

Supplementary Materials for **Origin of the blueshift of water molecules at interfaces of hydrophilic cyclic compounds**

Katsufumi Tomobe, Eiji Yamamoto, Dušan Kojić, Yohei Sato, Masato Yasui, Kenji Yasuoka

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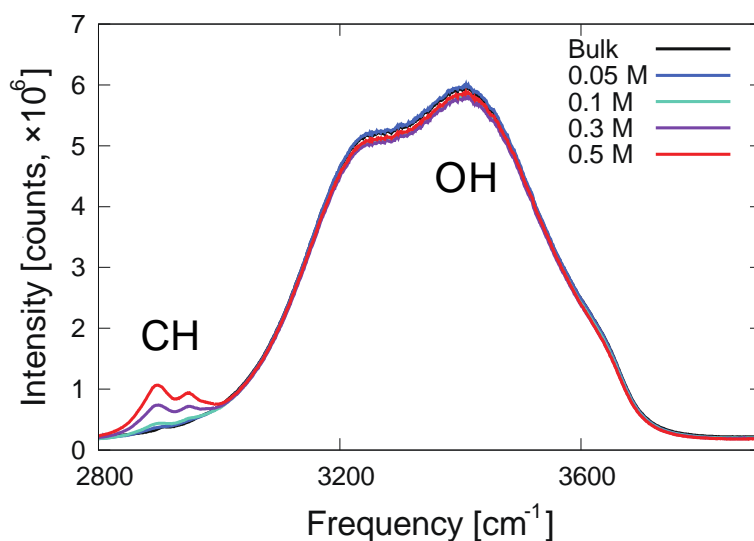


fig. S1. Raman spectra of D-glucose solutions at concentrations between 0 and 0.5 M.

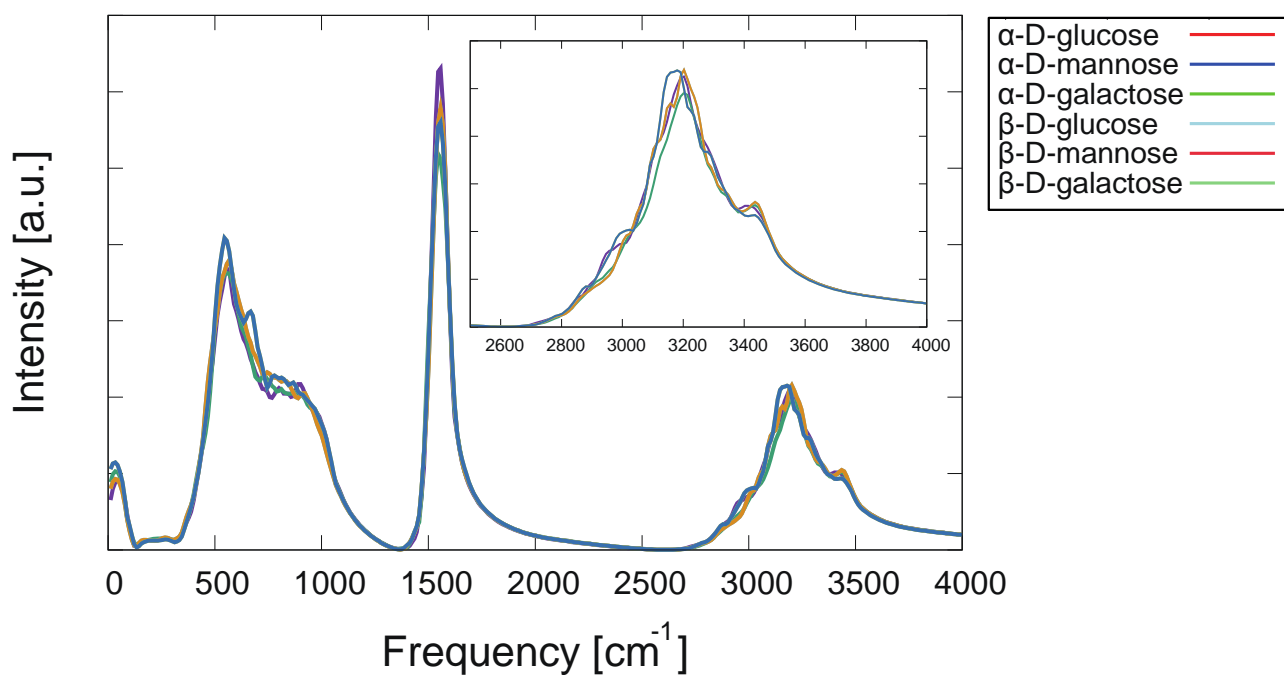


fig. S2. OH vibrational spectra for all water molecules in the system obtained by CPMD simulations. The spectra were obtained by the Fourier transform of the OH relative velocity correlation function. The Loess method was used for smoothing. The results are in good agreement with the water spectra obtained experimentally¹.

