Supporting Material

Proton Transfer between Tryptophan and Ionic Liquid Solvents Studied with Molecular Dynamics Simulations

Marco Klähn,* Abirami Seduraman and Ping Wu

Institute of High Performance Computing, 1 Fusionopolis Way, #16-16, Connexis, Singapore 138632, Rep. of Singapore

* To whom correspondence should be addressed. Phone: (65) 6419 1468. Fax: (65) 6463 2536.
E-mail: marco@ihpc.a-star.edu.sg.

TABLE S1: Solvation Free Energies of $HTrp^+$ in BMIM-PF_6 from Simulations that Contained Only One Solute

Replica no.	ΔG_{solv}^{IL} [kcal/mol]
1	-88.1
2	-85.5
3	-94.6
4	-89.3
5	-89.0
6	-90.1
7	-83.9
8	-91.5
9	-94.7
10	-87.6
average	-89.4 ± 1.1[a]

[a] The solvation free energy of $HTrp^+$ in BMIM-PF_6 that was obtained from simulations in which ten solutes were decoupled from the solvent simultaneously was -88.3 kcal/mol (unscaled value) for comparison. This confirms that for the calculation of solvation free energies interactions among the solutes were negligible.

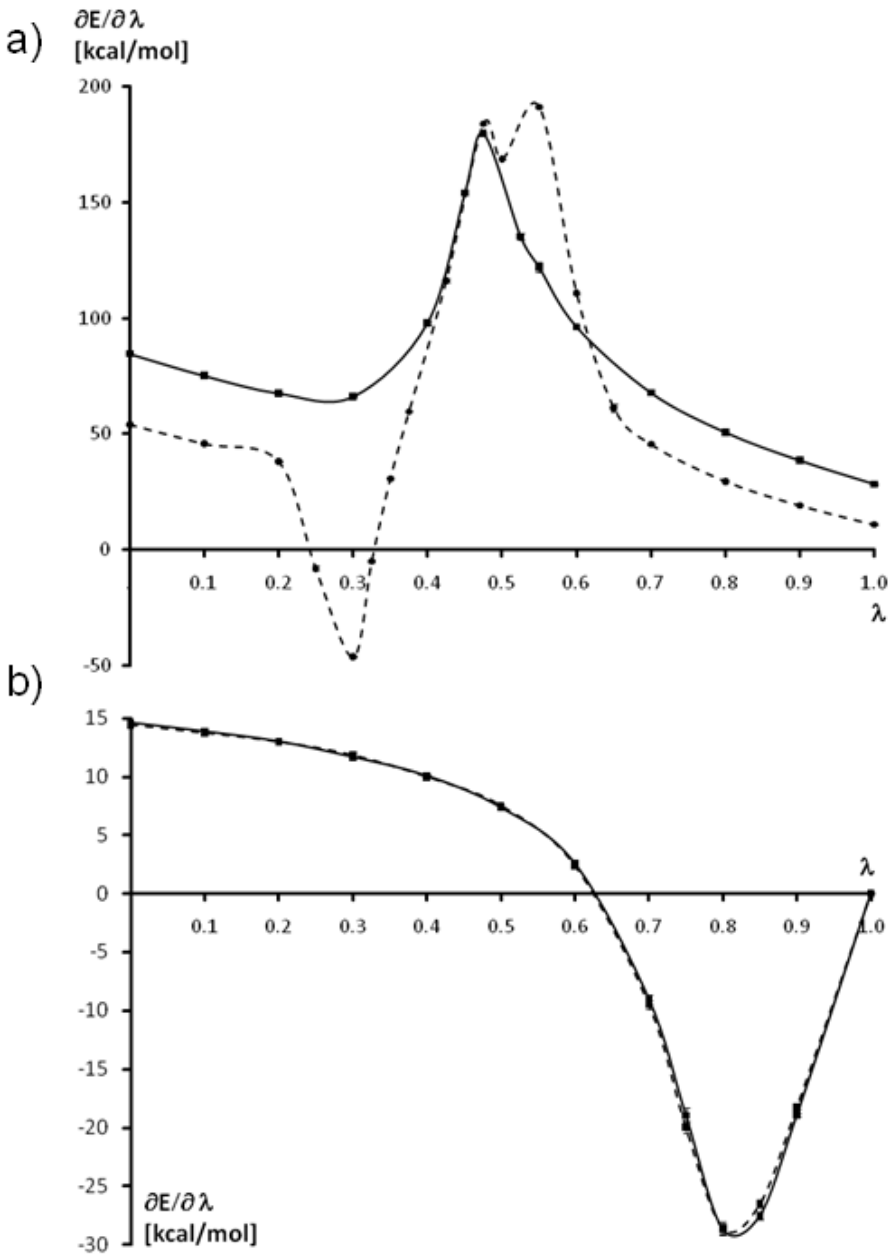

Figure S1. Values of $\partial E / \partial \lambda$ as a function of λ for the Coulomb contribution (a) and the van der Waals contribution (b) of $HTrp^+$ (straight line) and Trp (broken line) in water. Integrals of these curves were used to determine the solvation free energy. Error bars were omitted because they were too small to be discernible.

