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Special Issue

Conformations of Oligo- and Poly-saccharides

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Editor: Derek Horton

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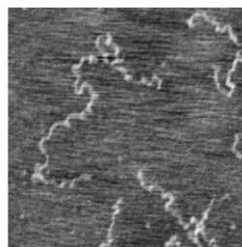
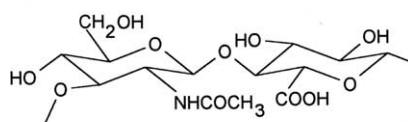
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Mary K. Cowman* and Shiro Matsuoka



Hyaluronan

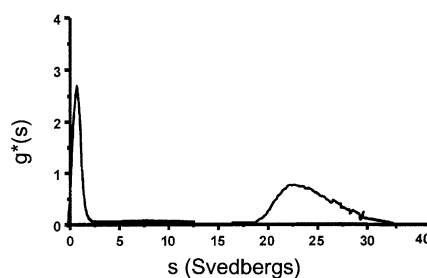
AFM image

Critical review of the literature on experimental analysis of hyaluronan structure and properties.

Challenges for the modern analytical ultracentrifuge analysis of polysaccharides

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Stephen E. Harding



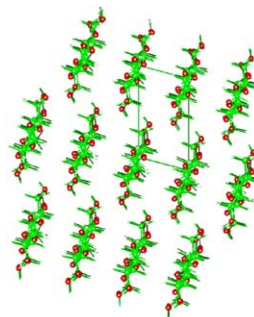
FULL PAPERS

Determining the crystal structure of cellulose III_I by modeling

pp 827–833

Zakhia M. Ford, Edwin D. Stevens, Glenn P. Johnson and Alfred D. French*

The minimized energies of 54 similar minicrystals were calculated to determine the most probable structure of cellulose III_I.

**Polysaccharide structures from powder diffraction data: molecular models of arabinan**

pp 835–839

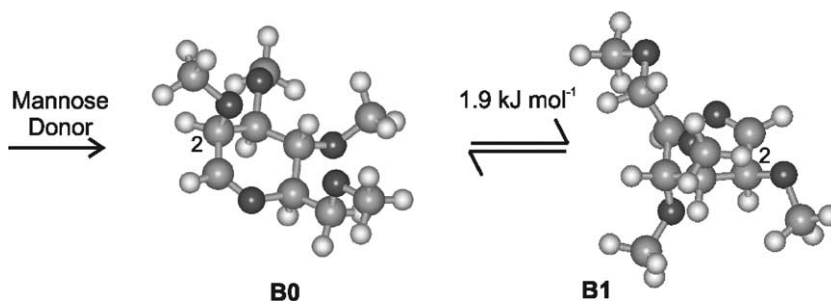
Srinivas Janaswamy and Rengaswami Chandrasekaran*

Molecular models of debranched arabinan, $[\rightarrow 5)\text{-}\alpha\text{-L-Araf-(1}\rightarrow)_n$, have been analyzed using X-ray powder diffraction data.

The two-conformer hypothesis: 2,3,4,6-tetra-*O*-methyl-mannopyranosyl and -glucopyranosyl oxacarbenium ions

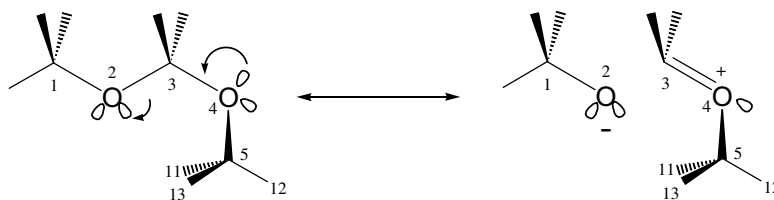
pp 841–852

Tomoo Nukada, Attila Bérces, LiJie Wang, Marek Z. Zgierski and Dennis M. Whitfield*

