OMICS International
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J Glycobiol 2015, 3:3
http://dx.doi.org/10.4172/2168-958X.S1.003

# Glycobiology World Congress

August 10-12, 2015 Philadelphia, USA

## Conformational properties of the antigenic determinant of a *Salmonella* polysaccharide using enhanced sampling MD simulations

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*Salmonella* infection is a common bacterial disease that causes approximately 1.2 million illnesses in the US according to the Centers for Disease Control and Prevention. Antibodies targeting the O-antigen of *Salmonella* can mediate bacterial killing and thus vaccine development has been investigated using O-polysaccharide conjugates. The O-antigen consists of multiple repeating units of tetrasaccharide, [(3)-D-Galp--(12)[D-Abep--(13)]-D-Manp--(14)-D-Rhap--(1]$_n$. To provide more insights on the structural features of this polysaccharide and potentially facilitate the design of more potent vaccines, we studied the conformational preference of the O-polysaccharide with 3 repeating units in the absence and presence of the bound antibody or with O-acetylation at the C2 position of Abep and Rhap residues using the CHARMM36 force field with the recently developed replica exchange with concurrent solute scaling and Hamiltonian biasing method. Results suggest preferred conformations existing in different conditions the may be related to the antigenic potential of the polysaccharide.

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## Design and development of glycopeptides as multiple sclerosis diagnostic probe

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Post translational modifications such as glycosylation may play a fundamental role for specific auto antibody recognition. In particular glycoproteins may be recognized as not-self molecules by antibodies triggering the onset of severe autoimmune diseases. We have previously demonstrated that an aberrant N-glucosylation is a fundamental determinant of auto-Ab recognition in multiple sclerosis (MS). The N-glucosylated Asn present in the 30-50 fragment of the myelin oligodentrocyte glycoprotein (MOG (30-50)) is an immunogenic epitope responsible for the interaction with MS auto antibodies. Starting from this sequence we identified CSF114 (Glc) biomarker, a glycopeptides able to recognize by ELISA, specific IgM auto Abs in the sera of MS patient population. CSF114 was improved in its specificity and sensitivity leading to the optimized glycopeptides SP077. This showed a higher homology with CSF114 (Glc) but was able to detect higher antibody titers as compared to CSF114 (Glc). NMR and ESR experiments supported by computer simulations allowed characterizing the sequence of events that rule the antigenic activity of the mentioned immunogenic peptides. These studies show that the glycosidic moiety plays a pivotal role, first ruling the binding of the probe to the membrane and then in coordinating the interaction with the antibody. Our findings provide valuable hints to develop new effective MS glycosylated probes and propose an innovative methodological approach that is instrumental to investigate the functional mechanism of other biologically relevant glycopeptides.

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