DISSERTATION
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Bioinformatics Methods and Tools for Glycomics

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Abstract: Glycomics is the study of the structure and function of carbohydrates in biological systems. In comparison to the expansion of the more established fields of genomics and proteomics, the integration of glycans and glycomics in biomedical research has lagged far behind. Glycomics has the potential to be included as another foundational science in the study of human disease, since glycans play have major roles in certain hereditary diseases, infectious diseases, and cancer. The structural and functional complexity of glycans coupled with the lack of robust bioinformatics impedes the integration of glycoscience into the scientific mainstream. The central objective of this thesis is to develop novel computational methods and bioinformatics tools to advance the understanding of structure and function relationships of glycans and their recognition and binding by Glycan Binding Proteins (GBPs).

We have developed a method to automate the interpretation of glycan microarray data to identify the glycan determinants that are necessary for binding. We evaluate this method against GBPs of known specificities to validate the results. We demonstrate this approach revealed new recognition motifs that had not been previously reported.

We also present a novel computational approach to automate the sequencing of glycans based on a method known as Metadata-Assisted Glycan Sequencing (MAGS), which combines analyses of glycan structures by mass spectrometry (MS) and glycan microarray technology to fully characterize glycan sequences. We target the soluble glycans in the human milk glycome as the first meta-glycome to be defined using this method.

To facilitate access by scientists to glycomics information, we developed an open-source, web-based bioinformatics platform for glycan microarray analysis. The platform provides interactive visualization features to view, search, and compare experimental data and also includes glycan motif mining and analysis.

In addressing these research areas, we have developed novel methods, algorithms, and software tools applied to the field of glycomics. These contributions will aid in the elucidation of the human glycome and a greater understanding of the diverse and important biological functions of glycans.

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