

A STRUCTURAL MODEL FOR THE ANTIGENICITY OF TYPE III GROUP B *STREPTOCOCCUS*

Renuka Kadirvelraj¹, Jorge Gonzalez-Outeiriño¹, Meredith L Beckham²,
Michael G Ford³ and Robert J Woods^{1*}

¹*Complex Carbohydrate Research Center, University of Georgia, 315 Riverbend Road, Athens, Georgia 30602, USA.* ²*Hansen Life Sciences Research Building 421, 201 S. University Street, Purdue University, West Lafayette, Indiana 47907, USA.*

³*Department of Molecular Cardiology/NB20, Lerner Research Institute, Cleveland Clinic Foundation, 9500 Euclid Avenue, Cleveland, Ohio 44195, USA*
rwoods@ccrc.uga.edu

Group B Streptococcus is the leading cause of neonatal sepsis and meningitis. To establish the structural origin for the observed variation of antigenicity with capsular polysaccharide (CPS) sequence, a model for the minimal immune complex between the CPS of the most virulent serotype (III) and the variable fragment (Fv) of monoclonal antibody 1B1 is presented. The structure was generated through a combination of comparative modeling, molecular docking, and molecular dynamics simulation. The relationship between CPS sequence and antigenicity has been quantified and the mechanism whereby the neuraminic acid residues mediate affinity established. Based on the similarity of the solution conformation of the CPS with that in the theoretical antibody Fv-CPS complex, the origin of the reported conformational epitope is established.