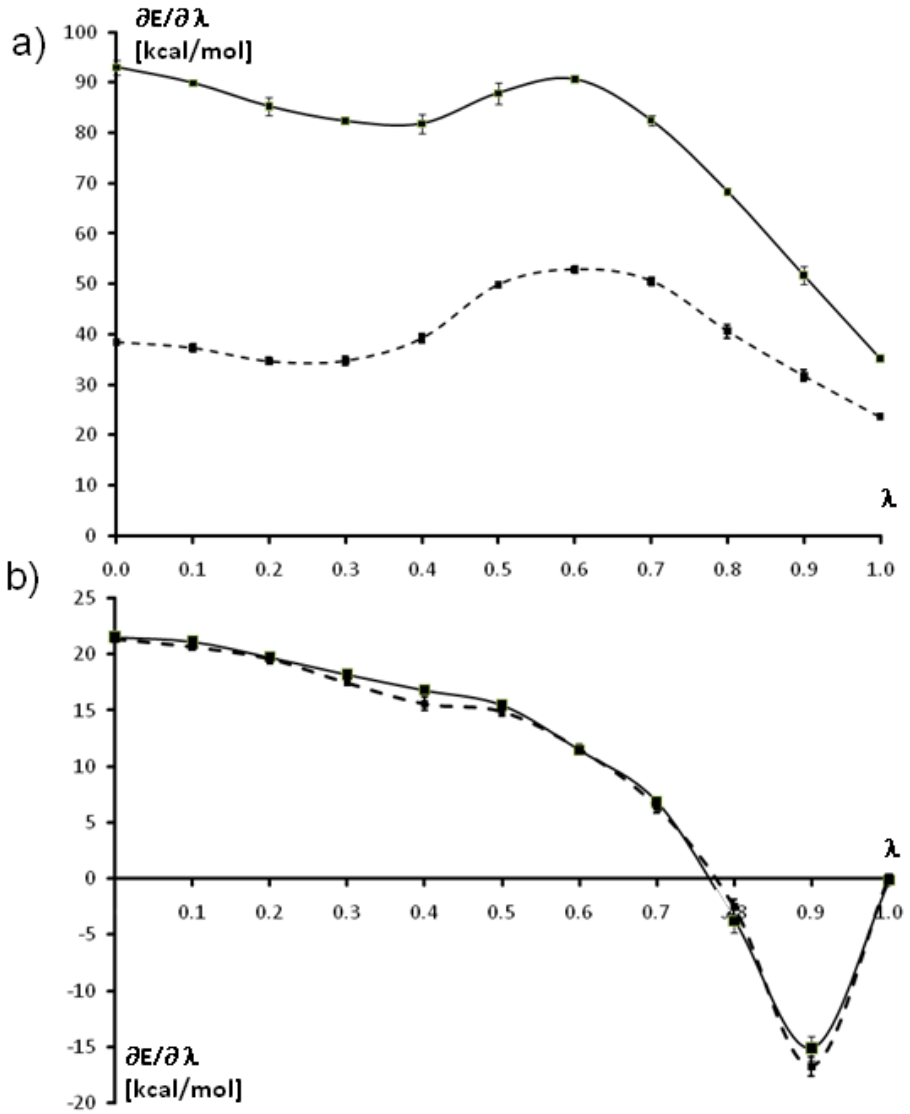

Figure S2. Values of $\partial E / \partial \lambda$ as a function of λ for the Coulomb contribution (a) and the van der Waals contribution (b) of $HTrp^+$ (straight line) and Trp (broken line) in BMIM-PF_6. Integrals of these curves were used to determine the solvation free energy. Error bars are displayed for each λ-point.

