Cooperative Adsorption of Trehalose to DPPC Monolayers at the Water-Air Interface Studied with Vibrational Sum Frequency Generation

Katie A Link,[a] Gabrielle N. Spurzem,[a] Aashish Tuladhar,[c] Zizwe Chase,[d] Zheming Wang,[c] Hongfei Wang[e] and Robert A. Walker[a,b]*

a. Department of Chemistry and Biochemistry, Montana State University, Bozeman, MT 59717, USA

b. Montana Materials Science Program, Montana State University, Bozeman, MT, 59717, USA

c. Physical Sciences Division, Physical and Computational Sciences Directorate, Pacific Northwest National Laboratory, Richland, Washington, 99352, USA

d. Department of Physics and Astronomy, Howard University, Washington, D.C., 20059, USA

e. Department of Chemistry and Shanghai Key Laboratory of Molecular Catalysis and Innovative Materials, Fudan University, Shanghai, 200433, China

Corresponding Author: rawalker@montana.edu

Supporting Information

Supporting Information

VSFG spectra were acquired in the OH stretching region from DPPC monolayers at two different surface coverages on top of solutions containing different amounts of the disachharide trehalose. Spectra were acquired under SSP polarization conditions using an EKSPLA spectrometer assembly (EKSPLA PL2251A-50) at the Environmental Molecular Sciences Laboratory (EMSL) at the Pacific Northwest National Laboratory (Richland, WA). Briefly, this spectrometer (EKSPLA) utilizes a Nd:YAG laser (EKSPLA PL2251A-50) with a 29 ps pulse at 10 Hz. Part of this fundamental output is converted from 1064 nm to a visible (532 nm) beam. The remaining fundamental is sent to an OPA to produce IR light that is tunable from 650 cm^{-1} to 4300 cm^{-1}. One point to note is that data acquired with the scanning SFG system were not referenced to any external standard so band intensities, especially at the extreme edges of the spectral range covered, were subject to greater uncertainties in their relative concentrations.

[1] O-H Region Spectra

Additional spectra were taken in the OH region using methods and instruments that have been described in previous publications.[1-6] Intensity in the water region did not vary considerably due to changes in Tre subphase concentration.

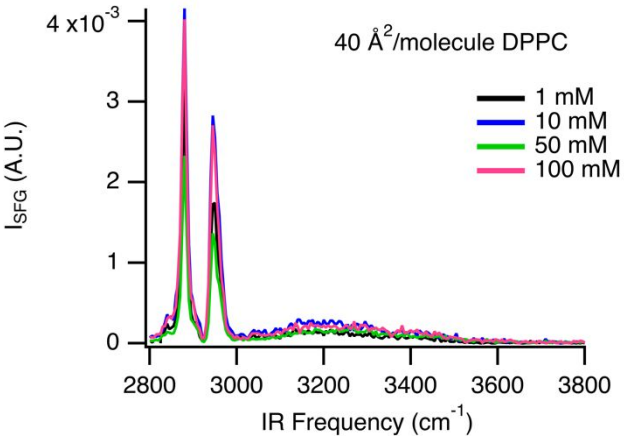

Figure S1: O-H vibrational region for 40 Å^2/molecule DPPC on various concentrations of Tre/Millipore solutions. In these experiments, the SFG spectrometer was optimized to collect data in the O-H stretching region.

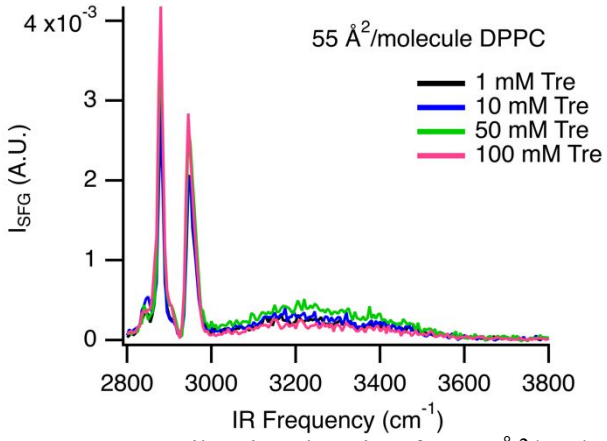

Figure S2: O-H vibrational region for 55 Å^2/molecule DPPC on various concentrations of Tre/Millipore solutions.

1. Burrows, S. M.; Gobrogge, E.; Fu, L.; Link, K.; Elliott, S. M.; Wang, H.; Walker, R., OCEANFILMS-2: Representing coadsorption of saccharides in marine films and potential impacts on modeled marine aerosol chemistry. *Geophysical Research Letters* **2016,** *43* (15), 8306-8313.
2. Link, K. A.; Spurzem, G. N.; Tuladhar, A.; Chase, Z.; Wang, Z.; Wang, H.; Walker, R. A., Organic Enrichment at Aqueous Interfaces: Cooperative Adsorption of Glucuronic Acid to DPPC Monolayers Studied with Vibrational Sum Frequency Generation. *J Phys Chem A* **2019,** *123* (26), 5621-5632.
3. Liu, W.; Fu, L.; Wang, Z.; Sohrabpour, Z.; Li, X.; Liu, Y.; Wang, H. F.; Yan, E. C. Y., Two Dimensional Crowding Effects on Protein Folding at Interfaces Observed by Chiral Vibrational Sum Frequency Generation Spectroscopy. *Phys. Chem. Chem. Phys.* **2018,** *20* (35), 22421-22426.
4. Lu, Z.; Karakoti, A.; Velarde, L.; Wang, W. N.; Yang, P.; Thevuthasan, S.; Wang, H. F., Dissociative Binding of Carboxylic Acid Ligand on Nanoceria Surface in Aqueous Solution: A Joint In Situ Spectroscopic Characterization and First-Principles Study. *J. Phys. Chem. C* **2013,** *117* (46), 24329-24338.
5. Mifflin, A. L.; Velarde, L.; Ho, J.; Psciuk, B. T.; Negre, C. F.; Ebben, C. J.; Upshur, M. A.; Lu, Z.; Strick, B. L.; Thomson, R. J.; Batista, V. S.; Wang, H. F.; Geiger, F. M., Accurate Line Shapes From sub-1 cm(-1) Resolution Sum Frequency Generation Vibrational Spectroscopy of Alpha-Pinene at Room Temperature. *J. Phys. Chem. A* **2015,** *119* (8), 1292-1302.
6. Olenick, L. L.; Chase, H. M.; Fu, L.; Zhang, Y.; McGeachy, A. C.; Dogangun, M.; Walter, S. R.; Wang, H. F.; Geiger, F. M., Single-Component Supported Lipid Bilayers Probed Using Broadband Nonlinear Optics. *Phys. Chem. Chem. Phys.* **2018,** *20* (5), 3063-3072.