

Accurate Modelling and Effective Visualization of Carbohydrate Conformation

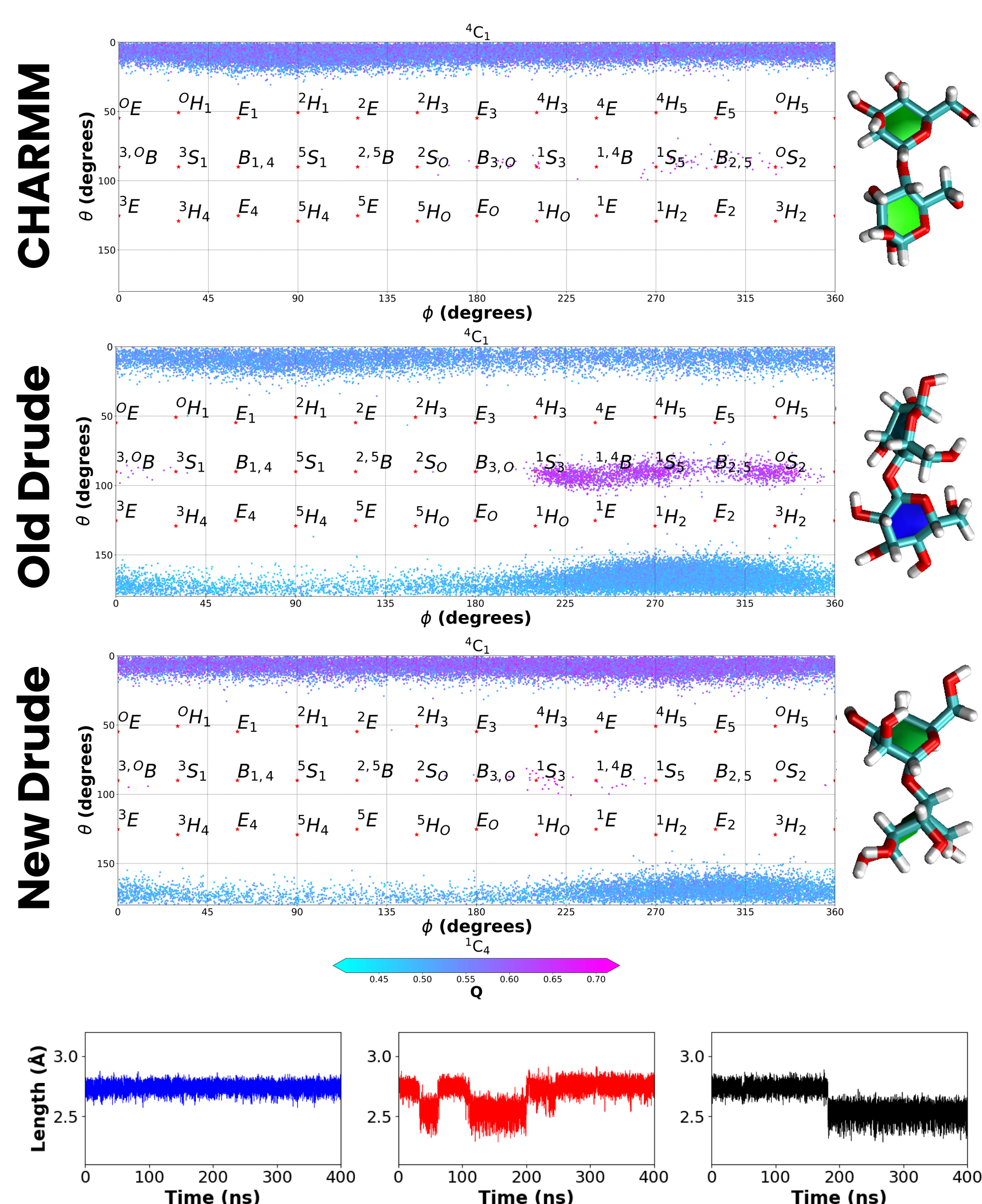
Introduction

Carbohydrates play critical roles in biological processes, and their interactions depend on their 3D shapes, or conformations. Understanding these conformations, through computer modelling and visualization, is therefore key to modern drug and vaccine design.

