# Supporting Information:

# Effect of Acetylation on the Nanofibril Formation of Chitosan

Aarion Romany,[†] Gregory F. Payne,[‡] and Jana Shen[*,†]

† *Department of Pharmaceutical Sciences, University of Maryland School of Pharmacy, Baltimore, MD 21201*

‡ *Institute for Bioscience and Biotechnology Research, University of Maryland, College Park, MD 20742*

E-mail: jana.shen@rx.umaryland.edu

# List of Figures

# Supplemental figures

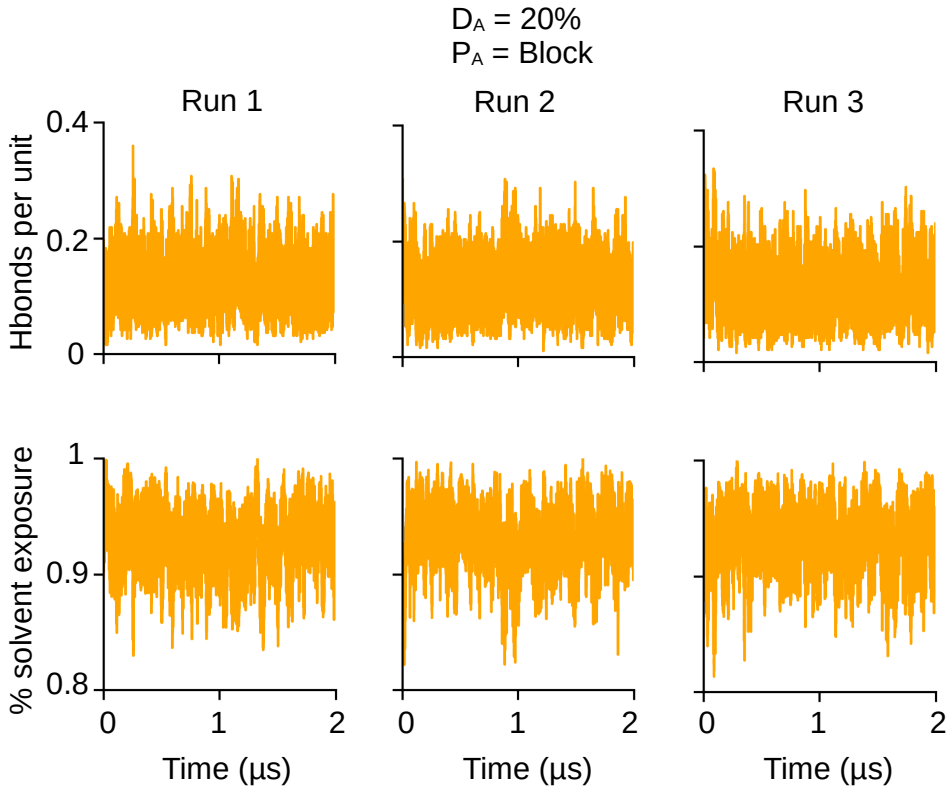


Figure S1: **Number of the interchain hydrogen bonds per acetylglucosamine (GlcAc) unit and percent solvent exposure at 20% DA as a function of simulation time.** A hydrogen bond is considered present if the heavy-atom donor-acceptor distance is below 3.5 Å and the donor-hydrogen-acceptor angle greater than 135°. Note, all 24 chains were used at each temperature. % solvent exposure is calculated as the solvent accessibility surface area (SASA) divided by the SASA of a fully solvent exposed chain. SASA is calculated using the LCPO algorithm of Weiser et al.[?]

