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Carbohydrate
RESEARCH

Carbohydrate Research Vol. 339, No. 5, 2004

Special Issue

Molecular Modeling of Carbohydrates

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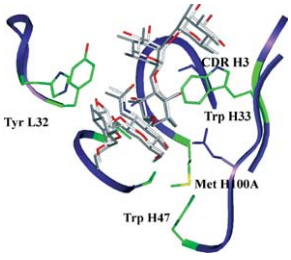

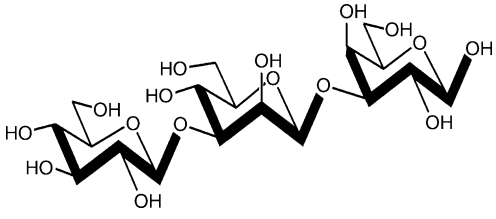

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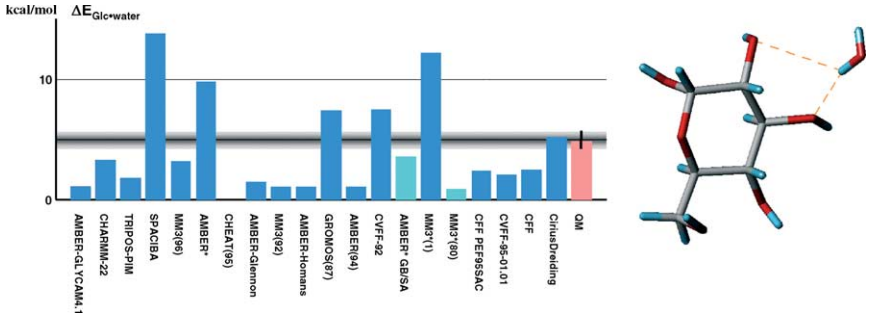
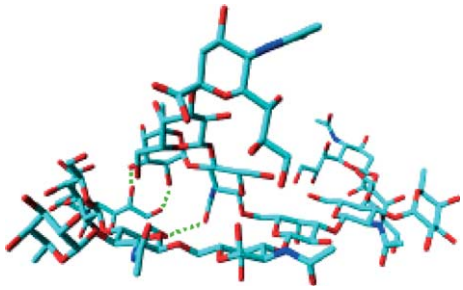
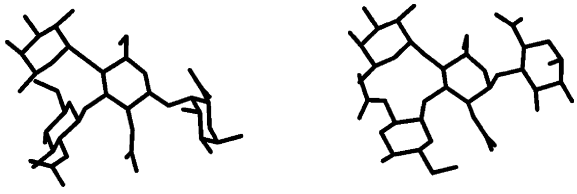
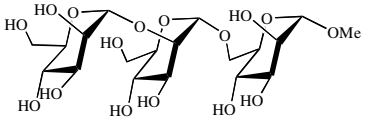
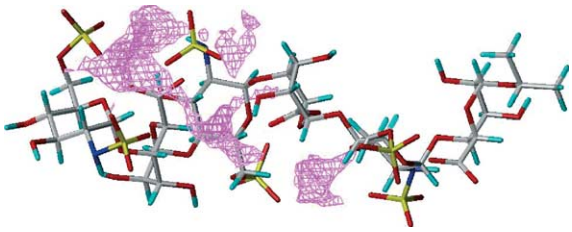


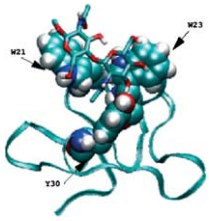


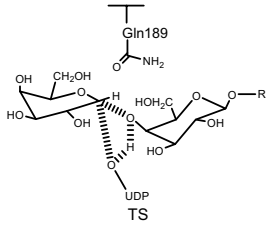


The minimum energy conformations of the branch tetrasaccharides of the two studied O-antigens—*E. coli* 159 (left) and *S. dysenteriae* type 4 (right).

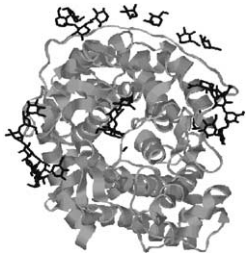








The catalytic mechanism of the retaining glycosyltransferases LgtC was investigated using high level ab initio calculations. The preferred pathway is predicted to proceed by an unique $A_ND_NA_HD_H$ type of mechanism. The determined structure of the transition state, in which the hydrogen bond between 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.



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ⓘ+ 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.

Indexed/Abstracted in: Chem. Abstr.: Curr. Contents: Phys., Chem. & Earth Sci. Life Sci. Current Awareness in Bio. Sci (CABS). Full texts are incorporated in CJELSEVIER, a file in the Chemical Journals Online database which is availabe on STN® International.

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ISSN 0008-6215