Mass Spectrometry Tools

Description

Mass Spectrometry is one of the main analytical techniques currently used in the structural analysis of glycans. In particular, MALDI and ESI MS methods are well suited to detect various glycoconjugates' glycosylation profiles. It is worth considering that tandem mass spectrometry, often combined with liquid chromatography and applied on complex mixtures, provides a large amount of raw data to be analysed to identify the molecular structures. Thus, it is not surprising that in the years, different libraries and tools have been developed for helping the determination of glycan structures, especially from a eukaryote, starting from an analysis of MS data.

Among the plethora of existing tools in this field, the GlycoWorkbench is a widespread open-source software that contains an extensive library of fragmentation types, which allows the simulation of glycans mass spectra. In addition to the library of fragments, this software supports many annotation options, so it is used in the building of UniCarb-DB, an archival database of analytical data mainly focused on mass spectrometry. It provides an open-access LC-MS/MS library of N- and O- linked glycans released from glycoproteins that have been annotated, facilitating structure elucidation. (54) Of note, this glycomic spectra library has implemented the MIRAGE guidelines for reporting. MIRAGE stands for Minimum Information Required for a Glycomics Experiment and aims to develop sample preparation, analysis, and publication guidelines to ease the interaction and exchange between structural glycomic data.

Among the different Mass spectrometry methods useful for the analysis of glycans, also the GC-MS (by electron ionisation) come to the aid of taking the first steps of the structural determination of glycans and it is especially used in the analysis of bacterial oligo- and polysaccharides.

Despite a plethora of different libraries and platforms containing a large amount of annotated and validated mass spectra, have been developed to facilitate structure elucidation of eukaryotic glycans, less has been done for the analysis of the microbial glycans, preventing from easily gaining glycosidic and cross-ring fragmentation ions, retention times, and associated experimental metadata descriptions that would instead help in the determination of the glycan structure. In this regard, two small but very informative databases come to the aid of taking the first steps of the structural characterisation of bacterial oligo- and polysaccharides. The first is included in the e-chapter "Gas Chromatography-Mass Spectrometry for Glycosciences" published on Glycopedia (www.glycopedia.eu), where different mass spectra of four types of derivatives are reported, permitting to achieve the monosaccharide composition and to establish the linkage pattern of each residue and its absolute configuration. The second mini-database is available on the Complex Carbohydrate Research Center of the University of Georgia (www.ccrc.uga.edu) and furnishes useful information for the interpretation of mass spectra obtained of chemical derivatisation of bacterial oligo- and polysaccharides.

A list of the main tools useful for the analysis of glycan MS spectra is here reported.

GlycoWorkBench: Downloadable software suite containing tools to draw glycans and assist MS

results with different information about environments or fragmentation, among others. (http://www.eurocarbdb.org/applications/ms-tools.)
Glycopedia e-chapters: Online database that provides information about different fields involving glycans. It is possible to find different e-chapters classified depending on the required knowledge level, not only about MS but also about NMR or just glycans knowledge. (https://www.glycopedia.eu/)

CCRC spectral database: Database that provides useful information about MS fragmentation patterns of different derivatives. (https://www.ccrc.uga.edu/specdb/ms/pmaa/pframe.html)

Glycomod: Online tool to predict monosaccharide composition of free or derivatised oligosaccharides from their experimental data. (https://web.expasy.org/glycomod/)

GlycoStore: Chromatographic, electrophoretic and MS database. The data is classified into different collections where descriptions, samples and analytical techniques are also defined. (https://glycostore.org/)

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