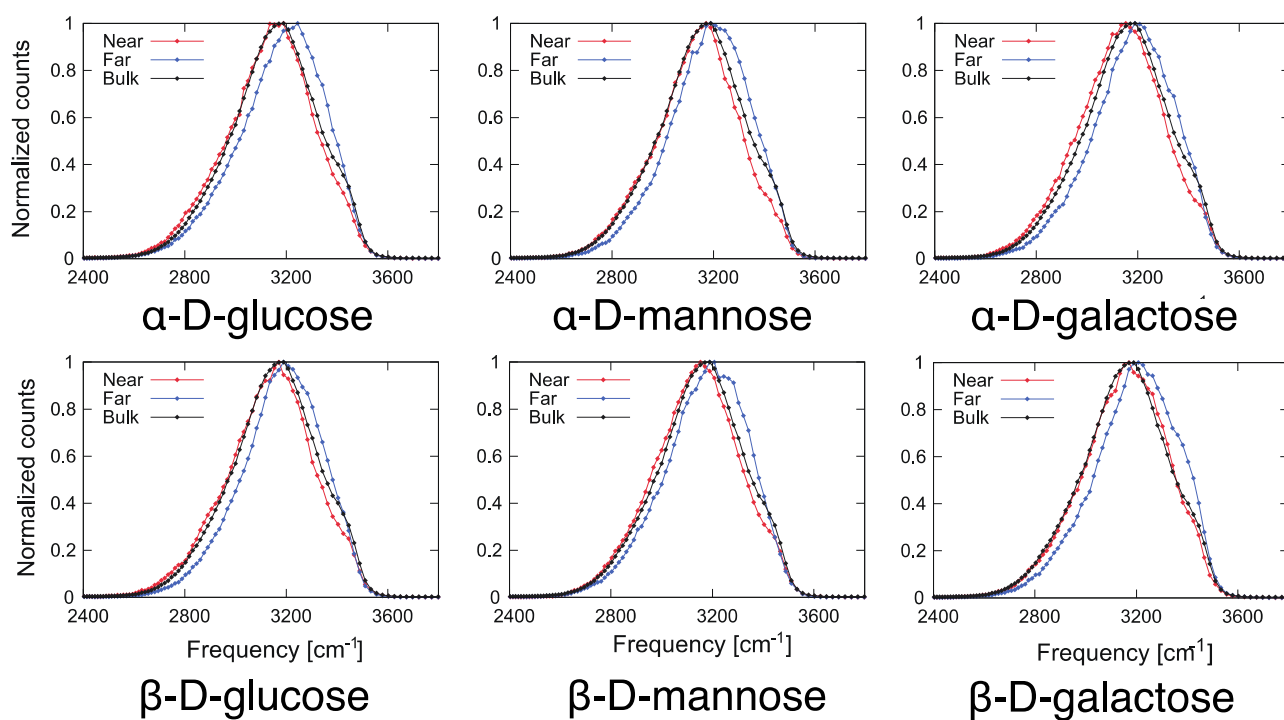


fig. S3. OH vibrational spectra of water molecules within 3.5 Å of all isomers. The spectra were obtained by the wavelet analysis. Red and blue lines show “near” and “far” OH bonds from monosaccharide oxygen atoms.

