Dr. Norbert Pienta

Editor, *Journal of Chemical Education*

Department of Chemistry

The University of Georgia

Athens, Georgia 30602-2556

Dear Dr. Pienta,

Acting on behalf of myself and my co-author, I have uploaded a manuscript and associated files to the ACS Paragon Plus system for consideration for publication in the *Journal of Chemical Education.* The manuscript, titled “Calculating Properties of Bulk Water with Molecular Dynamics,” describes a computational chemistry activity for calculating diffusion coefficients and radial distribution functions from a molecular dynamics simulation. Comparisons to literature values allow students to assess the relative strengths of the TIP3P water model for describing real water’s structure and dynamics. Generally, computational models of water must proritize among the qualitites: fast, accuract depiction of structure of the solid, accurate depiction of structure of the liquid, and accurate depiction of dynamics. One purpose of this lab is to let students determine which of these properites the TIP3P water model has prioritized.

Although laboratory experiments have been published in the *Journal* calculating separately distribution functions,1 transport properties,2 and simulations of water,3 this is the first paper to combine these calculations into an examination of the efficacy of computational chemistry to model real properties.Giventhe ever-increasing use of computational chemistry in the undergraduate curriculum, it is vital that students learn not only how to use common calculational tools (like Amber), but also learn how to evaluate the validity of the models built into those tools. We are confident that our manuscript will be interesting to the *Journal*’s readers, especially those who design or conduct physical chemistry laboratories.

We have included all the necessary input files to run dynamics in Amber, the scripts and code to process trajectories from Amber, and a detailed handout for use in the laboratory.

For review of the manuscript, we recommend the following people:

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Thank you for considering our manuscript. We look forward to hearing from you.

Sincerely,

Carrie S. Miller

Associate Professor

Department of Biology and Chemistry

Azusa Pacific University

1. Speer, O. F.; Wengerter, B. C.; Taylor, R. S. Molecular Dynamics Simulations of Simple Liquids. *J. Chem. Ed*. **2004**, *81*(9), 1330
2. Eckler, L. H.; Nee, M. J. A Simple Molecular Dynamics Lab to Calculate Viscosity as a Function of Temperature. *J. Chem. Ed*. **2016**, *93*(5), 927-931
3. Salz, E.; Tarazona, M. P. Molecular Dynamics and the Water Molecule: An Introduction to Molecular Dynamics for Physical Chemistry Students. *J. Chem. Ed*. **1997**, *74*(11), 1350