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Classification of oligosaccharides using molecular networks based on ion mobility

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Molecular networking of high-resolution tandem ion mobility spectra: A structurally relevant way of organizing data in glycomics?
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Contacts

David Ropartz, Simon Ollivier and Hélène Rogniaux
UR BIA
david.ropartz@inrae.fr
simon.ollivier@inrae.fr
helene.rogniaux@inrae.fr

Context

Carbohydrates are one of the most important chemical classes in the living world. They also have applications in various fields, such as biofuels or the food, pharmaceutical and cosmetic industries. However, minor chemical variations can have a major impact on their properties. While there is currently no satisfactory approach to finely characterise polysaccharides, particularly in complex extracts, mass spectrometry (MS) has emerged as a powerful tool for the structural analysis of other types of biopolymers, notably proteins. However, the methods cannot be directly transposed to carbohydrates, which contain many structural elements that do not affect their mass (a phenomenon known as isomerism). As a result, these isomers are invisible to MS – which detects only mass. Today, technological advances are making it possible to start lifting this analytical barrier. More specifically, molecules can be separated according to their 3D conformations by combining ion mobility spectrometry with MS (IM-MS).

Results

We developed a method exploiting the latest advances in IM-MS to identify structural groups of oligosaccharides. This method is inspired by a strategy used in metabolomics, called molecular networking. Classically, the strategy uses tandem mass spectrometry (MS/MS): the molecule of interest is isolated according to its mass and then broken down into fragments – akin to a structural signature of the molecule. A bioinformatics comparison allows similar spectra (and thus related structures) to be linked in the network. Unfortunately, this approach is not very informative for oligosaccharides because of the above-mentioned isomeric situations.

Our approach allows molecular networks to be constructed in which the mass of the fragments is replaced by their ion mobility. We tested this approach on several dozen oligosaccharides, representative of the carbohydrates found in plants. The constructed network proved to be superior in grouping oligosaccharides according to informative structural characteristics, chiefly related to their backbone.

Future outlook

This new method should simplify the analysis of carbohydrates in biological media by grouping similar species and making the data less complex. Future research will improve the approach by making maximum use of the two dimensions available in the data, namely fragment mass and mobility.

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