Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

Critical role of dimer formation in monosaccharide binding to human serum albumin

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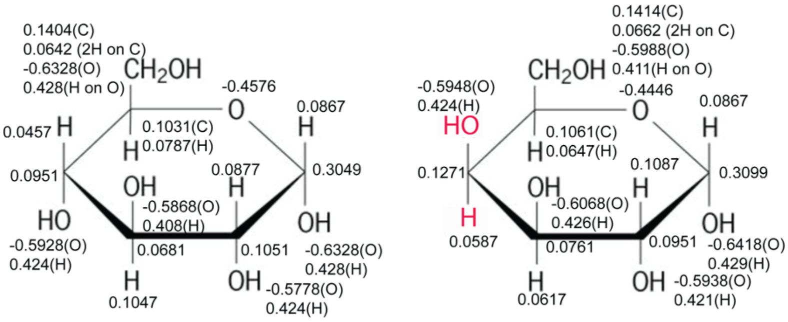
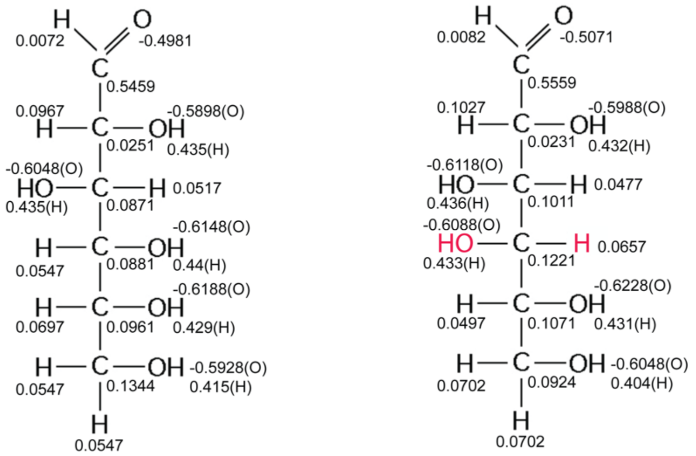


Glucose (GLC)

Galactose (GAC)



Glucose (GLO)

Galactose (GAO)

Figure S1. Calculated AM1-BCC charges of all glucose and galactose molecules.

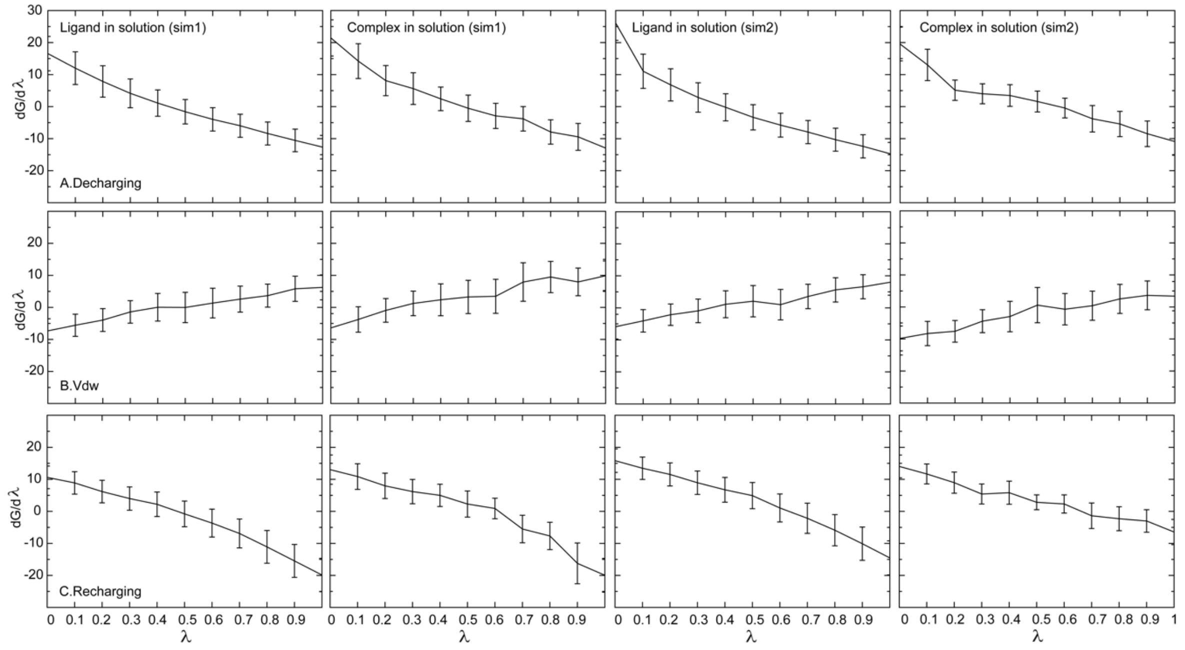


Figure S2. dG/dλ as a function of λ in the free energy perturbation calculations. Top, middle, and bottom rows are the steps for removing charges, changing vdW potentials and atom types, and recovering charges, respectively, and left to right columns describe the ligand (Sim1), ligand-HSA complex (Sim1), ligand (Sim2), and ligand-HSA complex (Sim2).