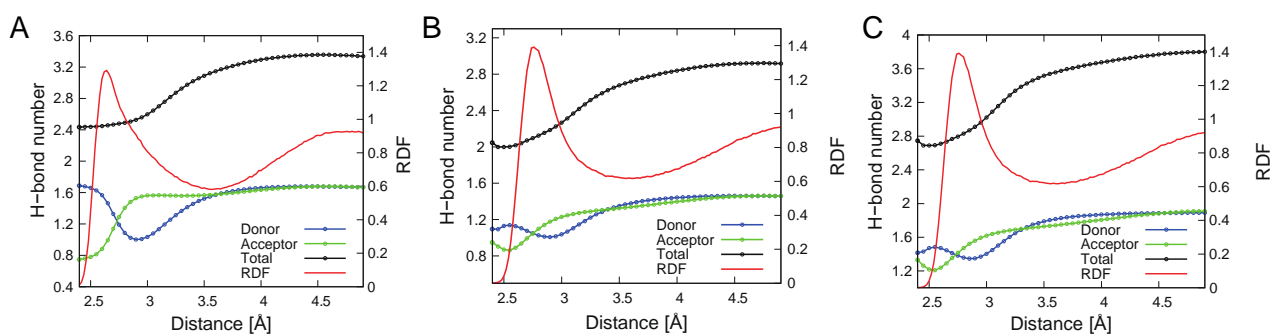


fig. S4. Average number of H-bonds between water molecules and RDF as a function of the distance between the oxygen atoms of monosaccharide and water molecules. (A) These results were obtained by the classical MD simulations of α -D-glucose solution at 298 K and 0.1 M using TIP5P water model. (B)(C) Different H-bond criteria using TIP3P water model with (B) $R_{oo} \leq 3.3$ Å, and $\theta \leq 25^\circ$ and (C) $R_{oo} \leq 3.7$ Å, and $\theta \leq 35^\circ$.

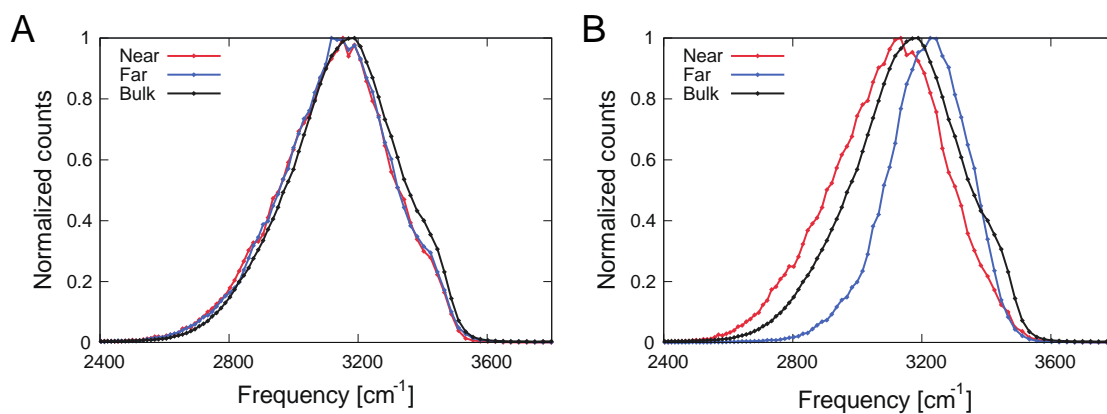


fig. S5. Spectra and water arrangement of water molecules in the NaBr solution. (A and B) “near” and “far” OH vibrational spectra of water molecules in the first hydration shell of Na⁺ and Br⁻, respectively.

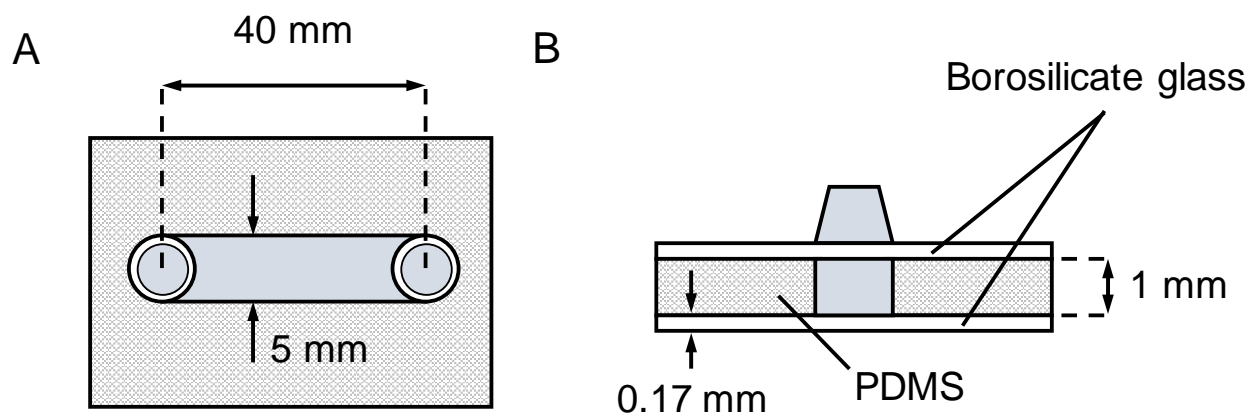


fig. S6. I-shaped channel used for Raman experiments. (A) top view and **(B)** cross sectional view of the I-shaped channel are illustrated.