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Sugar stereochemistry effects on water structure and on protein stability: The templating concept

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The stability of macromolecules in food and other systems strongly depends on modulation of water structure by co-solutes. It is well-known that sugars protect proteins; however, the mechanisms of protection have been elusive. Herein we propose that the better a template a sugar isomer is for cooperative hydration, the higher its hydration number and protein-protective effect. We developed unique atomistic Monte Carlo (MC) simulation that quantifies energetic and spatial compatibility of sugars with ideal tetrahedral water structure, as embodied in hexagonal ice. Studying four isomeric sugars, we found the following compatibility order with ice: D-galactose > D-glucose > D-mannose > D-talose. We found the same order in terms of sugar hydration number in liquid, both experimentally and by molecular dynamics (MD) simulation, and found important evidence for the cause of sugar kosmotropicity: the hydrogen bonds between sugar and water are shorter, on average, than water-water H-bonds, supporting our basic hypothesis that the first hydration layer of a sugar is more tightly bound. The simulation showed second and third hydration layers that are more ordered around galactose compared to talose (the best and least compatible isomers, respectively), further supporting the validity of our 'templating for cooperative-hydration' concept. The same order was also found for the protective effect of the sugars against thermal denaturation of a protein, supporting our proposed templating concept as fundamental in explaining nonionic solute effect on water structure and on protein stability. This study may pave the way for rationally designing more powerful protein stabilizers, by synthesizing molecules of optimized structure for water-structure templating.

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