JCTC Journal of Chemical Theory and Computation

ERRATUM

Minimalist Explicit Solvation Models for Surface Loops in Proteins. [J. Chem. Theory Comput. 2008, 4, 1] [*J. Chem. Theory Comput. 2*, 1135−1151 (2006)]. By Ronald P. White and Hagai Meirovitch*. Department of Computational Biology, University of Pittsburgh School of Medicine, 3064 Biomedical Tower 3, Pittsburgh, Pennsylvania 15260

Page 1150. Before the last sentence of the paper (starting "One such method...") should appear the following two sentences that have been omitted by mistake:

The calculation of such extensive variables (e.g., *E*, *F*, and *S*) with enough accuracy is possible because of the relatively small size of the system. For example, the average energy (over the five trajectories) with $N_W = 120$ ($R_{cap} =$ 18 Å) is -1587.4 ± 0.6, -1505.2 ± 0.7, -1894.9 ± 8.3, and -1727.9 ± 0.6 kcal/mol for the loop of RNase, ser-proteinase, and loops 1 and 2 of proteinase, where $R_{temp} =$ 15, 13, 13, and 13 Å, respectively.

CT600317D

10.1021/ct600317d
Published on Web 11/18/2006