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Erratum: "Investigating the role of non-covalent interactions in conformation and assembly of triazine-based sequence-defined polymers" [J. Chem. Phys. 149, 072330 (2018)]

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**Erratum: "Investigating the role of non-covalent interactions in conformation and assembly of triazine-based sequence-defined polymers" [J. Chem. Phys. 149, 072330 (2018)]**

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In our publication<sup>1</sup>, when producing the free energy landscapes for the replica exchange molecular dynamics (REMD) simulations<sup>2</sup>, the multistate Bennett acceptance ratio (MBAR), specifically the Python implementation by Shirts and Chodera, was used<sup>3</sup>. The incorrect input file (replica\_temp.xvg instead of replica\_index.xvg from GROMACS<sup>4</sup>) was used for MBAR and produced an incorrect free energy landscape and an incorrect most stable conformation for each triazine hexamer and one triazine trimer. Fig. 6, Fig. 7, Fig. 8, Fig. 9, and Fig. 10 show the correct free energy landscape and the most stable conformation obtained for the trimer with S-ethyl side chains (2 hydrogen bonds and 3 *trans* bonds), the hexamer with S-ethyl side chains (6 hydrogen bonds and 3 *trans* bonds), the hexamer with amino-ethyl-sulfide side chains (4 hydrogen bonds and 6 *trans* bonds), the hexamer with amino-ethyl side chains (5 hydrogen bonds and 7 *trans* bonds), and the hexamer with amino side chains (7 hydrogen bonds and 8 *trans* bonds), respectively.

Since the correct most stable conformation for the hexamer with amino-ethyl-sulfide side chains was also the nanorod structure but with a different number of *trans* bonds than previously stated (6 instead of 3), a more thorough search for nanorod structures was conducted. The nanorod structures are the same as previously stated but three out of the four hexamers can take various number of hydrogen bonds and *trans* bonds than previously stated to form the nanorod structure. Specifically, the hexamer with amino-ethyl-sulfide side chains is the nanorod structure when it has 4 hydrogen bonds and 3-6 *trans* bonds; the hexamer with amino-ethyl side chains is the nanorod structure when it has 4, 6 hydrogen bonds and 5, 7 *trans* bonds (previously stated as 6 hydrogen bonds and 6 *trans* bonds but should be 6 hydrogen bonds and 5 *trans* bonds); the hexamer with amino side chains is the nanorod structure when it has 4 hydrogen bonds and 3, 5 *trans* bonds or 6 hydrogen bonds and 5, 7 *trans* bonds.

This erratum does not change the rest of the results and any of the conclusions and discussions in our publication. The correct input file (replica\_temp.xvg) was used to calculate the average number of round trips in a given observation time  $\tau = 10$  ns, so the REMD simulations remain as converged simulations.

## SUPPLEMENTARY MATERIAL

The figure numbers correspond to the figures in the original article. Corrected PSE files for the triazine trimer and all of the triazine hexamers are available. The files can be viewed using Pymol.

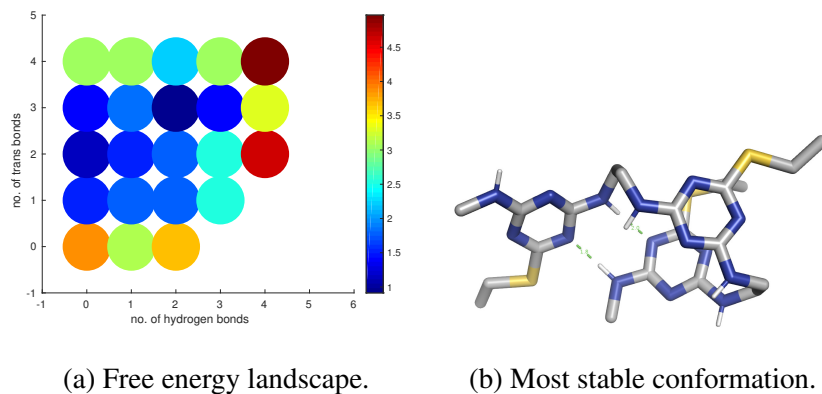


FIG. 6. Free energy landscape and most stable conformation of a single triazine trimer with S-ethyl side chains and amino backbone from REMD simulations. Figure (a) plots the free energies in log scale or  $-k_B T \ln P$  (kcal/mol), where  $P$  denotes the weight, truncated at 5 kcal/mol, and the color bar indicates which colors correspond to which free energies in log scale (kcal/mol). Figure (b) shows the most stable conformation (2 hydrogen bonds and 3 *trans* bonds).

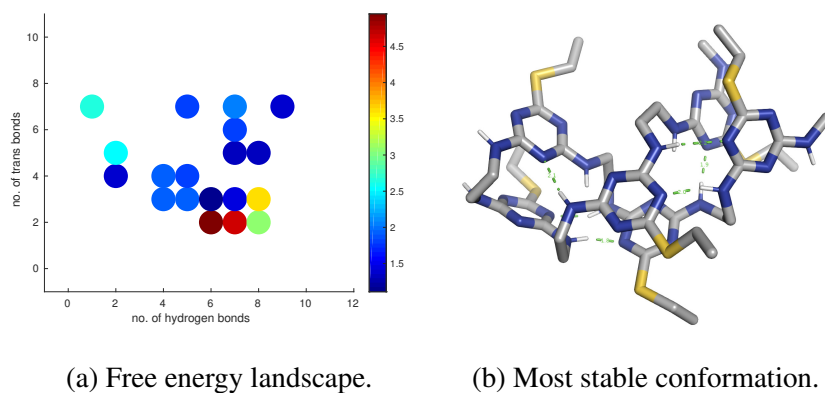


FIG. 7. Same as Fig. 6 but for a single triazine hexamer with S-ethyl side chains.

