

Ice recrystallization inhibition by disaccharides

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Ice formation, mainly consisting of ice nucleation and growth, is a ubiquitous phenomenon. Controlling its formation is a most sought-after task for a wide range of industrial needs, from cryopreservation of cells, to preservation of food and to de-icing of infrastructures. Nature has developed unique ways of controlling ice formation by producing proteins with the ability of promoting ice nucleation or inhibiting its growth. Due to the many drawbacks in the use of natural occurring proteins, for example high cost of extraction and toxicity for human cells, the development of efficient synthetic alternatives to natural proteins has become of utmost importance.

The role of polysaccharides as ice nucleating and antifreeze molecules has only recently started to come to the surface, and the tremendous amount of available experimental data on their activity has opened a number of very important questions on their mechanism of action. While these questions cannot be answered with state-of-the-art experimental techniques, molecular simulations have the right spatial and temporal resolution to discriminate between the wide number of mechanisms hypothesized from experimental results, and can contribute to the unravelling the essential molecular motifs responsible for ice-controlling activities. Here I carry out a computational investigation to elucidate the mechanism by which the disaccharides recognize ice, bind to it, and halt its growth.