**The external-anomeric torsional effect**

pp 853–862

Jenn-Huei Lii, Kuo-Hsiang Chen, Glenn P. Johnson, Alfred D. French* and Norman L. Allinger*

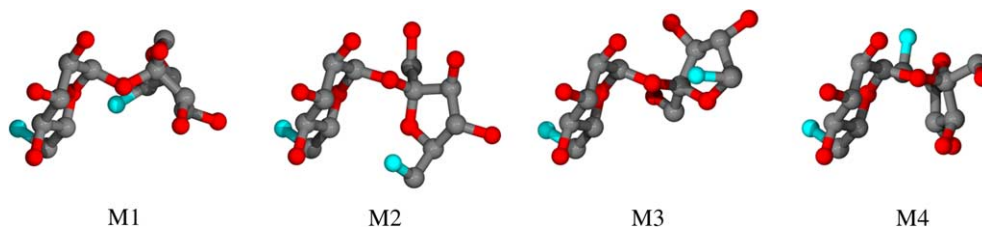


Torsional energies for rotation of an aglycon depend on the *exo*-anomeric conformation.

The utility of residual dipolar couplings in detecting motion in carbohydrates: application to sucrose

pp 863–874

Richard M. Venable, Frank Delaglio, Scott E. Norris and Darón I. Freedberg*

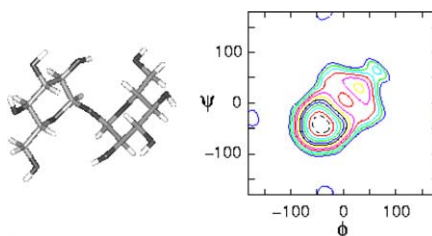


The solution structure and dynamics of sucrose are examined using a combination of NMR residual dipolar coupling and molecular mechanics force fields.

Ramachandran free-energy surfaces for disaccharides: trehalose, a case study

pp 875–879

Michelle M. Kuttel and Kevin J. Naidoo*

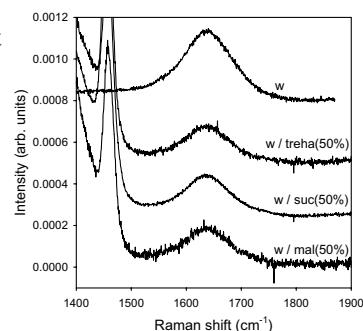


Free-energy surfaces for trehalose reveal that it is restricted to a single minimum-energy conformation in both vacuum and solution thus providing a molecular rationale for the antidesiccant properties of trehalose glasses.

Influence of homologous disaccharides on the hydrogen-bond network of water: complementary Raman scattering experiments and molecular dynamics simulations

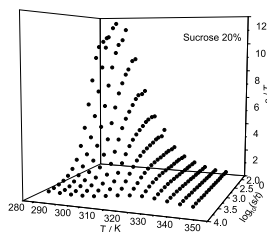
pp 881–887

Adrien Lerbret,* Patrice Bordat, Frédéric Affouard,
Yannic Guinet, Alain Hédoux, Laurent Paccou, Dominique Prévost
and Marc Descamps

