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Special Issue

Conformations of Oligo- and Poly-saccharides

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Editor: *Derek Horton*

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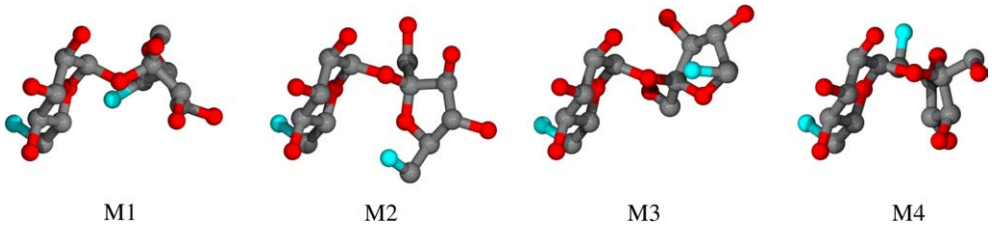
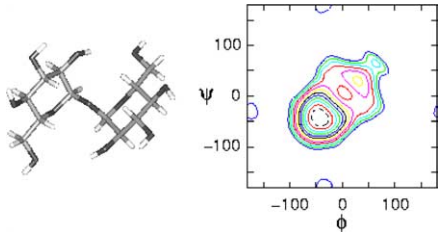
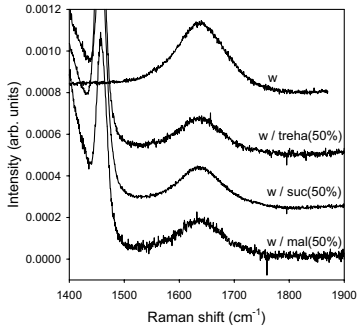
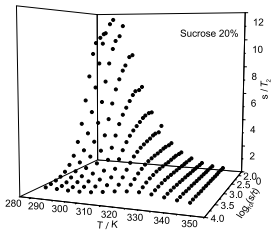


The solution structure and dynamics of sucrose are examined using a combination of NMR residual dipolar coupling and molecular mechanics force fields.

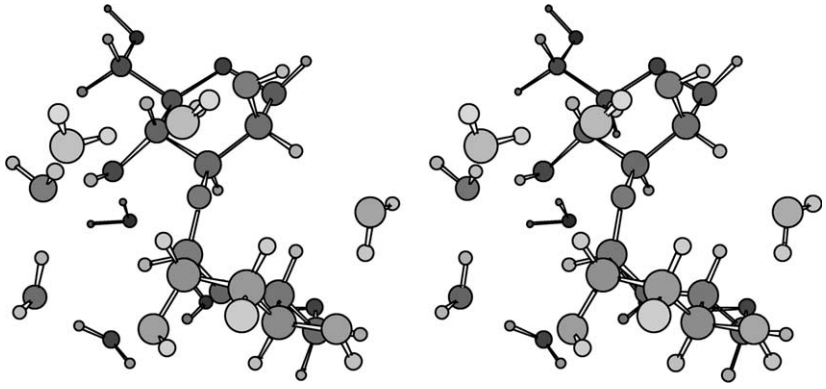


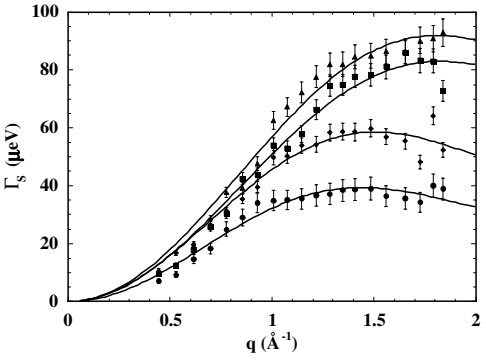
Free-energy surfaces for trehalose reveal that it is restricted to a single minimum-energy conformation in both vacuum and solution thus providing a molecular rationale for the antidesiccant properties of trehalose glasses.

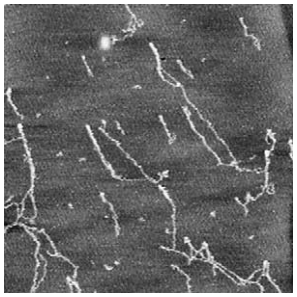


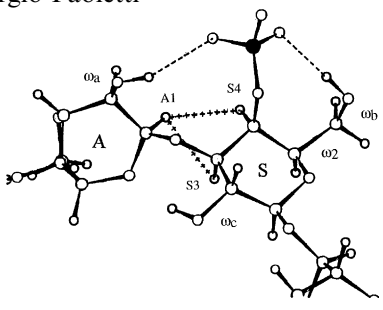


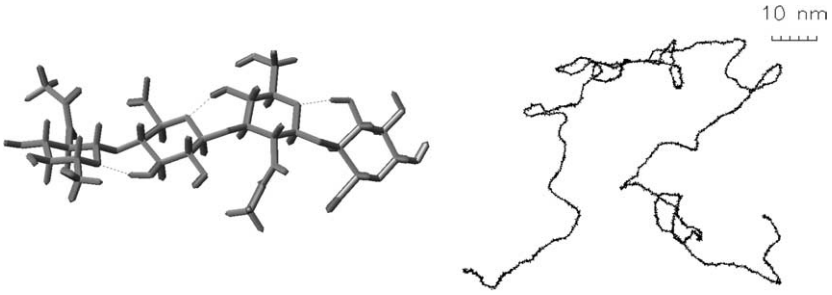
Proton NMR spin–spin relaxation rate dispersion curves, $1/T_2$ versus $\log_{10}(1/\tau)$, for a 20% w/w sucrose solution in water, measured by the CPMG pulse sequence, as a function of temperature, T.