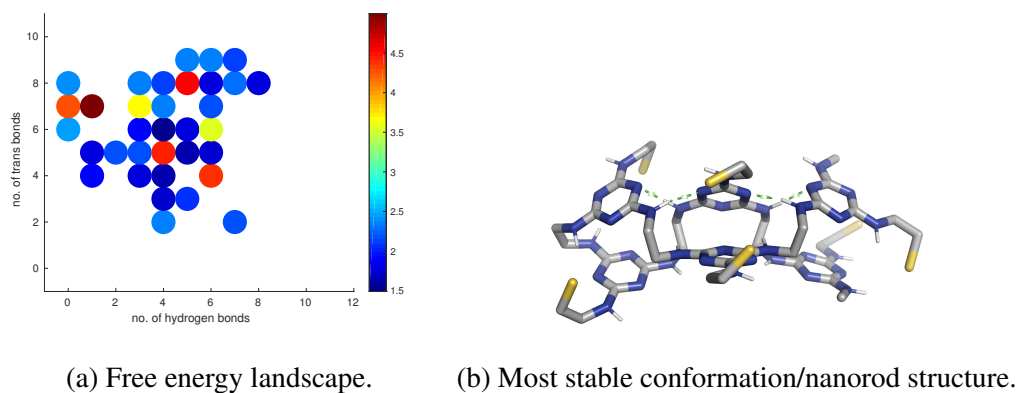


FIG. 8. Same as Fig. 6 but for a single triazine hexamer with amino-ethyl-sulfide side chains.

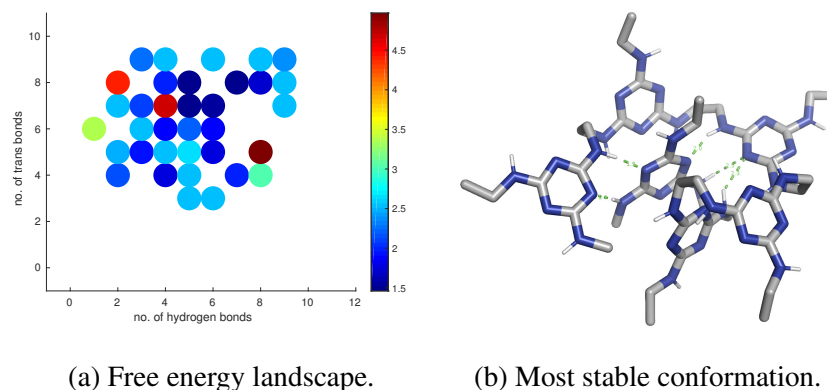


FIG. 9. Same as Fig. 6 but for a single triazine hexamer with amino-ethyl side chains.

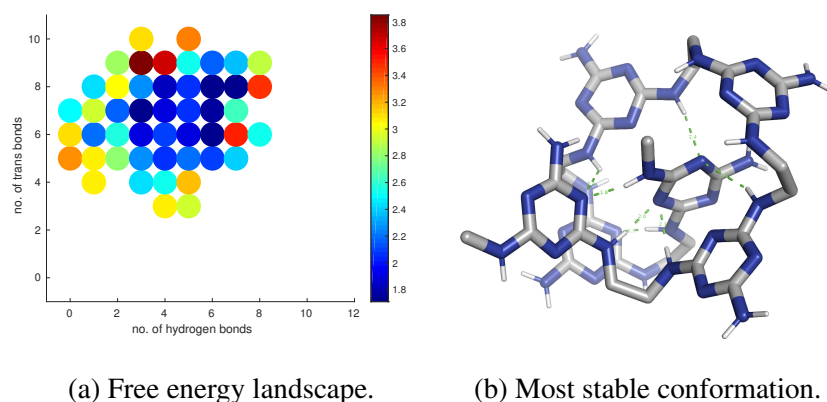


FIG. 10. Same as Fig. 6 but for a single triazine hexamer with amino side chains.

## REFERENCES

- <sup>1</sup>S.-H. Ahn, J. W. Grate, and E. F. Darve, “Investigating the role of non-covalent interactions in conformation and assembly of triazine-based sequence-defined polymers,” *The Journal of Chemical Physics* **149**, 072330 (2018).
- <sup>2</sup>Y. Sugita and Y. Okamoto, “Replica-exchange molecular dynamics method for protein folding,” *Chemical Physics Letters* **314**, 141–151 (1999).
- <sup>3</sup>M. R. Shirts and J. D. Chodera, “Statistically optimal analysis of samples from multiple equilibrium states,” *The Journal of Chemical Physics* **129**, 124105 (2008).
- <sup>4</sup>S. Pronk, S. Páll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M. R. Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, *et al.*, “Gromacs 4.5: a high-throughput and highly parallel open source molecular simulation toolkit,” *Bioinformatics* **29**, 845–854 (2013).