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Erratum

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Correction to Enhanced Conformational Sampling Using Replica Exchange with Collective-Variable Tempering

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Recently we have found an error in the *demux.pl* analysis tool of Gromacs 4.6.7. This tool is used to obtain the trajectories across the replica ladder which we used to compute the distributions of the root-mean-square deviation (RMSD) showed in Figure S6 of the Supporting Information of ref 1. More precisely, the processed trajectories are not reliable if the simulations exceed 100 ns per replica. We recomputed the distributions with a corrected version of the script. A significant change in the level of agreement of the trajectories can be appreciated when comparing Figure S6 of ref 1 with the new Figure 1 where the histogram of the RMSD deviation from a representative structure has been computed with the properly processed trajectories. Three replica exchange molecular dynamics (REMD) protocols are compared in the figure, namely, temperature REMD (T-REMD), dihedral-scaling REMD (H_{dih}-REMD), and the newly introduced replica exchange with collective-variable tempering (RECT) method. In general, for the three compared methods the agreement between the trajectories across the replica ladder is much lower than in Figure S6 of ref 1. This indicates that all of the simulations are still not fully converged. However, when looking at the comparison between the methods, this change affects mostly our previous assessment of the H_{dih}-REMD method. Here the agreement decreases significantly and the method behaves thus in a way similar to that of T-REMD. Trajectories from RECT still show a better agreement among them than trajectories from T-REMD.

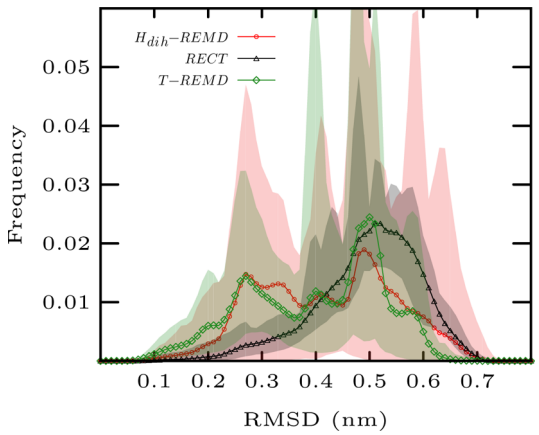

Figure 1. Empirical probability distribution of heavy atom RMSD from the canonical A-form as computed from the trajectories across the replica ladder, shown for all REMD methods. Average probability is shown in solid line, and range between maximum and minimum probability among all trajectories is shaded. It can be appreciated that the agreement among the conformational distributions of trajectories from T-REMD and H_{dih}-REMD is poorer than the one of those obtained with RECT. We notice that RECT samples a very different generalized ensemble from those of T-REMD and H_{dih}-REMD schemes.

Therefore, none of the main discussions and conclusions of the original article[1] is affected. Figure S6 should be replaced with Figure 1 included here. Moreover, the sentence, "*As it can be appreciated in Figure S6, for H_{dih}-REMD and RECT the empirical distribution of RMSD is very similar for all the trajectories in the generalized ensemble, indicating that, for each method, all of them sampled the same conformational space.*" from the first paragraph of the subsection Tetranucleotide of the section Results, should read instead, "*As it can be appreciated in Figure S6, for RECT the trajectories in the generalized ensemble are more consistent than those obtained with the other methods.* ".

REFERENCES

(1) Gil-Ley, A.; Bussi, G. *J. Chem. Theory Comput.* **2015**, *11*, 1077−1085.

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