

Corrections to “Do Molecular Dynamics Force Fields Capture Conformational Dynamics of Alanine in Water?”

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Article Recommendations

We report three corrections to our original publication.

Correction 1:

The incorrect NSF grant proposal number was acknowledged in our original publication. The corrected acknowledgment is

“This material is based upon work supported by the National Science Foundation under Grant No. MCB-1817650.”

Correction 2:

All MD simulations of GAG and AAA within CHARMM were performed using the CHARMM36m version of the force field.¹

Correction 3:

On page 512, in Methods (subsection MD Simulations) an incorrect pressure equilibration time of 20 ns was reported. The actual pressure equilibration time was 20 ps.

REFERENCES

(1) Huang, J.; Rauscher, S.; Nawrocki, G.; Ran, T.; Feig, M.; de Groot, B. L.; Grubmüller, H.; MacKerell, A. D., Jr. CHARMM36m: an improved force field for folded and intrinsically disordered proteins. *Nat. Methods* **2017**, *14*, 71–73.