Computational Tools for the Structural Elucidation

Description

Determining the glycan structure, presents many challenges, mainly related to glycan's complexity and diversity, together with the non-templated nature of glycan biosynthesis. Simple sugar monosaccharides can be assembled through linkages at many different sites, forming complex polymers which can adopt a wide variety of shapes. (46) A major difficulty occurs when dealing with bacterial glycans due to many different constituent monosaccharides. As mentioned above, over one hundred different sugar building blocks have indeed been identified in bacteria, including many non-conventional monosaccharides, often modified with noncarbohydrate substituents.

Thus, the full characterisation of glycans, spanning from the primary structure's elucidation to the determination of glycoconjugates' three-dimensional dynamical features, is an intricate work constituted by different steps. It implies complex bench organic and analytical organic chemistry procedures using different analytical techniques, mainly mass spectrometry and NMR spectroscopy. (47) The procedure to reach the full characterisation of complex glycan structures should be seen as a puzzle. The different techniques provide a piece of information, and only putting them together allows obtaining the final image, thus the glycan structure and architecture.
The implementation of bioinformatics tools represents a key aspect of making the structural analysis easier, faster, and more reliable, helping assess all the items necessary to get glycans' chemical structure. Consequently, to support the increment of information in this field is mandatory to have easy ways to organise, unify and share in a user-friendly way these amounts of data within the scientific community, as it is vital for the development of modern glycomics and glycoproteomics. (48, 49) Thus, it is no coincidence that, in the years, several tools emerged as useful methods to address the limitations of existing techniques for the determination of glycans structure. Here we report the current bioinformatics resources available to analyse and characterise complex glycans, focusing on bacterial polysaccharides.

Category

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