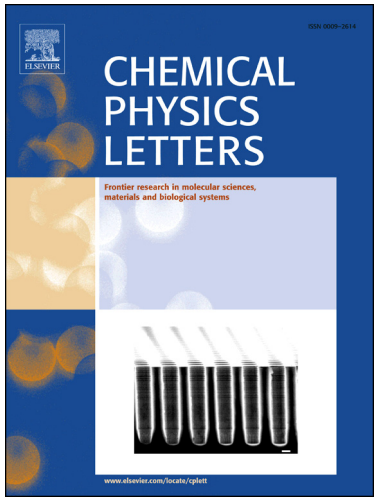

Research paper

Resolving Solvophobic Interactions Inferred from Experimental Solvation Free Energies and Evaluated from Molecular Simulations

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PII: S0009-2614(16)30926-5
DOI: http://dx.doi.org/10.1016/j.cplett.2016.11.038
Reference: CPLETT 34345

To appear in: *Chemical Physics Letters*

Received Date: 13 September 2016
Revised Date: 2 November 2016
Accepted Date: 18 November 2016

Please cite this article as: J. Wesley Barnett, A. Bhutta, S.C. Bierbrier, N. da Silva Moura, H.S. Ashbaugh, Resolving Solvophobic Interactions Inferred from Experimental Solvation Free Energies and Evaluated from Molecular Simulations, *Chemical Physics Letters* (2016), doi: http://dx.doi.org/10.1016/j.cplett.2016.11.038

Resolving Solvophobic Interactions Inferred from Experimental Solvation Free Energies and Evaluated from Molecular Simulations

J. Wesley Barnett[1], Amna Bhutta[2], Sarah C. Bierbrier[1], Natalia da Silva Moura[1], Henry S. Ashbaugh[1,*]

[1]Department of Chemical and Biomolecular Engineering, Tulane University, New Orleans, LA 70118

[2]Department of Chemical and Biochemical Engineering, Rutgers University, Piscataway, NJ 08854

Abstract

Ben-Naim estimated the solvent-mediated interaction between methanes based on experimental solvation free energy differences between chemically similar hydrocarbons. Interactions were predicted to be strongest in water, dominated by characteristic entropic gains. We use molecular simulations in combination with an empirical interpolation procedure that bridges interactions from outside methane's excluded volume down to overlap to test Ben-Naim's estimates. While Ben-Naim's approach captures many distinctive trends, the alchemical differences between methane and a methyl unit play a non-trivial role on the predicted association strength and the sign of enthalpic and entropic components of the interaction free energy in water and ethanol.

* corresponding author: hanka@tulane.edu