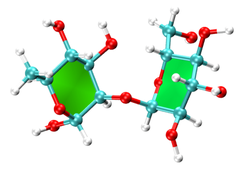
Molecular Modelling of Mannan-Latching

A molecular dynamics study of Carbohydrate-Carbohydrate Interactions



1 INTRODUCTION

Cell surfaces are adorned with diverse biomolecules, and of immediate interest are carbohydrates which make up large portions of the molecules found on cell surfaces.

Although there is evidence for carbohydrate carbohydrate interactions (CCI) mediating cell adhesion, cell signalling and cell recognition events, their specific role remains undetermined.

We investigate a type of CCI called mannose latching which occurs when there is a net attractive force between two interacting mannose molecules and the separation between the interacting molecules is at an equilibrium distance.

2 METHODS

We use molecular dynamics (MD) simulations to study the potential for CCI and their functional role in glycobiology. In particular, we are interested in mannans and glucans (i.e. linear homopolysaccharides consisting of D-mannose and D-glucose residues, respectively).

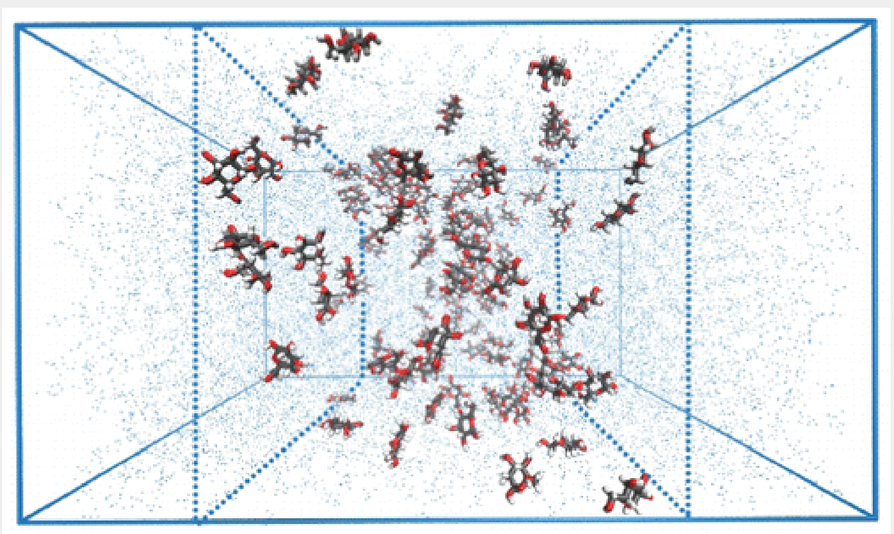


Figure 1: An illustration of a simulation setup for CCI

In MD, atoms are represented as balls and covalent bonds are represented as springs. A harmonic potential function is then employed to describe dynamic interactions between molecules.

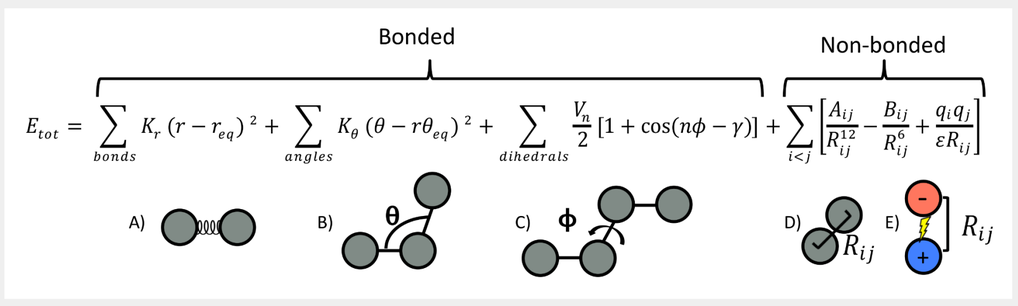


Figure 2: A representation of the molecular mechanics model for bonded and non-bonded atoms.

3 RESULTS AND DISCUSSION

We find that 1000ns MD simulations of CCI show little to no aggregation, as shown in Figure 3. The Glycosidic torsions of the carbohydrate simulations are in agreement with known experimental/simulation results, as shown in Figure 4. This confirms the validity and correctness of our model.

This project is still in progress, therefore there is still scope for improvement. So far, the simulations indicate that carbohydrates show very weak interactions strengths.