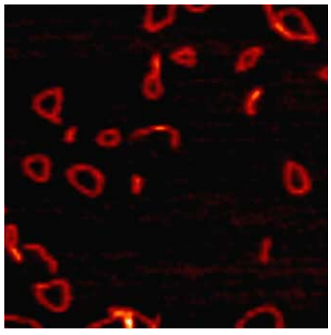


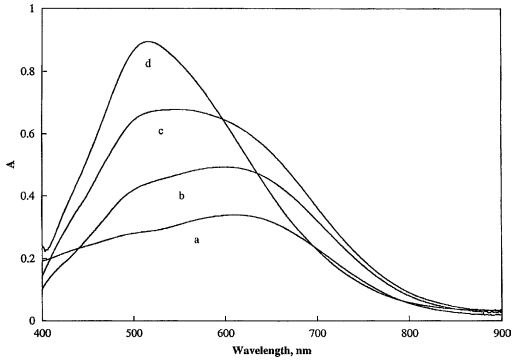


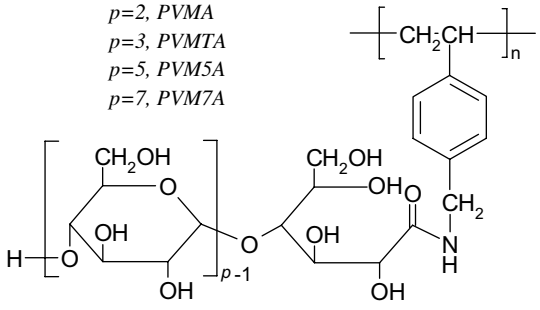


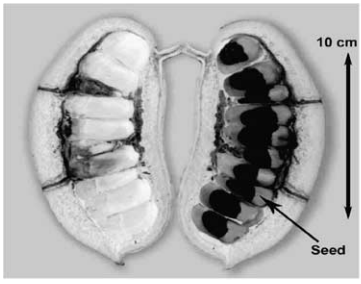




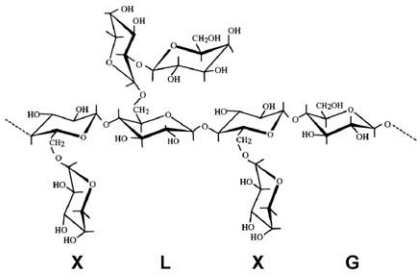




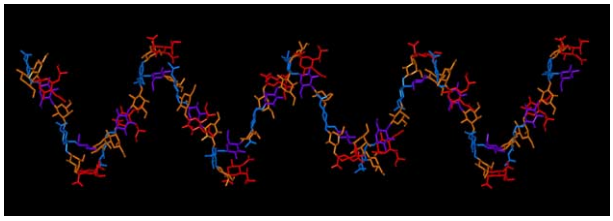




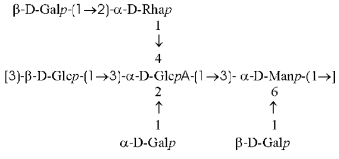
Afzelia africana **Se. Pers.** Pod and Seeds



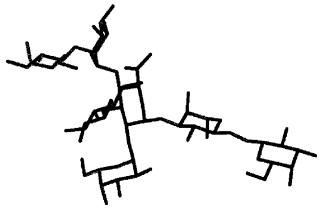
Representative xyloglucan tetrasaccharide unit



Helical structure (diameter of 29.3 Å and a pitch 89.5 Å) of the capsular polysaccharide from group B *Streptococcus* (serotype III), predicted by 50 ns MD simulations. The sialylated side-chains are arrayed on the exterior surface of the helix while the immunodominant epitope lines the core.



Sequence and minimum energy conformation of the repeating unit.



Molecular mechanics and molecular dynamics studies were carried out on Cepacian, the exopolysaccharide produced by the majority of clinical strains of the opportunistic pathogen *B. cepacia* involved in cystic fibrosis pulmonary infections.

*Corresponding author
Supplementary data available via ScienceDirect

COVER

Model of blood group A trisaccharide in the binding site of the *Dolichos biflorus* lectin as established by a combination of theoretical and experimental approaches. Molecular modeling of the oligosaccharide demonstrated that two different conformations could be adopted by the trisaccharide in the binding site. NMR experiments using transferred nuclear Overhauser effects (TRNOE) displayed intermolecular contacts (blue arrows) corresponding to only one of the two theoretical conformations. This work is a collaboration between Anne Imberty (CERMAV, Grenoble) and Thomas Peters (University of Lübeck) and was presented during the XXIInd International Carbohydrate Symposium (Glasgow, 2004) on the occasion of the Whistler award.

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