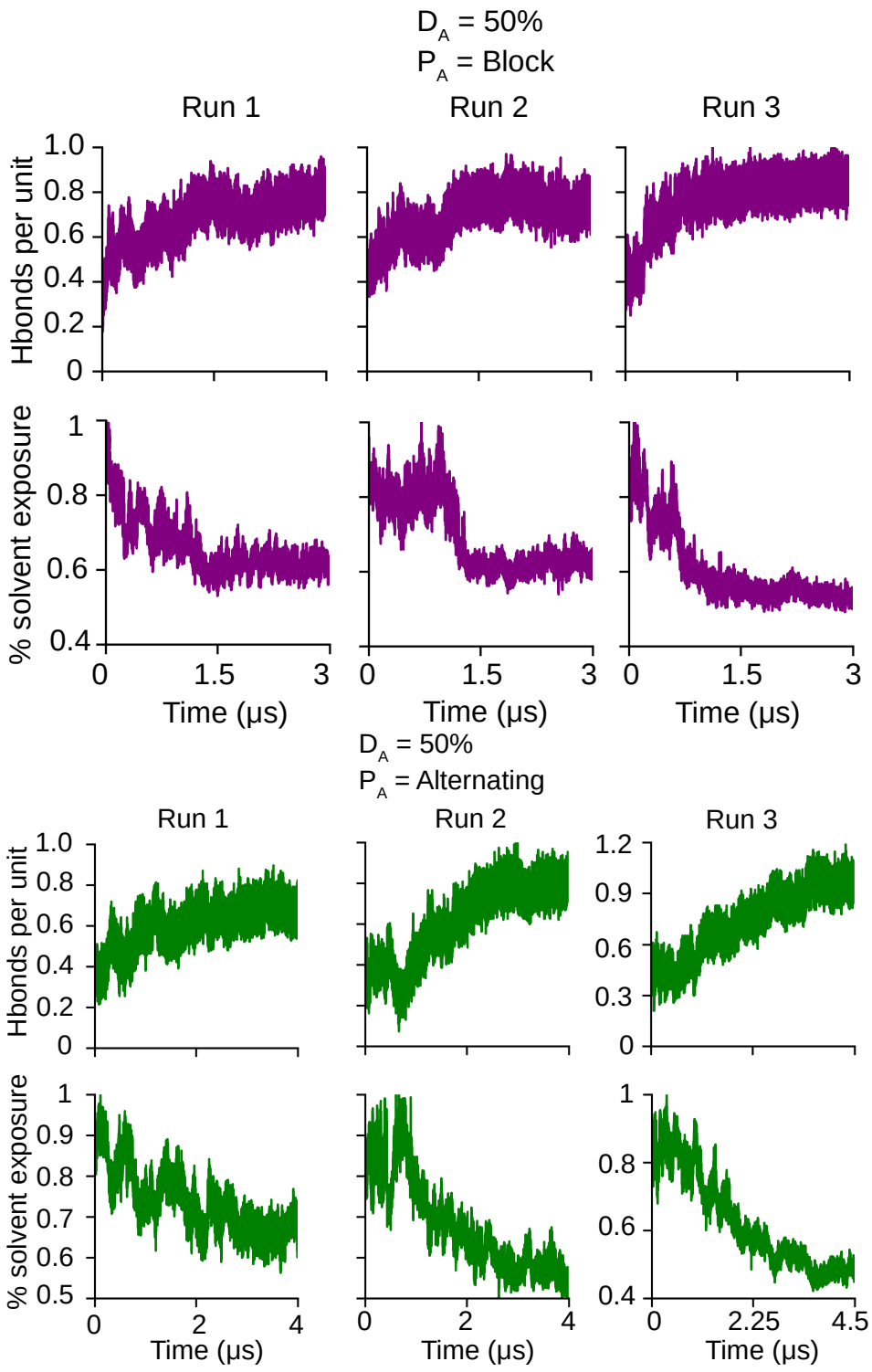


Figure S2: **Number of the interchain hydrogen bonds per acetylglucosamine (GlcAc) unit and percent solvent exposure as a function of simulation time for 50% DA chitosan chains with the block (top) and alternating (bottom) PA.**

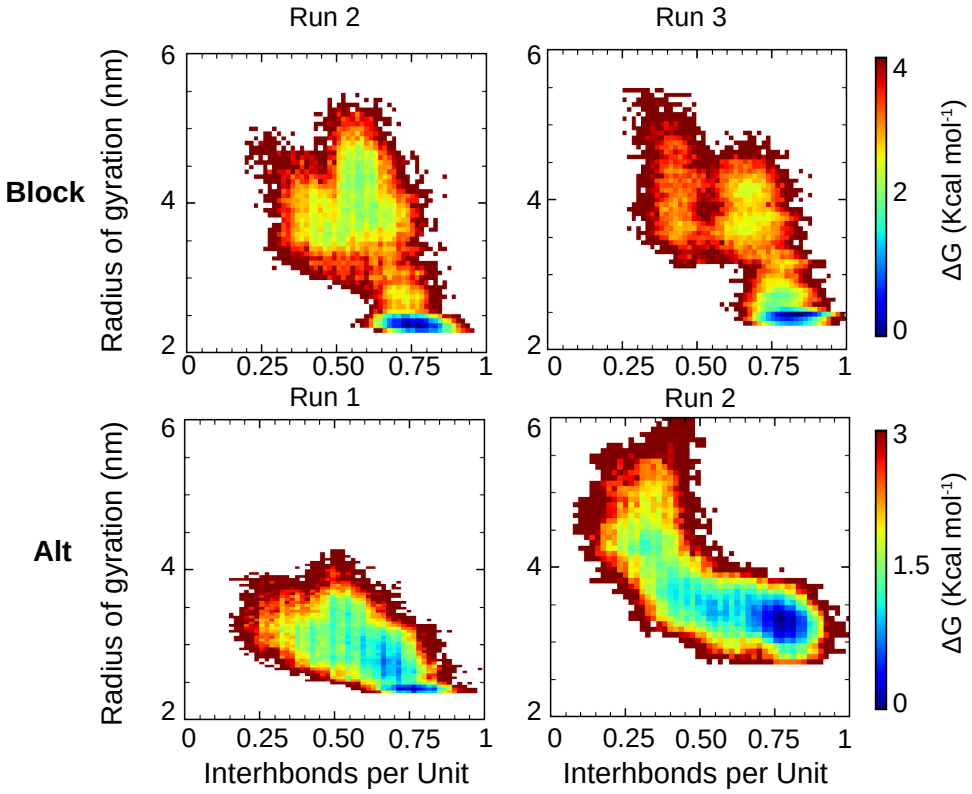


Figure S3: **Free energy as a function of the radius of gyration and intermolecular hbonds per unit for all runs of block and alternating pattern chitosan at 50% DA.** The entire simulation length was used in this calculation for each run.