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Correction to "Massively Parallel Implementation of Steered Molecular Dynamics in Tinker-HP: Comparisons of Polarizable and Nonpolarizable Simulations of Realistic Systems"

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While performing routine tests using the newly released GPUs version[1] of the Tinker-HP package,[2] we noticed that there was an error in the potential of mean force (PMF) calculation procedure described in our paper. Indeed, a scripting error led to the introduction of wrong SMD vector components for Figure 9b. This does not change the discussion concerning the differences between forces fields and the conclusion of this section of the paper. Nevertheless, in Figure 1 we provide here the corrected PMF for the stretching process of ubiquitin's β strand computed using various force fields since the new results open a discussion about the convergence of the SMD simulations.

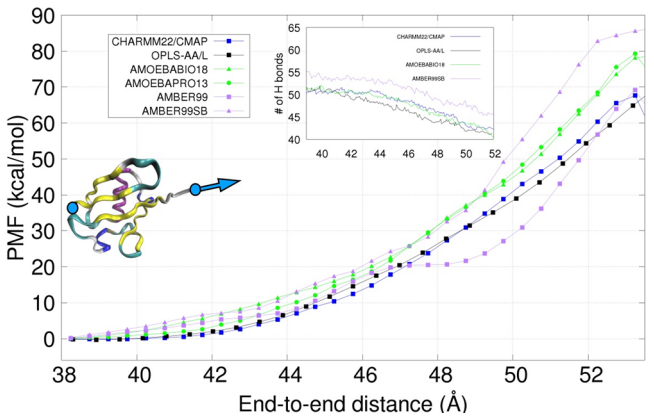

Figure 1. Corrected Figure 9b.

As Table 2 of the paper is directly associated with Figure 9, the corrected relative values for Table 2 are also provided here in Table 1.

Analyzing these new numbers, we can stress that the relatively high values of the standard deviation work (SDW) could tend to show that our SMD calculations are not fully converged. Although SDWs are only partial indicators of convergence, we decided to perform further simulations. Indeed, a previous work performed by Pai-Chi et al.[3] using umbrella sampling (US) coupled to the CHARMM22/CMAP force field showed that they obtained a smaller free energy barrier of approximatively 31 kcal/mol. In this direction, we decided to decrease the SMD velocity by a factor 10, from 0.01 to 0.001 Å/ps. Thanks to GPUs,[1] additional PMFs have been calculated for the nonpolarizable force field CHARMM22/CMAP and the polarizable force field AMOEBABIO18. We also completed these results with additional US simulations to check the convergence of our new SMD results. The setup of the US simulations (time step, integrator, thermostat, ...) was similar to that of the SMD simulations. The new results are depicted in Figure 2.

Table 1. Corrected Table 2

force field	free energy barrier (kcal/mol)	SDW (kcal/mol)
AMBER99	79.2	5.93
AMBER99SB	82.1	5.46
OPLS-AA/L	71.0	6.35
CHARMM22/CMAP	68.9	4.68
AMOEBAPRO13	79.9	4.89
AMOEBABIO18	78.8	5.00

With this update, we observe that we obtain the same free energy barrier as the one previously obtained by Pai-Chi et al.[3] It is also in good agreement with our respective US results. We also observe that the free energy barrier obtained with AMOEBABIO18 is in agreement with its corresponding PMF obtained using US simulations. Furthermore, it is worth noting that the free energy difference between CHARMM22/CMAP and AMOEBABIO18 amounts to 10 kcal/mol, which is similar to the PMF obtained with a faster SMD velocity (i.e., 0.01 Å/ps).

We can then conclude, on the basis of the literature and on our US simulations that we reached a satisfactory convergence for the ubiquitin system with both CHARMM22/CMAP and AMOEBABIO18 using a slower SMD velocity (0.001 Å/ps). Since the free energy differences between force fields are not impacted by the use of two different SMD velocities (and have

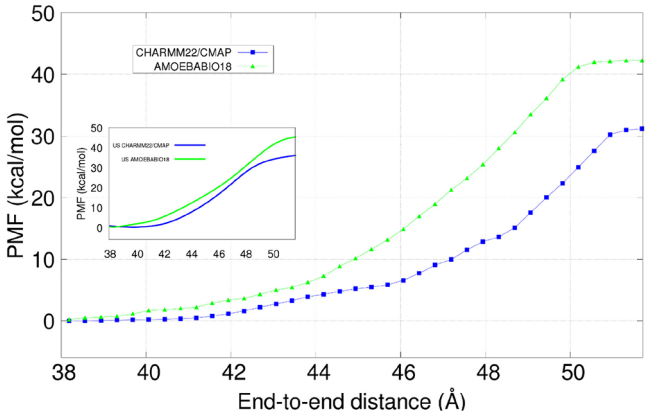

Figure 2. Potential of mean force computations using SMD and umbrella sampling for the ubiquitin protein system (PDB: 1UBQ) using the polarizable AMOEBA and CHARMM22/CMAP force fields. US results are enclosed in the left inset.

been compared to umbrella sampling computations), the conclusions concerning the comparisons between nonpolarizable and polarizable force fields discussed our paper are not affected by the bias induced by the initial excessive SMD velocity.

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