Critical Importance of Length Scale Dependence in Implicit Modeling of Hydrophobic Interactions

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Supplementary Materials

I. Complete Reference 16: MacKerell, A. D., Jr. et al., *J. Phys. Chem. B*, **1998**,102, 3586–3616.

A. D. MacKerell, Jr., D. Bashford, M. Bellott, R. L. Dunbrack, J. D. Evanseck, M. J. Field, S. Fischer, J. Gao, H. Guo, S. Ha, D. Joseph-McCarthy, L. Kuchnir, K. Kuczera, F. T. K. Lau, C. Mattos, S. Michnick, T. Ngo, D. T. Nguyen, B. Prodhom, W. E. Reiher, III, B. Roux, M. Schlenkrich, J. C. Smith, R. Stote, J. Straub, M. Watanabe, J. Wiorkiewicz-Kuczera, D. Yin, and M. Karplus. *J. Phys. Chem. B* **1998**, 102, 3586–3616.

II. Dimer and Trimer Configurations: atomic coordinates can be requested from the authors.

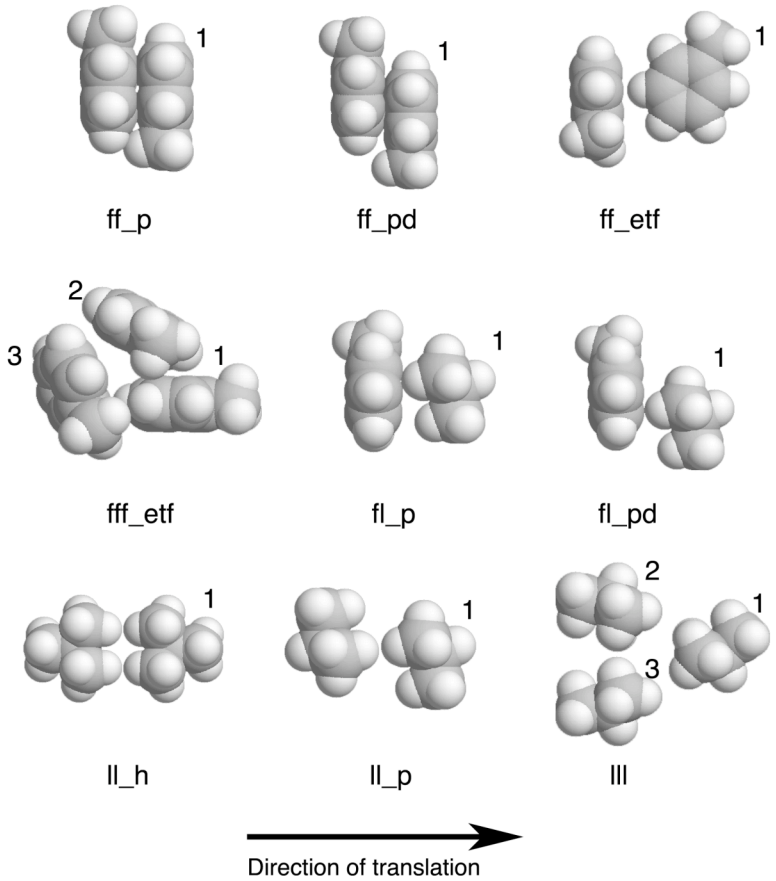

Figure 1 Configurations of dimeric and trimeric clusters. Monomers marked as "1" were the translated during the PMF calculations. For the two trimeric clusters (fff_etf and lll), additional pair-wise PMFs were computed between monomers 12 and 13 by deleting either monomer 2 or monomer 3.

III. Production sampling time and Convergence of PMFs: numerical results of the full PMFs are available upon request from the authors.

Cluster	sampling[1]	convergence[2]
ff_p	2.0	0.1
ff_pd	2.0	0.05
ff_etf	2.0	0.03
fff_etf	2.0	<0.01
fff_p12	2.0	0.06
fff_p13	2.0	0.04
fl_p	1.0	0.03
fl_pd	1.0	0.05
ll_h	1.0	0.03
ll_p	1.0	0.1
lll	2.0	0.05
lll_p12	2.0	<0.01
lll_p13	2.0	<0.01

[1] in nanoseconds [2] in kcal/mol

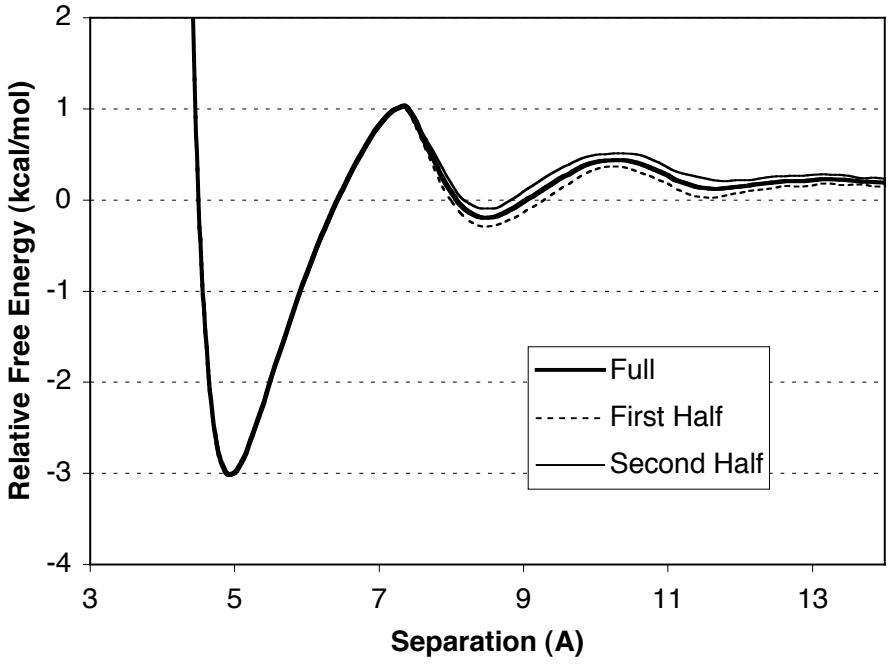

Figure 2. PMFs of trimeric Leu sidechain analog association, computed using all 2 ns (thick line), the first 1 ns (dashed line) and the second 1ns (thin line) of sampling.