Supporting Information: Modeling Ion Specific Effects: Toward the Correlations with Hydrophobic Solvation via Aqueous Interfacial Fluctuations

Shu-Ching Ou

Sealy Center for Structural Biology and Molecular Biophysics,

University of Texas Medical Branch, 301 University Boulevard, Galveston, Texas 77555, USA

Di Cui and Sandeep Patel*

Department of Chemistry and Biochemistry, University of Delaware, Newark, Delaware 19716, USA

*Corresponding author. E-mail: sapatel@udel.edu

I. POTENTIAL OF MEAN FORCE: SINGLE ALKANE & ALCOHOL TRANSFERRING THE AIR-WATER INTERFACE

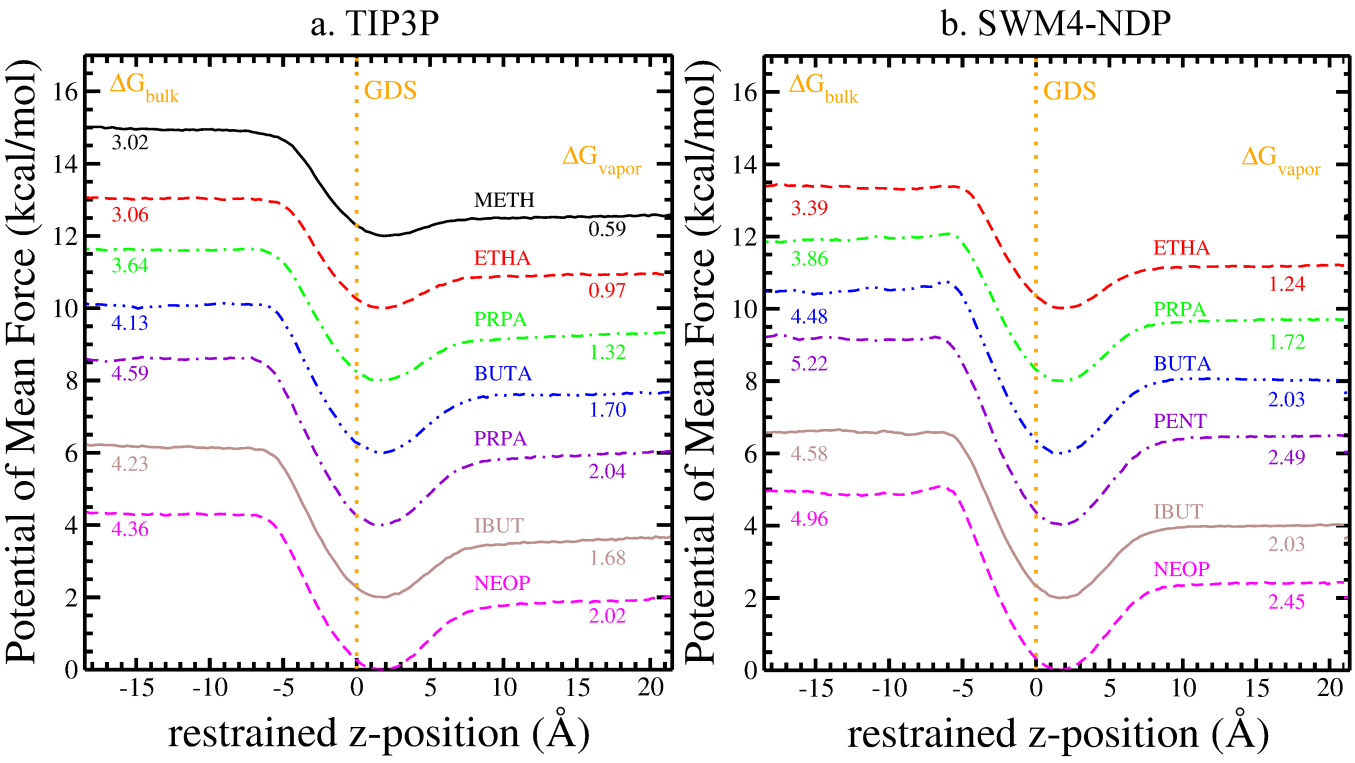

FIG. S1: Potential of mean force as a function of the z-position of a single alkane along the direction normal to the (a) TIP3P (b) SWM4-NDP water surface. An offset of 2 kcal/mol is added at the minimum state for clarity. Numbers below the PMF's indicate the free energy difference between bulk/vapor state (z = -18 or 22 Å) and the global minimum, which are marked as $\Delta G_{\rm bulk}/\Delta G_{\rm vapor}$. Reproduced from ref[1] with permission from the PCCP Owner Societies.

