Research Group: Laboratory of Biochemistry – GQBB

Project: SURFACE GEOMETRY–BASED DETECTION AND CLASSIFICATION OF GLYCAN BINDING SITES

Brief description:

Protein-carbohydrate interactions are fundamental to a wide range of biological processes, from cell-cell communication and immune response to infection and cancer progression. Glycans are the most structurally diverse biomolecules, and their recognition by proteins plays a crucial role in numerous physiological and pathological mechanisms. Despite their importance, many aspects of protein-glycan interactions remain elusive due to the intrinsic complexity of glycans, their dynamic nature, and the challenge of studying their binding mechanisms at high resolution.

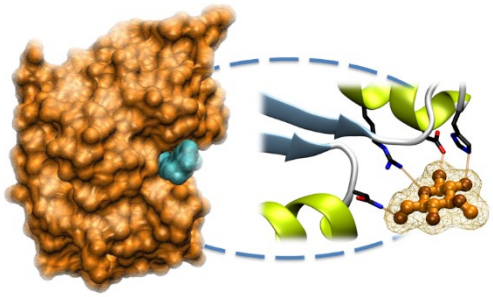

Figure 1. A) *Example of a glycan binding pocket specific to β-glucose.*

In this project you will contribute to advance the molecular understanding of protein–glycan recognition by developing computational methods to identify and classify glycan-binding sites on protein surfaces. This will involve exploring mathematical models that describe surface geometry and reveal features relevant to carbohydrate recognition. These geometric descriptors will serve as the foundation for machine learning models that can learn and predict glycan-binding specificity, potentially enabling the automated detection of protein–glycan interfaces across diverse protein structures. By integrating structural biology, mathematical modeling, and data science, this project has the potential to accelerate the discovery of new glycan-targeted therapies and to support innovations in biotechnology, biomedicine, and sustainable industry. https://gqbb.iqs.edu/

Objective:

This project aims to develop a robust computational framework to classify glycan-binding sites based on the structural and geometric features of protein surfaces at the interface. By extracting meaningful descriptors from the topology and shape of protein surfaces. The classification method will allow the detection of protein-glycan interfaces and, eventually, predicting carbohydrate specificity for any given protein. By applying methodologies similar to those used for protein-protein interaction prediction, the goal is to harness the power of machine learning to gain insights into the molecular basis of carbohydrate recognition by proteins.

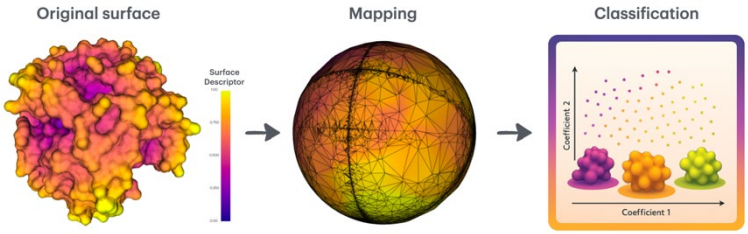

Figure 2. Surface-to-shape workflow: *From molecular surface to mapped representation and classification based on geometric descriptors.*

Technical skills:

You will learn how to apply a variety of computational techniques to address a biologically relevant problem, including:

- Protein Surface Analysis and Geometric Descriptors
- Molecular Modeling and Structural Bioinformatics
- Data Processing and Visualization
- Machine Learning and Classification Methods
- Python Programming and Scientific Libraries

The project will be tailored to your background, with flexibility to focus more on surface modeling, algorithm development, or application of machine learning tools, depending on your interests and experience.

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