Contribution ID : **47** Type : **Oral**

Studying Polysaccharides in Solution with SAXS and Molecular Dynamics

Friday, 26 November 2021 13:30 (20)

Polysaccharides are semi-flexible polymers composed of sugar residues with a myriad of important functions in-vivo, including structural support, energy storage and immunogenicity. The local conformation of such chains is a crucial factor governing their interactions. Traditionally this conformation has only been directly accessible in the solid-state, using crystallographic techniques such as fibre diffraction. However, improvements in the quality of synchrotron-based X-ray scattering data means that conformation-dependent features can now be measured in solution. In tandem, scattering predictions based on structures initiated from existing fibre x-ray diffraction data, and then re-animated using molecular dynamics, can now be performed.

Our group has recently measured the detailed small-angle x-ray scattering from a variety of anionic oligo- and poly-saccharides in solution. This talk will specifically present data obtained from experiments carried out on homogalacturonan, alginate and carrageenan and discuss their comparison with predictions based on our molecular dynamics simulations. The remarkable agreement found provides unequivocal evidence for the validity of our real-space atomistic models of the solution state structures. This technique is expected to be universally applicable for polysaccharides that consist of comparatively stiff glycosidic linkages, and to have extensive relevance for a number of biological macromolecules, including glycosylated proteins.

Level of Expertise

Experienced Researcher

Presenter Gender

Man

Pronouns

Which facility did you use for your research

Australian Synchrotron

Students Only - Are you interested in AINSE student funding

Do you wish to take part in the Student Poster Slam

Condition of submission

Yes

Primary author(s) : Dr IRANI, Amir (School of Fundamental Sciences, Massey University, NZ); Mr WESTBERRY, Ben (School of Fundamental Sciences, Massey University, NZ); Dr MANSEL, Bradley (Department of Chemical Engineering, National Tsing Hua University, Taiwan); Prof. WILLIAMS, Martin (Bill) (Massey University, MacDiarmid Institute, NZ); RYAN, Tim

Presenter(s) : Prof. WILLIAMS, Martin (Bill) (Massey University, MacDiarmid Institute, NZ)

Session Classification : Biomedicine, Life science & Food Science

Track Classification : Biomedicine, Life science & Food Science