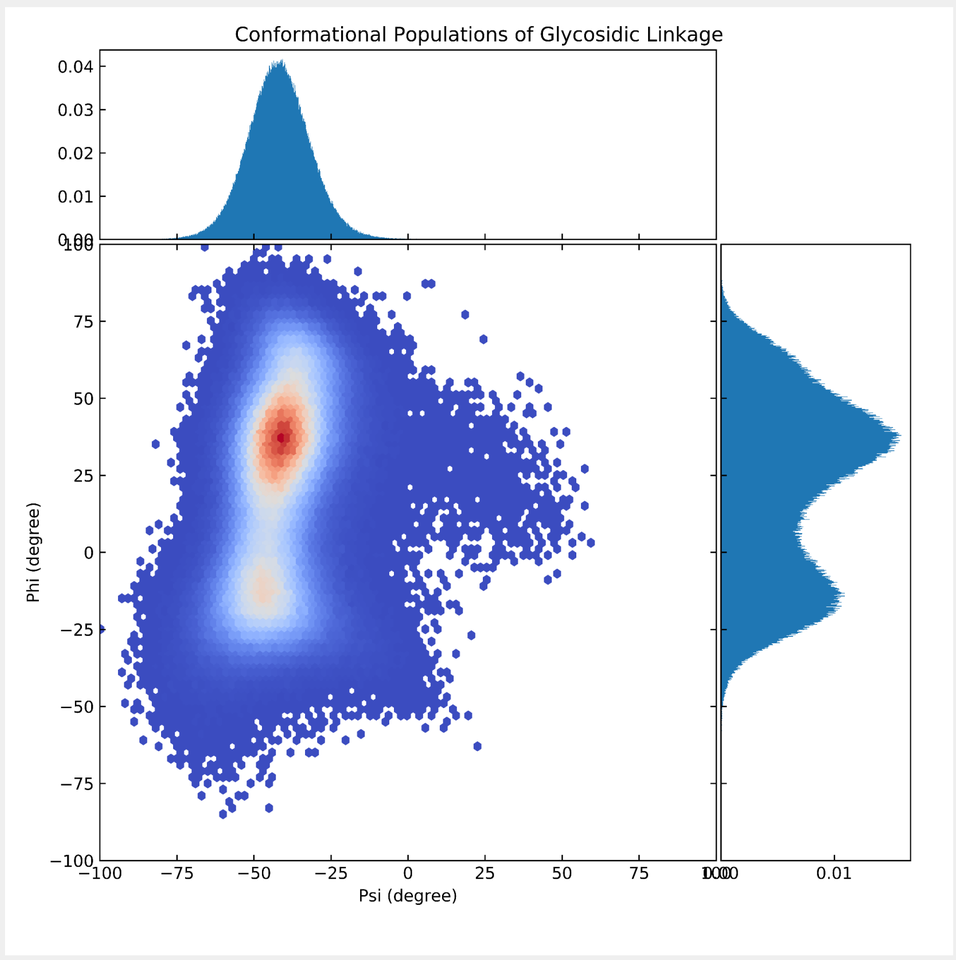


Figure 4: The conformational populations of glycosidic torsions in Mannose disaccharide linked through Carbon-1 and Carbon-2

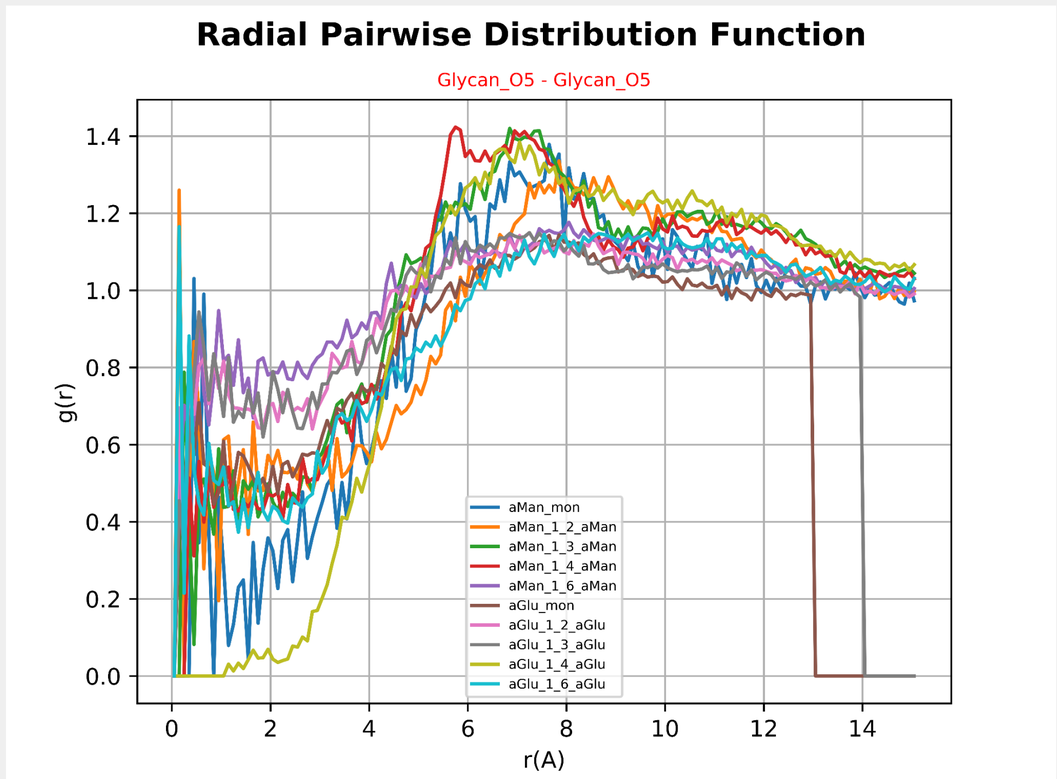


Figure 3: A radial pair distribution graph showing weak interactions between carbohydrate oxygen atoms.

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