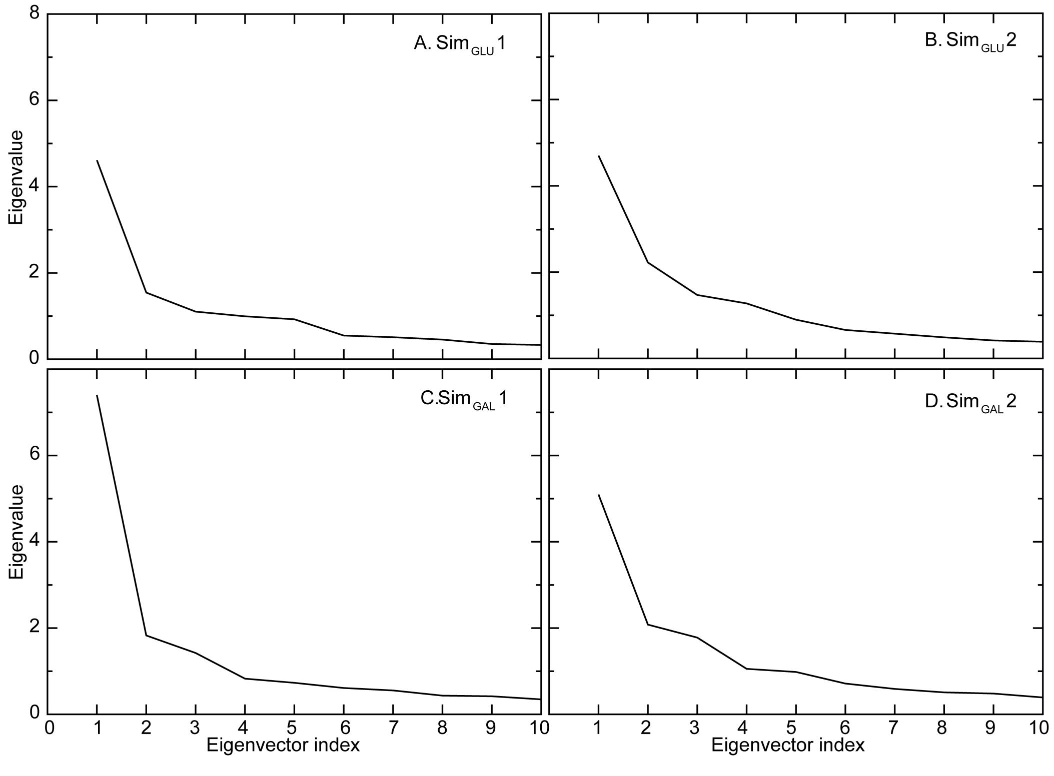


Figure S3. Eigenvalues from the principal component analysis applied to (A) Sim$_{GLU}$1, (B) Sim$_{GLU}$2, (C) Sim$_{GAL}$1, and (D) Sim$_{GAL}$2, respectively.

