Information	MS	NMR
Quali-quantitative analysis of composing sugars	✓ GC-MS	✓ NMR
Monosaccharide Absolute configuration	✓ GC-MS	✓ NMR
Size of the sugar ring	✓ GC-MS	✓ NMR
Anomeric configuration of monosaccharides	✗	✓ NMR
Linkage analysis	✓ GC-MS	✓ NMR
Monosaccharides sequences	✓ MALDI-MSn ✓ ESI-MSn	✓ 2D NMR
Determination of non-carbohydrate appendages	✓ GC-MS ✓ MALDI-MSn ✓ ESI-MSn	✓ 2D NMR
Repeating unit – Patterns occurring along the chain	✓ MS	✓ NMR
Molecular weight distribution	✓ MS	✓ NMR

Bioinformatics & Determination of Glycan Structures

Description

Above all, bioinformatics tools are useful for achieving the hard goal of elucidating complex glycans structure, making it easier to interpret the experimental data.

As mentioned above, these moleculesâ?? structural analysis implies a complex operation of bench organic and analytical organic chemistry. Only once extracted and purified the polysaccharide material it is possible to proceed with specific derivatization to determine the nature of the constituting monosaccharide residues and the nature of the linkage to the neighbouring units. (53) This is far from trivial considering the plethora of monosaccharides that occur in nature, especially in the case of bacterial glycans.
In this regard, the home page of Stenutz (www.stenutz.eu) provides a collection of standardised procedures described as practical guides to the structural analysis of carbohydrates. In detail, from the main menu, it is possible to select specific procedures spanning from the purification to the structural analysis of polysaccharides, including a brief description of the method, the flow scheme of the reaction, if available, the list of the necessary reagents, the steps of the procedure and some comments and references.
Once extracted and purified the polysaccharide material, usually by following well-described procedures such as those reported on the website from Stenutz, it is necessary to proceed with the determination of the chemical structure of glycans that aims at defining several items: including i) the determination of the number, the nature and the position of the constituent monosaccharides, along with their absolute configuration; ii) the determination of the ring size of the monosaccharides, distinguishing between furanosidic and pyranosidic rings; iii) the description of the type and the anomeric configuration of the glycosidic linkages; iv) the identification of the monosaccharides sequence and if the glycan has a regular structure, the determination of the repeating unit; v) the identification of noncarbohydrate substituents; vi) the definition of their molecular size.
It is possible to reach all this information by taking advantage of different analytical techniques, mainly Mass Spectrometry (MS) and NMR spectroscopy. Complementing them with bioinformatic tools is a great help to ease the structural analysis (Table 1).

Information	MS	NMR
Quali-quantitative analysis of composing sugars	✓ GC-MS	✓ NMR
Monosaccharide Absolute configuration	✓ GC-MS	✓ NMR
Size of the sugar ring	✓ GC-MS	✓ NMR
Anomeric configuration of monosaccharides	✗	✓ NMR
Linkage analysis	✓ GC-MS	✓ NMR
Monosaccharides sequences	✓ MALDI-MSn ✓ ESI-MSn	✓ 2D NMR
Determination of non-carbohydrate appendages	✓ GC-MS ✓ MALDI-MSn ✓ ESI-MSn	✓ 2D NMR
Repeating unit – Patterns occurring along the chain	✓ MS	✓ NMR
Molecular weight distribution	✓ MS	✓ NMR

Table 1: Different analytical techniques, NMR and MS-based, used to obtain information for the structural determination of glycans

Category

1. News