**Water T_2 relaxation in sugar solutions**

pp 889–905

Deborah Fabri, Martin A. K. Williams and Thomas K. Halstead*

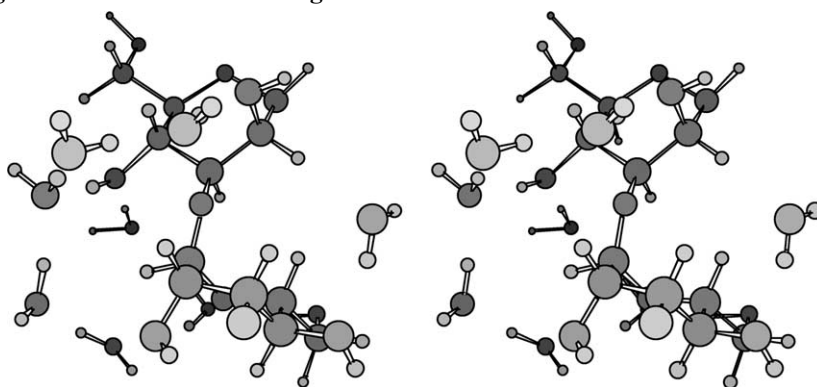


Proton NMR spin–spin relaxation rate dispersion curves, $1/T_2$ versus $\log_{10}(1/\tau)$, for a 20% w/w sucrose solution in water, measured by the CPMG pulse sequence, as a function of temperature, T .

Towards understanding the interaction between oligosaccharides and water molecules

pp 907–920

Andrew Almond

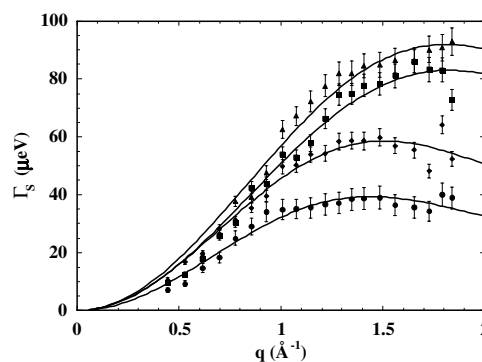


Proton fluctuations and water diffusion in dextran chemical hydrogels studied by incoherent elastic and quasielastic neutron scattering

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Gaio Paradossi,* Francesca Cavalieri and Ester Chiessi

Proton fluctuations related to local motions of the glycosidic linkages of chemically crosslinked dextran hydrogels with well defined pore-size distributions are studied by static and dynamic neutron-scattering approaches.

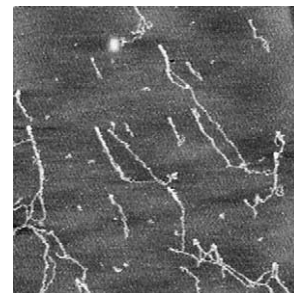


Hyaluronan conformations on surfaces: effect of surface charge and hydrophobicity

pp 929–941

Chiara Spagnoli, Alexander Kornikov, Abraham Ulman, Endre A. Balazs, Yuri L. Lyubchenko and Mary K. Cowman*

Extended, relaxed, condensed, and interacting forms of the polysaccharide hyaluronan on surfaces of mica and graphite have been observed by atomic force microscopy (AFM).

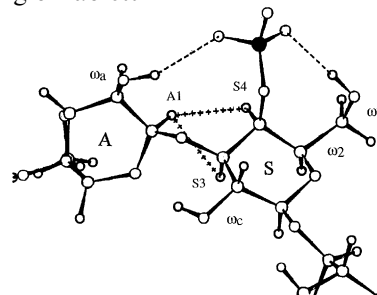


The disordered conformation of κ-carrageenan in solution as determined by NMR experiments and molecular modeling

pp 943–958

Marco Bosco, Annalaura Segre, Stanislav Miertus, Attilio Cesàro and Sergio Paoletti*

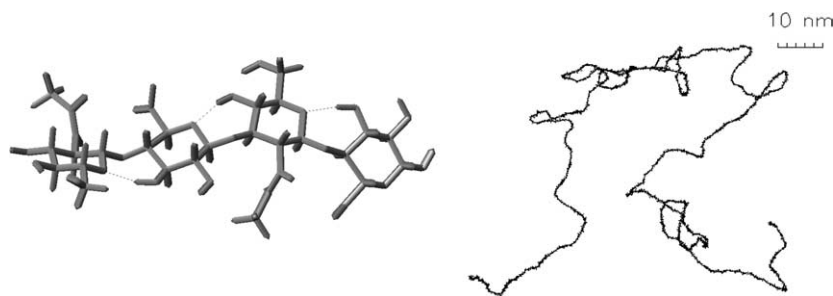
The conformation of κ-carrageenan in solution was studied combining ^1H and ^{13}C NMR with molecular mechanics.