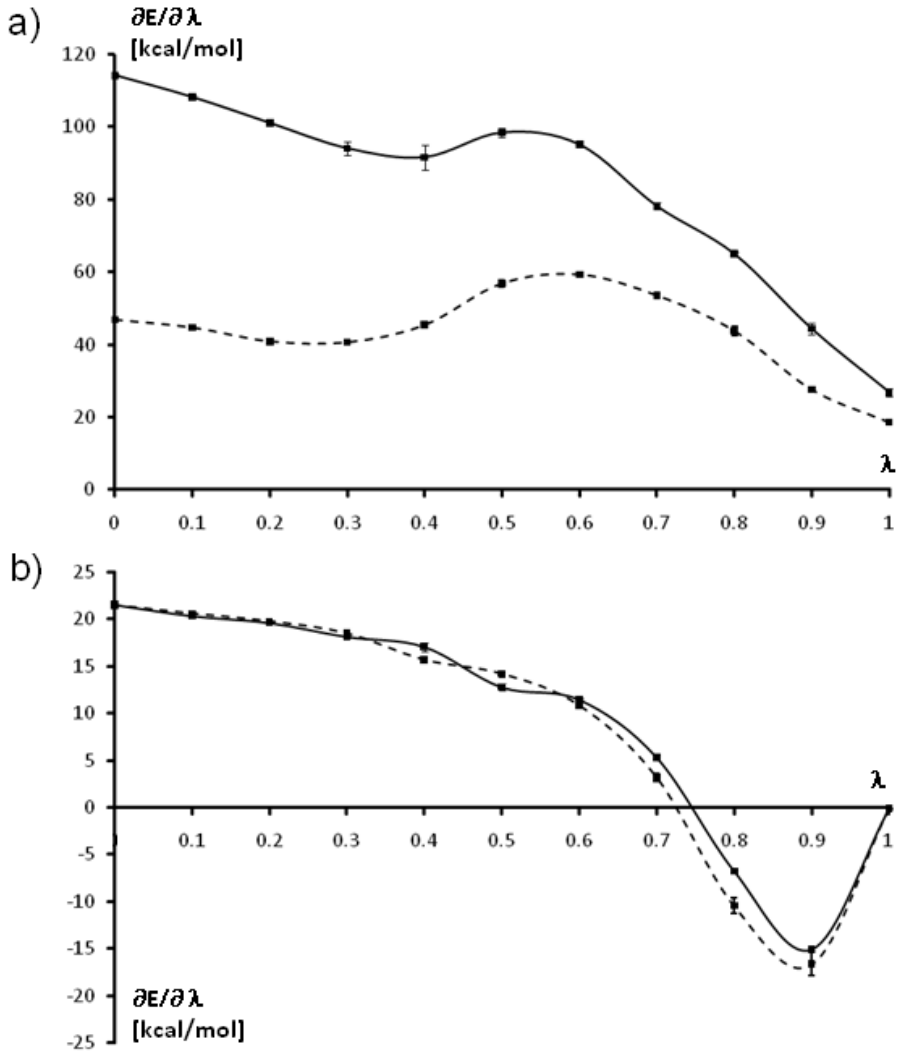

Figure S3. Values of $\partial E / \partial \lambda$ as a function of λ for the Coulomb contribution (a) and the van der Waals contribution (b) of $HTrp^+$ (straight line) and Trp (broken line) in BMIM-BF_4. Integrals of these curves were used to determine the solvation free energy. Error bars are displayed for each λ-point.