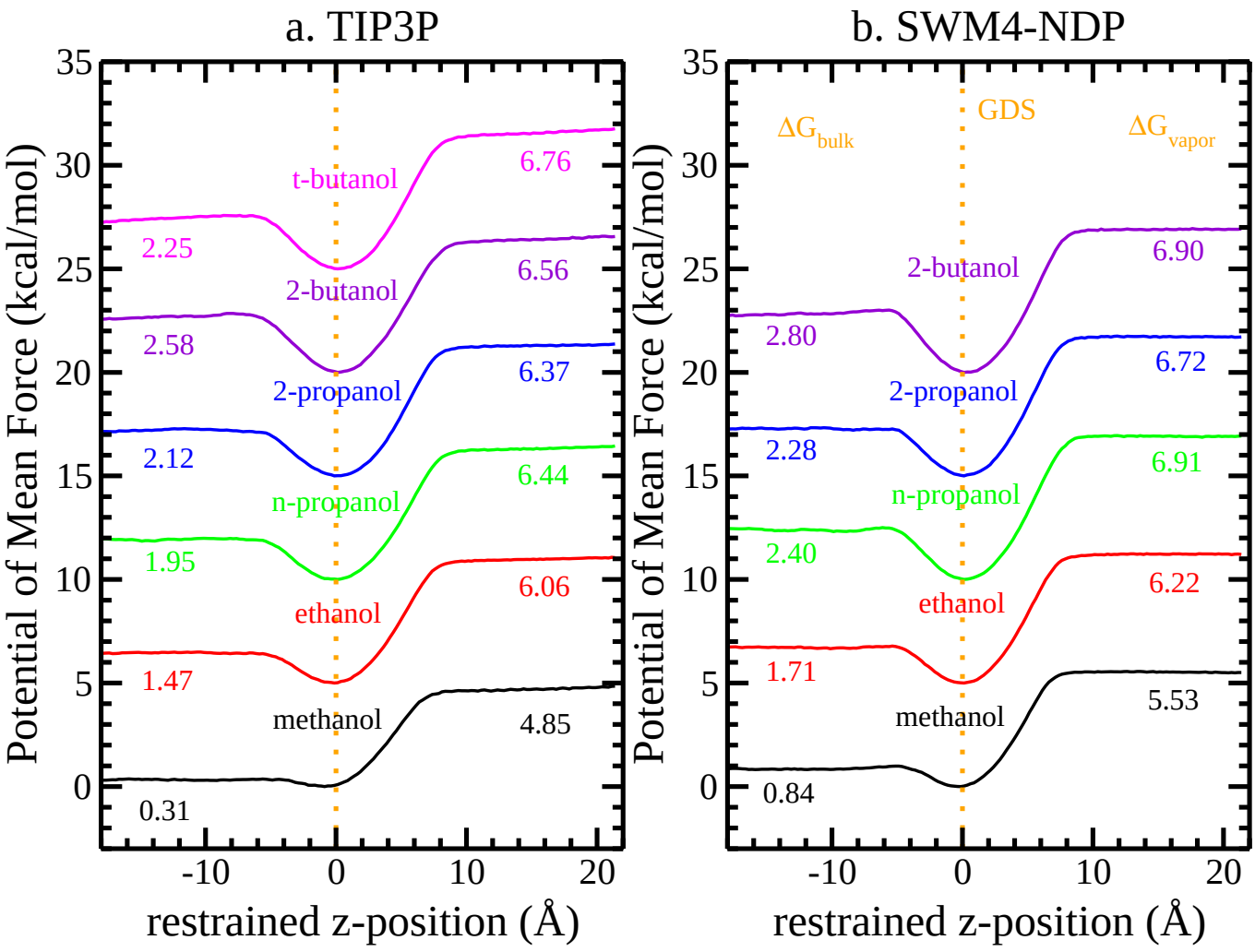

FIG. S2: Potential of mean force as a function of the z-position of a single alcohol along the direction normal to the (a) TIP3P (b) SWM4-NDP water surface. An offset of 5 kcal/mol is added at the minimum state for clarity. Numbers below the PMF's indicate the free energy difference between bulk/vapor state (z = -18 or 22 Å) and the global minimum, which are marked as $\Delta G_{\rm bulk}/\Delta G_{\rm vapor}$.

[1] S. C. Ou, D. Cui, and S. Patel, Phys. Chem. Chem. Phys. **16**, 26779 (2014).