Supplementary Material

The AGBNP2 Implicit Solvation Model

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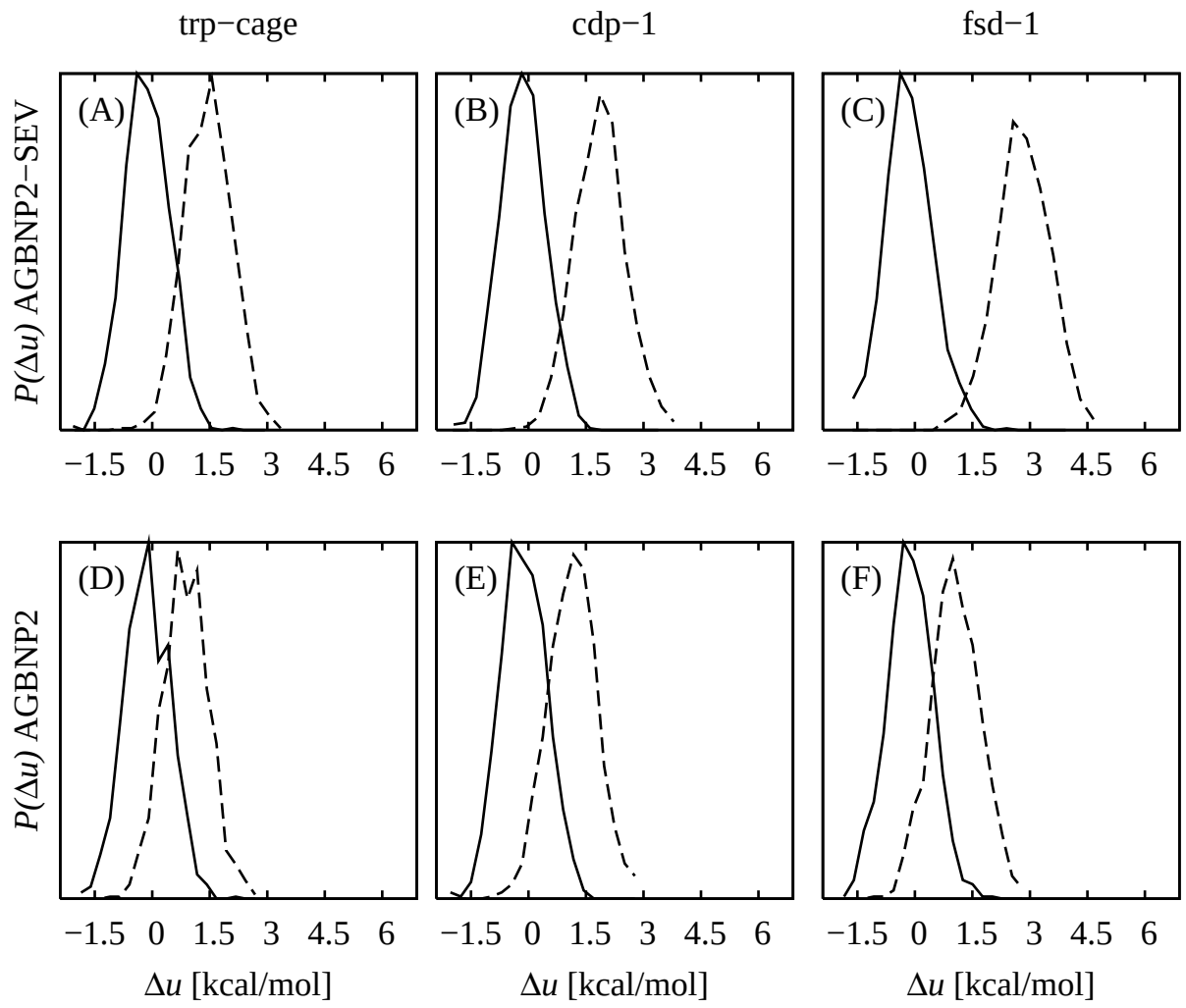

Figure 1: Potential energy distributions of the AGBNP1 (full line) and explicit solvent (dashed line) conformational ensembles for the the trp-cage (first column, panels A, D), cdp-1 (second column, panels B, E), and fsd-1 (third column, panels C, F) mini-proteins scored with the AGBNP2-SEV/OPLS-AA (first row, panels A, B, and C) and AGBNP2/OPLS-AA (second row, panels D, E, F) effective potentials. AGBNP2 is the current model and AGBNP2-SEV the current model without hydrogen bonding and surface tension corrections. The distributions are shown as a function of the energy gap per residue (Δu) relative to the mean effective potential energy of the implicit solvent ensemble distribution. Compared to Fig. 9A-C in the main text we see that the SEV model reduces significantly the energy gap between the AGBNP1 and explicit solvent distributions (first row of plots). The hydrogen bonding and surface tension corrections reduce the gap further (second row of plots).

Table 1: Experimental and AGBNP1 predicted hydration free energies of a set of small molecules.

Molecule	Exper.[a,b]	AGBNP1[a,c]
n-ethane	1.83	1.54
n-propane	1.96	1.72
n-butane	2.08	1.87
n-pentane	2.33	2.03
n-hexane	2.50	2.21
cyclo-pentane	1.20	1.95
cyclo-hexane	1.23	1.87
benzene	-0.87	1.29
toluene	-0.89	0.98
acetone	-3.85	0.04
acetophenone	-4.58	0.27
ethanol	-5.01	-4.18
phenol	-6.62	-2.32
ethandiol	-9.60	-7.46
acetic acid	-6.70	-1.35
propionic acid	-6.48	-1.05
methyl acetate	-3.32	1.17
ethyl acetate	-3.10	1.57
methyl amine	-4.56	-2.63
ethyl amine	-4.50	-1.76
dimethyl amine	-4.29	-1.66
trimethyl amine	-3.24	-0.75
acetamide	-9.71	-5.12
N-methylacetamide	-10.08	-3.20
pyridine	-4.70	-0.82
2-methylpyridine	-4.63	-0.24
3-methylpyridine	-4.77	-0.54
methanethiol	-1.24	-0.27
ethanethiol	-1.30	0.11
acetate ion	-79.90	-73.61
propionate ion	-79.10	-73.14
methylammonium ion	-71.30	-71.27
ethylammonium ion	-68.40	-68.93
methylguanidinium	-62.02[d]	-56.37

[a] In kcal/mol. [b] Experimental hydration free energy from reference 1 except where indicated.

[c] AGBNP1[2] predicted hydration free energy. [d] From reference 3.

References

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3. Vorobyov, I.; Li, L.; ; Allen, T. *J. Phys. Chem. B* **2008,** *112,* 9588–9602.