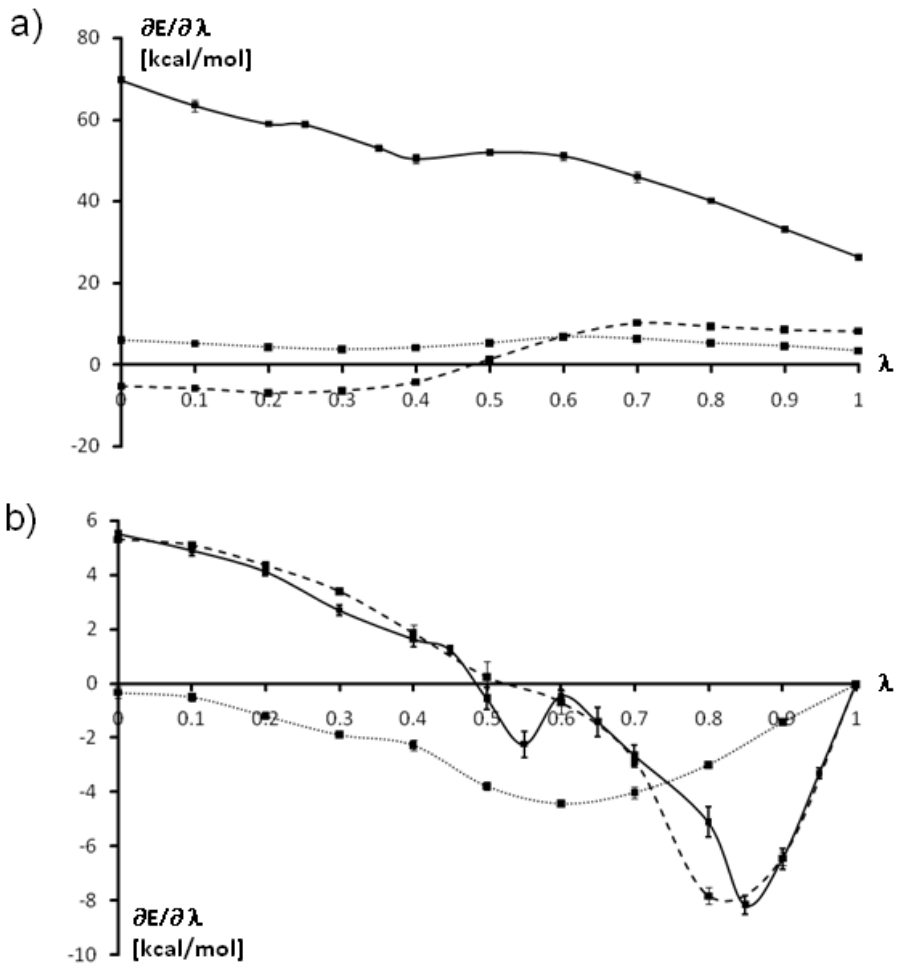

Figure S4. Values of $\partial E / \partial \lambda$ as a function of λ for the Coulomb contribution (a) and the van der Waals contribution (b) of PF_6^- (straight line), PF_5 (broken line) and HF (dotted line) in BMIM-PF_6. Integrals of these curves were used to determine the solvation free energy. Error bars are displayed for each λ-point.

