Hamilton Institute Student Seminar Series

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**Title:** **The Dynamics and Molecular Recognition of Complex Carbohydrates**

**Abstract:** Carbohydrates, most commonly known as sugars, play an essential role in human health and disease. The function of carbohydrates in human biochemistry is not limited to their role as a primary energy source; long chains of complex carbohydrates known as glycans, are attached to proteins and lipids, and cover the surface of most of our cells like a fur (the glycocalyx). These glycans facilitate the interaction between the cell and other cells, its surrounding environment, and its movement. Also, the interaction with the carbohydrates on the cell surface represents the first port of entrance for bacteria, viruses, and toxins into the cell, which allows for infection. Understanding the links between glycosylation patterns and the structure and function of the proteins they are attached to, is one of the most active research areas in pharmaceutical chemistry and glycobiology. Because glycans are not genetically encoded, it is difficult to identify their pattern of occurrence, and while experimental methods are used to identify the structure by enzyme digestion, it cannot capture the dynamics and significance of the intact glycan structure. With an overview of my work, I will show how computational methods like Molecular Dynamics (MD) and Quantum Mechanic (QM) calculations can be used to simulate the dynamics and conformational propensity of N-glycans and how these methods shed light on the sequence-to-structure dependance of N-glycans, which in turn affects the functionality of the associated proteins and biomolecules.