Hyaluronan chain conformation and dynamics

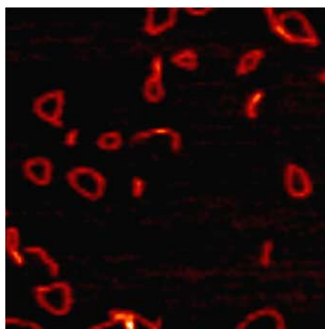
pp 959–970

Sara Furlan, Giovanni La Penna, Angelo Perico and Attilio Cesàro*

**Probing macromolecular architectures of nanosized cyclic structures of (1→3)-β-D-glucans by AFM and SEC-MALLS**

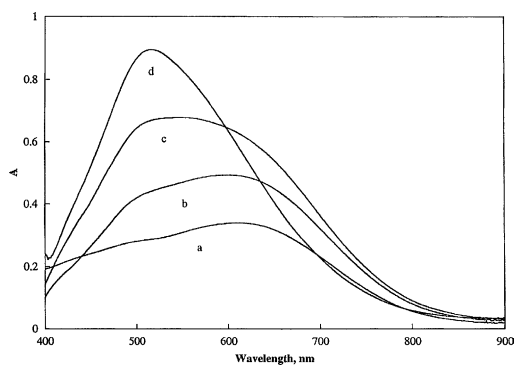
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Marit Sletmoen, Bjørn E. Christensen and Bjørn T. Stokke*

**The complex of xylan and iodine: the induction and detection of nanoscale order**

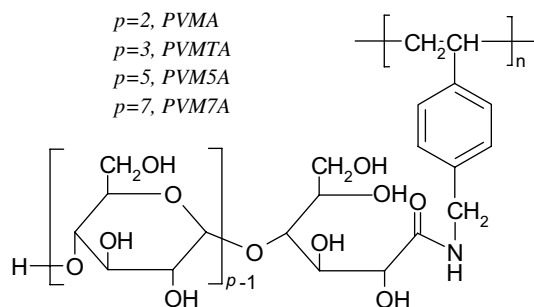
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Xiaochun Yu and Rajai H. Atalla*

**Effect of the carbohydrate side-chain on the conformation of a glycoconjugate polystyrene in aqueous solution**

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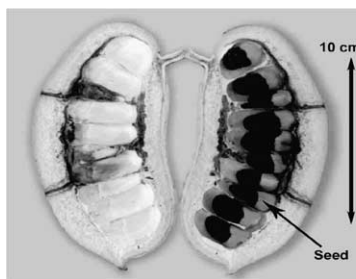
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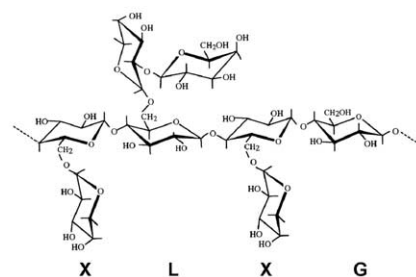
A novel xyloglucan from seeds of *Azelia africana* Se. Pers.—extraction, characterization, and conformational properties

pp 997–1005

Yilong Ren, David R. Picout, Peter R. Ellis,
Simon B. Ross-Murphy* and J. S. Grant Reid



Azelia africana Se. Pers. Pod and Seeds

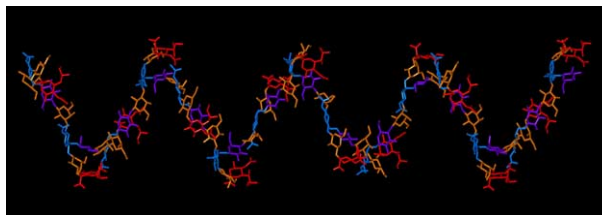


Representative xyloglucan tetrasaccharide unit

Structural elucidation of type III group B *Streptococcus* capsular polysaccharide using molecular dynamics simulations: the role of sialic acid