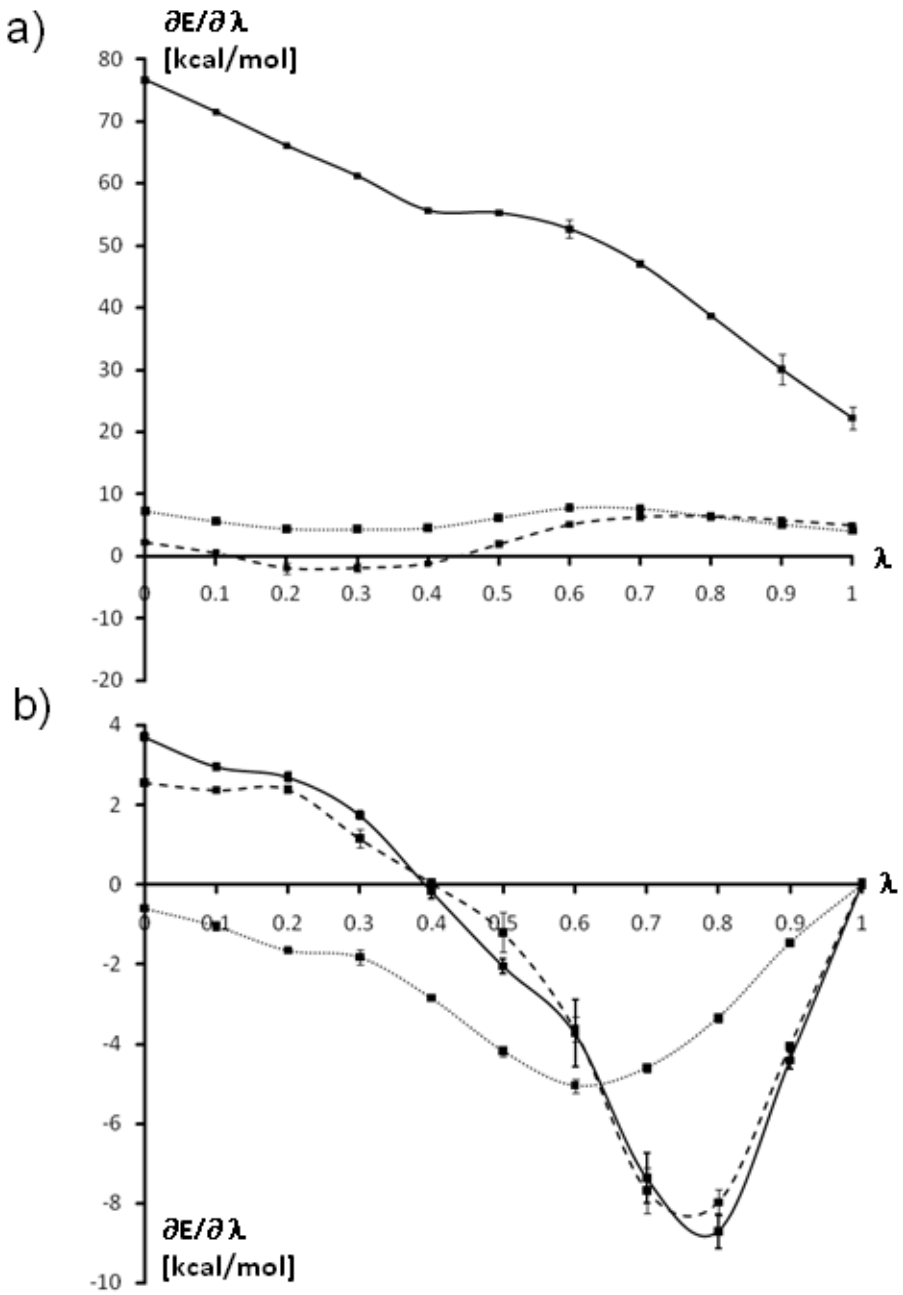

Figure S5. Values of $\partial E / \partial \lambda$ as a function of λ for the Coulomb contribution (a) and the van der Waals contribution (b) of BF_4^- (straight line), BF_3 (broken line) and HF (dotted line) in BMIM-BF_4. Integrals of these curves were used to determine the solvation free energy. Error bars are displayed for each λ-point.