Carbohydrate-Lectin Interactions - An Unexpected Contribution to Affinity

JournalArticle (Originalarbeit in einer wissenschaftlichen Zeitschrift)

ID 3719751
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Year 2017
Title Carbohydrate-Lectin Interactions - An Unexpected Contribution to Affinity
Journal ChemBioChem
Volume 18
Number 6
Pages / **Article-Number** 539-544
Uropathogenic E. coli exploit the PapG-II adhesin for infecting host cells of the kidney; moreover, the expression of PapG-II located at the tip of bacterial pili has been correlated with the onset of pyelonephritis in humans, a potentially life-threatening condition. It was envisaged that the blocking of PapG-II, and thus bacterial adhesion, embodies a viable therapeutic alternative to conventional antibiotic treatment. Within our search for potent PapG-II antagonists, we observed an increase in affinity when tetrasaccharide 1, the natural ligand of PapG-II in human kidneys, was elongated to hexasaccharide 2, although the additional Siaα(2-3)Gal extension is not in direct contact with the lectin. ITC studies suggest that the increased affinity results from partial desolvation of non-binding regions of the hexasaccharide, and is ultimately connected to the perturbation of outer hydration layers. Our results are in agreement with previous observations and suggest a general mechanism for modulating carbohydrate-protein interactions based on non-binding regions of the ligand.
Publisher Wiley
ISSN/ISBN 1439-4227 ; 1439-7633
edoc-URL http://edoc.unibas.ch/53270/
Full Text on edoc No;
Digital Object Identifier DOI 10.1002/cbic.201600615
PubMed ID http://www.ncbi.nlm.nih.gov/pubmed/28076665
ISI-Number WOS:000397472800009
Document type (ISI) Journal Article