The Effects of Glucosylation and O-Acetylation on the Conformation of Shigella Flexneri Serogroup 2 O-Antigen Vaccine Targets

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Supplementary Figure S1: Block averaging analysis calculated for the time series of end-to-end distance (a) and radius of gyration (b) of the 6 RU O-Ags. The blocked standard error (BSE) reaches a plateau for all the O-Ags, indicating convergence of the simulation. Further analysis reveals correlation times consistently less than 45 ns — much less than the simulation time of 1000 ns, indicating sufficient sampling.
Supplementary Figure S2: The 6 RU static models of the serotype Y backbone built by extrapolation of the dominant linkage conformations in the simulations which demonstrate the extremes in the polysaccharide motion. (a) A model with all linkages in the +ψ orientation. This creates an extended conformation and corresponds to the extended conformations (cluster Y1) only observed for Y. (b) The 6 RU model with linkages in the -ψ orientation produces a rounded conformation which corresponds to the conformations of 2a-3Ac. (c) The helical model produced by -ψ orientations in the A-B and B-C linkages with +ψ orientations in the C-D and D-A linkages which corresponds to the conformations observed in 2b.
Supplementary Figure S3: Vacuum PMF plots of the α-D-glucose-(1→4)-α-L-rhamnose linkage corresponding to the E-C linkages of 2a for: (a) the Glc-(1→4)-α-L-Rha disaccharide and (b) a full pentasaccharide 2a repeating unit. The presence of the adjacent rhamnose (residue B) sterically constrains the E-C linkage to two distinct conformations separated by an energy barrier of between 3-4 kcal.mol$^{-1}$. 