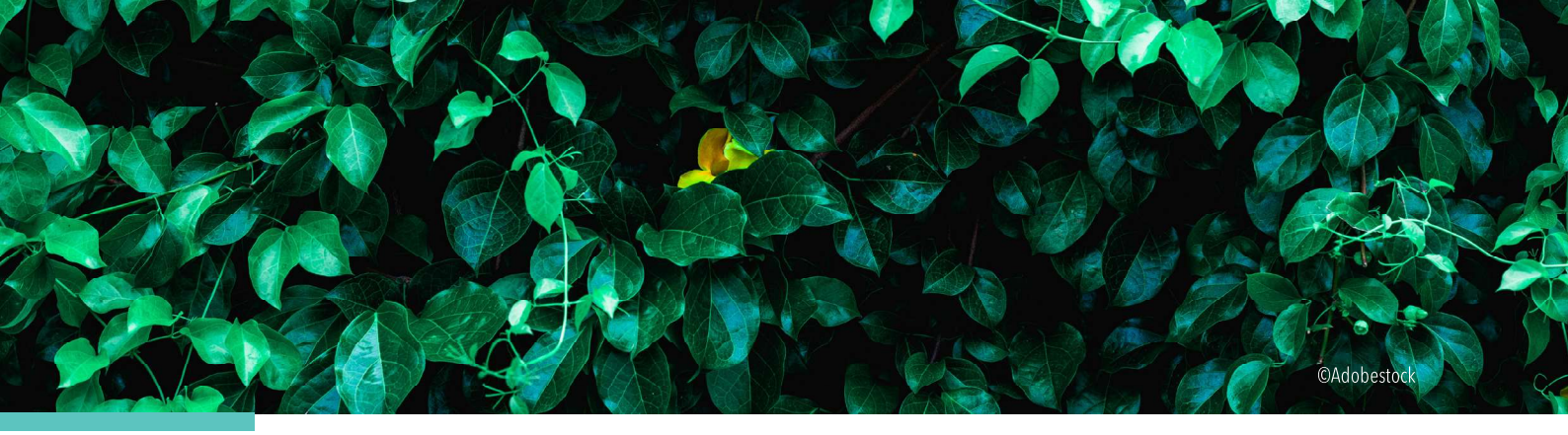


# Towards an automated workflow for reading the mass spectra of plant oligosaccharides

## Read more

Lollier V *et al.*

Oligator: a flexible interface to draw oligosaccharide structures and generate their theoretical tandem mass spectra.

Bioinformatics . 2021 - https://doi.org/10.1093/bioinformatics/btab412

## Mobilization and impact

These tools are publicly available in the GitHub source code repository.

A scope brief is being drafted to help mobilize these valuable software technologies.

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## Context

Glycans are the main plant cell wall components. They are known to have effects on nutrition and hold strong potential in green chemistry, but further applications are bottlenecked by the unmet challenge of resolving their precise structure. Tandem-mass spectrometry (MS/MS) is a mainstay analytical technique for resolving the structure of biopolymers. However, a shortage of good-quality reference leaves this high-throughput technology underequipped in terms of tools to support an automated workflow for reading mass spectra, especially for plant glycans. The structural analysis of these complex molecules demands specific methodological developments where the interpretation of mass spectra has to be done manually, which is a painstaking and laborious task that fails to capitalize on the powerful analyses carried out.

## Results

The BIBS platform has developed two software packages, Oligator and mzLabelEditor, to facilitate the interpretation of mass spectra and the collection of spectral reference data. These two software programs standardize the process of structural sketch-up and annotation of MS/MS spectra but keep the flexibility needed to explore new chemical forms of oligosaccharides.

Oligator provides a graphical interface to sketch up a candidate oligosaccharide structure and then produce its theoretical MS/MS spectrum based on the usual ion nomenclature. To store the structures and explore unreferenced chemical substitutions, Oligator uses the popular chemoinformatics notation 'simplified molecular input line entry system (SMILES)'.

MzLabelEditor is designed for building a library of reference spectra. The software interface can keep the instrumental information (manufacturer, ionization mode, fragmentation mode, etc.) associated with a given annotated spectrum. A spectrum is annotated by putting labels on the peaks of interest. MzLabelEditor is the only purpose-dedicated mass spectrometry tool that allows free-form editing of these annotations.

To facilitate the interpretation and annotation of a spectrum, mzLabelEditor proposes a workflow that compares it to a 'model', which is ideally a theoretical spectrum generated with the Oligator tool.

## Future outlook

The two programs used in tandem help to collect and compile reference data into a spectral library and raise prospects for an automated workflow for reading the MS/MS spectra of plant glycans.

Finally, most of the features of MzLabelEditor are essentially generic and it could readily support other MS/MS fragment nomenclatures in the comparative analysis module in order to extend the tool to other types of molecules.