pp 1007–1018

Jorge González-Outeiriño, Renuka Kadirvelraj and Robert J. Woods*



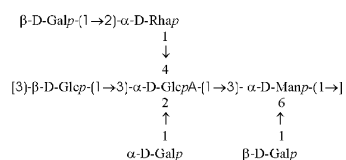
Helical structure (diameter of 29.3 Å and a pitch 89.5 Å) of the capsular polysaccharide from group B *Streptococcus* (serotype III), predicted by 50 ns MD simulations. The sialylated side-chains are arrayed on the exterior surface of the helix while the immunodominant epitope lines the core.



Conformation of the exopolysaccharide of *Burkholderia cepacia* predicted with molecular mechanics (MM3) using genetic algorithm search

pp 1019–1024

Francesco Strino, Abraham Nahmany, Jimmy Rosen, Graham J. L. Kemp,
Isabel Sá-correia and Per-Georg Nyholm*



Sequence and minimum energy conformation of the repeating unit.



Conformational features of cepacian: the exopolysaccharide produced by clinical strains of *Burkholderia cepacia*

pp 1025–1037

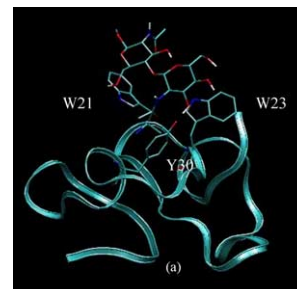
Carlos E. Sampaio Nogueira, Jose R. Ruggiero, Paola Sist, Paola Cescutti, Ranieri Urbani* and Roberto Rizzo

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.

A dynamic perspective on the molecular recognition of chitooligosaccharide ligands by hevein domains pp 1039–1049

Giorgio Colombo,* Massimiliano Meli, Javier Cañada, Juan Luis Asensio and Jesus Jimenez-Barbero*

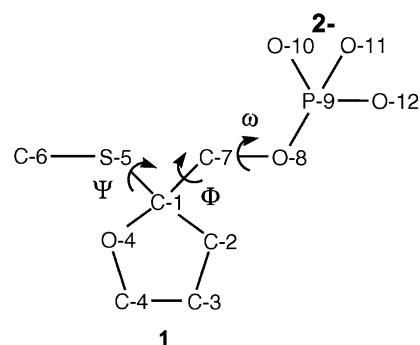
We study, through molecular-dynamics simulations, the complexes between hevein and different chitin oligomers, from the di- to the penta-saccharide.

**Potential transition-state analogs for glycosyltransferases. Design and DFT calculations of conformational behavior**

pp 1051–1057

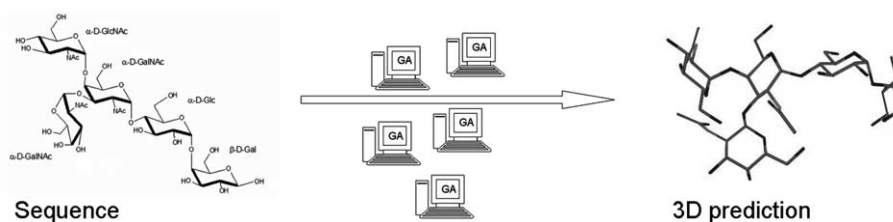
Michal Raab, Stanislav Kozmon and Igor Tvaroška*

The structure of a previously calculated transition state (TS) was used to design the [tetrahydro-2-(methylthio)furan-2-yl]methyl phosphate dianion (**1**) as a new scaffold for transition-state analogs of reactions catalyzed by the inverting glycosyltransferases.


**The use of a genetic algorithm search for molecular mechanics (MM3)-based conformational analysis of oligosaccharides**

pp 1059–1064

Abraham Nahmany, Francesco Strino, Jimmy Rosen, Graham J. L. Kemp and Per-Georg Nyholm*



*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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