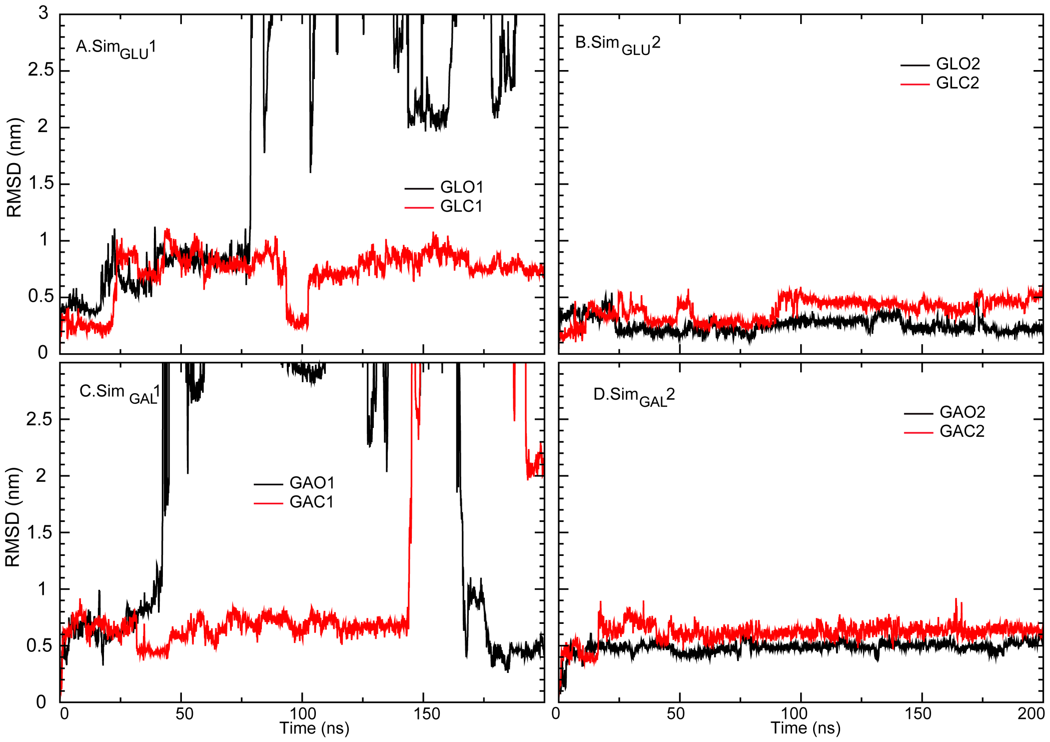


Figure S4. RMSDs of sugars calculated as a deviation from the snapshot at 0 ns. Each frame is first fitted to the structure at t=0 ns using C$_{\alpha}$ atoms, and the RMSD of sugar is evaluated without further fitting.

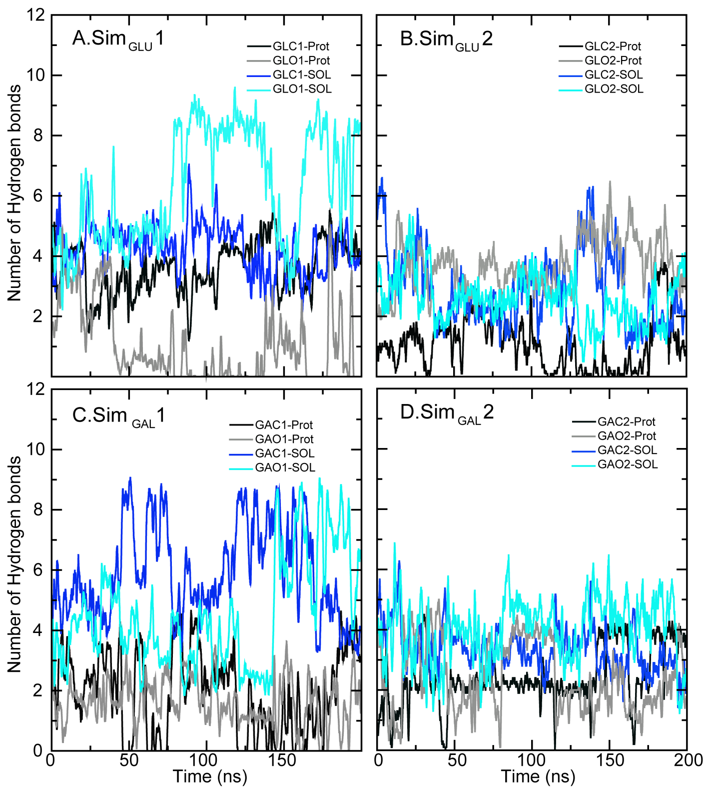


Figure S5. Number of sugar-protein and sugar-water hydrogen bonds found during the 200 ns-long simulations. Hydrogen bonds are counted as 1 when hydrogen-donor-acceptor angle is below 30º and the donor-acceptor distance is shorter than 0.35 nm.

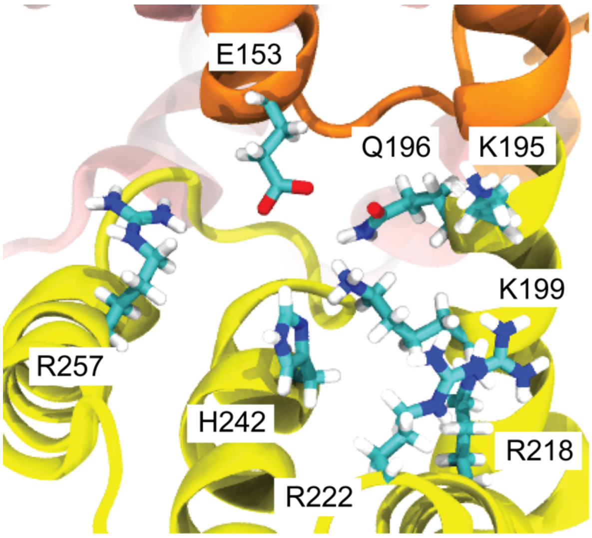


Figure S6. Key residues about the binding pocket inside subdomain IIA (yellow). Orange is subdomain IB.