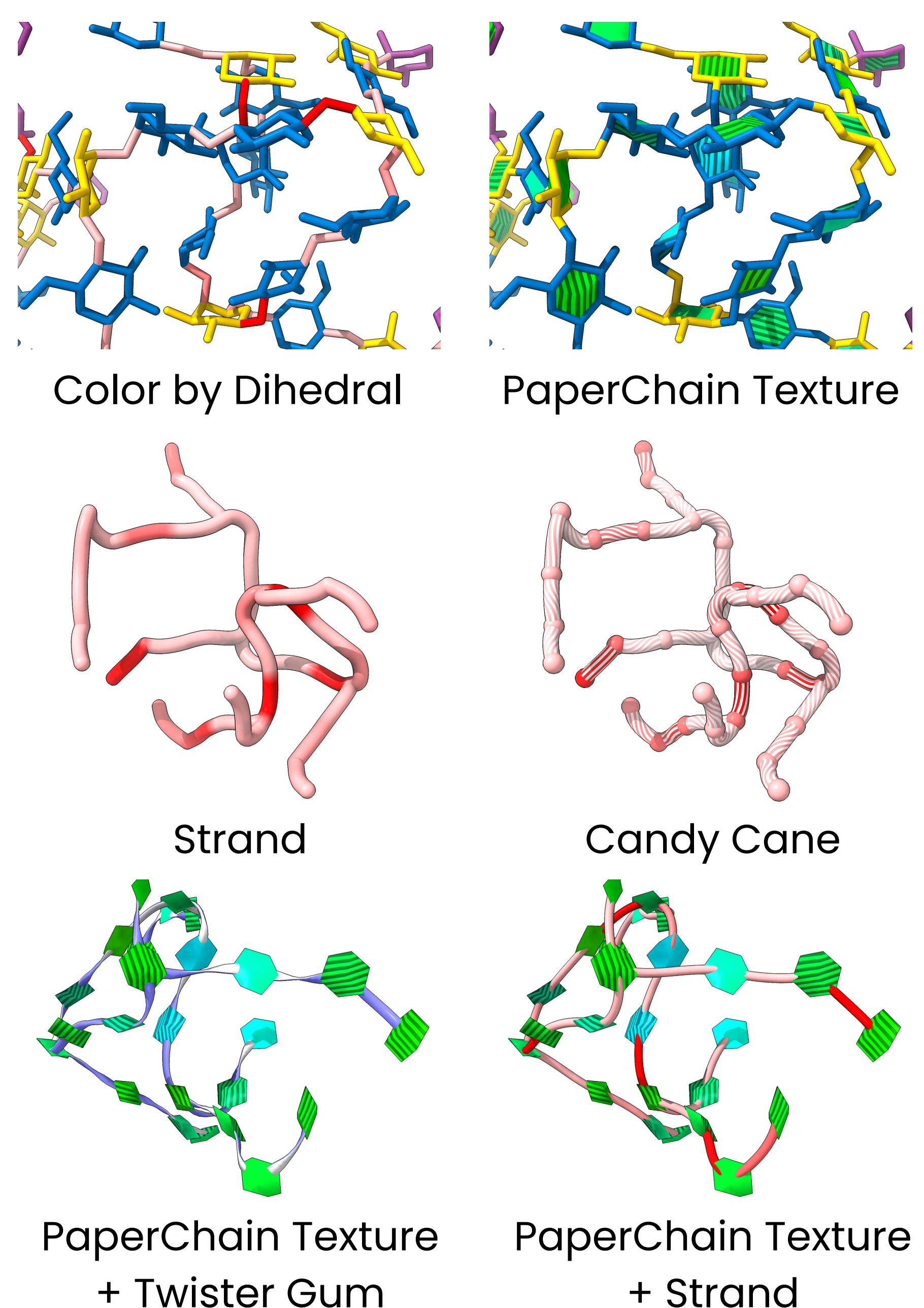
Objectives

- Compare the latest refinement of the Drude polarizable force field to its previous version and the well-established CHARMM force field for modelling oligosaccharides
- Design and evaluate new visualizations to enable more effective analysis of carbohydrate conformation

Simulation Results



Visualization Designs



Conclusions

The latest refinement of Drude significantly reduces the oversampling of non- 4C_1 ring pucker present in the previous version but does not align with CHARMM. The radius of gyration in New Drude is more stable than Old Drude but less stable than CHARMM.

Overall, the designs were found to effectively depict carbohydrate conformation. In particular, PaperChain Texture and Strand provided significant benefits over the existing PaperChain and Twister representations, particularly when used together.