

## **SIMULATING MASS SPECTRA: A STEP TOWARDS ANALYZING GLYCAN BIOSYNTHESIS**

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### **ABSTRACT**

The study of systems biology faces a typical problem of lack of experimental time-series data which quantify the system's properties versus time. The Complex Carbohydrates Research Center (CCRC) at the University of Georgia is currently studying glycan biosynthetic pathways in IDAWG<sup>TM</sup> experiments, which incorporate heavy nitrogen (<sup>15</sup>N) into glycans and provide quantitative time-series data that encode information regarding the appearance and lifetime of glycans. Successfully simulating the mass spectra of IDAWG<sup>TM</sup> experiments will help analyze and model glycan biosynthesis. In our work, the major issue is how to estimate the relative abundance levels of molecules involved in glycan biosynthesis, from experimental mass spectra collected from different time points. The proposed approach utilizes gradient search to minimize the difference between experimental and simulated spectra. These relative abundance levels are then fed into a pathway simulation model to analyze glycan biosynthesis. The preliminary results obtained so far are satisfactory and show robustness.