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Special Issue

Molecular Modeling of Carbohydrates

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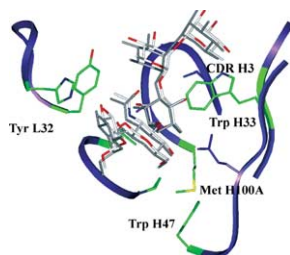
Contents

Foreword pp 905–906

REVIEWS

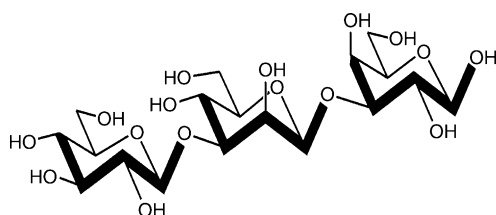
NMR spectroscopic and molecular modeling studies of protein–carbohydrate and protein–peptide interactions pp 907–928

Margaret A. Johnson and B. Mario Pinto*



Web resources for the carbohydrate chemist pp 929–936

Olivier Berteau and Roland Stenutz*

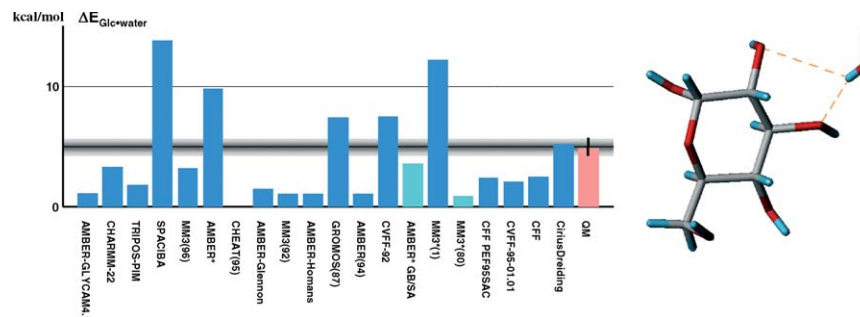


ARTICLES

Evaluation of carbohydrate molecular mechanical force fields by quantum mechanical calculations

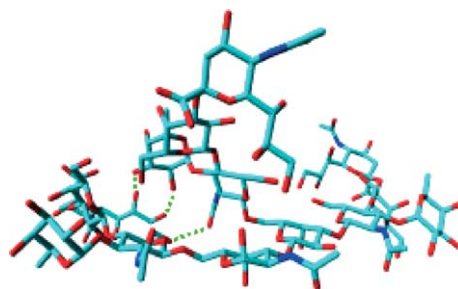
pp 937–948

Lars Hemmingsen,* Daniel E. Madsen, Anders L. Esbensen, Lars Olsen and Søren B. Engelsen

**Conformational analysis of complex oligosaccharides: the CICADA approach to the uromodulin O-glycans**

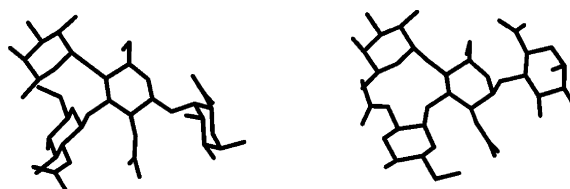
pp 949–959

Gianluca Cioci,* Alain Rivet, Jaroslav Koča and Serge Pérez*

**The conformations of the O-specific polysaccharides of *Shigella dysenteriae* type 4 and *Escherichia coli* O159 studied with molecular mechanics (MM3) filtered systematic search**

pp 961–966

Jimmy Rosen, Armin Robobi and Per-Georg Nyholm*

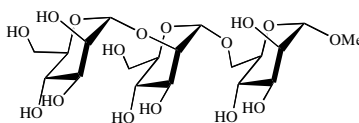


The minimum energy conformations of the branch tetrasaccharides of the two studied O-antigens—*E. coli* 159 (left) and *S. dysenteriae* type 4 (right).

Conformational analysis and dynamics of mannosides and mannotriosides using Monte Carlo/stochastic dynamics simulations

pp 967–973

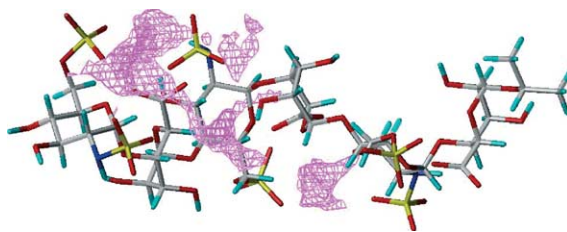
Anna Bernardi,* Andrea Colombo and Inmaculada Sánchez-Medina



The heparin–Ca²⁺ interaction: the influence of the O-sulfation pattern on binding

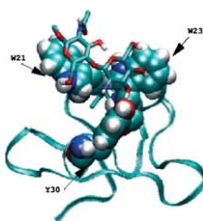
pp 975–983

Franck Chevalier, Ricardo Lucas, Jesús Angulo, Manuel Martin-Lomas and Pedro M. Nieto*

**Toward the understanding of the structure and dynamics of protein–carbohydrate interactions: molecular dynamics studies of the complexes between hevein and oligosaccharidic ligands**

pp 985–994

Giorgio Colombo,* Massimiliano Meli, Javier Cañada, Juan Luis Asensio and Jesús Jiménez-Barbero*

**Molecular dynamics simulations of glycosyltransferase LgtC**

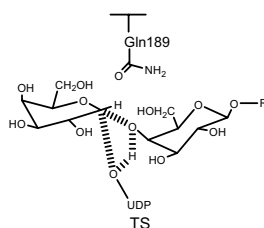
pp 995–1006

Lenka Šnajdrová, Petr Kulháněk, Anne Imberty and Jaroslav Koča*

**Molecular modeling insights into the catalytic mechanism of the retaining galactosyltransferase LgtC**

pp 1007–1014

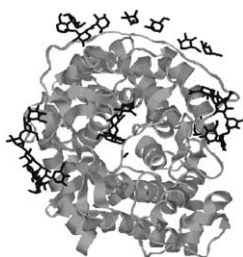
Igor Tvaroška*



The catalytic mechanism of the retaining glycosyltransferases LgtC was investigated using high level ab initio calculations. The preferred pathway is predicted to proceed by an unique A_ND_NA_HD_H type of mechanism. The determined structure of the transition state, in which the hydrogen bond between the nucleophile and the leaving group oxygens facilitates the attack of the acceptor O-4' from the same side of the transferred galactose is exceptional and provides valuable information for designing stable analogues of TS as potent inhibitors of the bacterial LgtC.

Data mining the protein data bank: automatic detection and assignment of carbohydrate structures**pp 1015–1020**

Thomas Lütteke,* Martin Frank and Claus-W. von der Lieth



*Corresponding author

i* Supplementary data available via ScienceDirect

COVER

Well-defined glycoforms of glycoproteins can easily be obtained by oxidative coupling of synthetic thioaldoses with proteins that have a cysteine moiety in lieu of an asparagine residue carrying natural N-linked oligosaccharides. In vitro glycosylation offers several advantages such as quantitative conjugation, incorporation of oligosaccharides that display high bioactivities and the possibility of using convenient bacterial or yeast protein expression systems. The figure is related to Geert-Jan Boons' *Carbohydrate Research Award* paper, *Carbohydr. Res.*, **2004**, 339, 181–193.



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