, 933, 1–9. <https://doi.org/10.1016/j.aca.2016.05.036>.
9. Ropartz, D.; Giuliani, A.; Hervé, C.; Geairon, A.; Jam, M.; Czjzek, M.; Rogniaux, H. High-Energy Photon Activation Tandem Mass Spectrometry Provides Unprecedented Insights into the Structure of Highly Sulfated Oligosaccharides Extracted from Macroalgal Cell Walls. *Anal. Chem.* 2015, 87 (2), 1042–1049. <https://doi.org/10.1021/ac5036007>.

Combination of the two techniques for the structural characterization of carbohydrates

10. Ropartz, D.; Fanuel, M.; Ollivier, S.; Lissarrague, A.; Benkoulouche, M.; Mulard, L. A.; André, I.; Guieysse, D.; Rogniaux, H. Combination of High-Resolution Multistage Ion Mobility and Tandem MS with High Energy of Activation to Resolve the Structure of Complex Chemoenzymatically Synthesized Glycans. *Anal. Chem.* 2022, 94 (4), 2279–2287. <https://doi.org/10.1021/acs.analchem.1c04982>.

DESIRED SKILLS AND QUALIFICATIONS

Required:

- A PhD degree in Chemistry, Physical-Chemistry or Biochemistry;
- Lab experience with mass spectrometry (HR-MS and MS/MS);
- Lab experience with ion mobility mass spectrometry;
- A publishing record with at least one first-author publication;
- Proficiency in English;
- Capacity to quickly acquire new knowledge and master new skills;
- Interest in both hands-on research activities and data analysis;
- Ability to work independently and as a member of a research team;

Preferred:

- Lab experience with Waters Corp.™ instruments
- Lab experience with liquid chromatography hyphenated to MS
- Knowledge of carbohydrates chemistry and their structural analysis

EMPLOYER

INRAE (www.inrae.fr)

INRAE is a world-leading institute for research on agriculture, food and the environment, with a responsibility to address the global challenges of our time, namely climate change, food insecurity and biodiversity loss. Through an integrated approach, INRAE is able to identify and develop solutions with multiple applications to achieve the agro-ecological, nutritional and energy transitions we need to make.

INRAE is committed to nurturing an inclusive culture and a welcoming atmosphere. The Institute has made the "Social and Environmental Responsibility" a collective priority, in line with its commitment to sustainable development. This strategy should lead the Institute's research and internal practices to converge with ambitious values of environmental responsibility, solidarity and equity.

CONDITIONS OF EMPLOYMENT

Contract: 18-month.

The pay is commensurate with experience and ranges from 2,370 to 2,920 EUR per month.

By joining us, you will benefit from:

- 30 + 15 days of annual leave (for full-time employees, meaning 38.5h/week);
- Support for parenthood;
- Skills development programmes;
- Social support, holiday and leisure services;
- Sport and cultural activities.

APPLICATION PROCEDURE

Interested candidates are invited to submit a cover letter, an up-to-date CV and the contact details of at least one reference to david.ropartz@inrae.fr and helene.rogniaux@inrae.fr

Deadline for application: November 1, 2023

Contract start date: January 1, 2024 (Adjustable depending on availability of the selected candidate)