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Glycan Analyzer: Software to Annotate Glycan Structures from Exoglycosidase Experiments

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Abstract : Glycoproteins and their covalently bonded glycans play critical roles in the immune system, cell communication, disease and disease prognosis. Ultra performance liquid chromatography (UPLC) coupled with mass spectrometry is conventionally used to qualitatively and quantitatively characterise glycan structures in a given sample. Exoglycosidases are enzymes that catalyze sequential removal of monosaccharides from the non-reducing end of glycans. They naturally have specificity for a particular type of sugar, its stereochemistry (α or β anomer) and its position of attachment to an adjacent sugar on the glycan. Thus, monitoring the peak movements (both in the UPLC and MS1) after application of exoglycosidases provides a unique and effective way to annotate sugars with high detail - i.e. differentiating positional and linkage isomers. Manual annotation of an exoglycosidase experiment is difficult and time consuming. As such, with increasing sample complexity and the number of exoglycosidases, the analysis could result in manually interpreting hundreds of peak movements. Recently, we have implemented pattern recognition software for automated interpretation of UPLC-MS1 exoglycosidase digestions. In this work, we explain the software, indicate how much time it will save and provide example usage showing the annotation of positional and linkage isomers in Immunoglobulin G, apolipoprotein J, and simple glycan standards.

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