Spencer Sabatino

706 Linn St. | Ithaca, NY | (330)-354-2191 | spencersabatino17@gmail.com

EDUCATION

PhD in Chemical Engineering
Cornell University, Ithaca, New York
GPA – 3.87
Advisor: Shuwen Yue

MS in Chemical and Biomedical Engineering
Miami University, Oxford, Ohio
GPA – 3.87
Thesis Title – "Predicting Octanol/Water Partition Coefficients Using Molecular Simulation for the SAMPL7 Challenge: Comparing the Use of Neat and Water Saturated 1-Octanol"
Advisor: Andrew Paluch

BS in Chemical Engineering*, cum laude*
Miami University, Oxford, Ohio
Minors: Paper Science
University Honors Program
Major GPA – 3.80
Cumulative University GPA – 3.73

RELEVANT EXPERIENCE

Miami University – Research Assistant **Sept 2019-May 2022**

- Worked in a research lab under Dr. Andrew Paluch, leading teams of 5 undergraduate students
- Assisted Dr. Paluch in writing research papers, running simulations, and developing methods to solve modern problems in thermodynamics.
- Extensively uses high-performance computing power to run simulations of thousands of molecules at once, extracting key information from the system.

Miami University – Teaching Assistant **Feb. 2021-May 2022**

- Worked as a teaching assistant for CSE 273, CPB 204, CPB 244, CPB 314, and CPB 324 in the CPB and CSE departments.
- Held office hours and graded assignments for over two hundred students.

PROJECTS

SAMPL7 Challenge **Sept. 2020-March 2021**

- Competed in community challenge with research mentor to predict various thermodynamic properties for a set of 37 complex molecules.
- Managed thousands of gigabytes data for the project in the Ohio Supercomputing Center.
- Placed first in the contest in computational methods category using given models.
- Presented findings and process at international conferences in November 2020 and April 2021 with 400 people attending virtually.
- Published a paper detailing our findings in Journal of Computer Aided Molecular Design.

Assessment of SMD, SM8, and SM12 Models **Sept. 2019-Apr. 2020**

- Worked in a team of 4 to compile data for over 160 compounds using SMD, SM8, and SM12 solvation models.
- Spearheaded efforts to design a graphical user interface to harbor the data and display it for users.
- Published a paper detailing our findings in the Processes journal.

PUBLICATIONS

- Rodriguez, S.A., Tran, J., Sabatino, S.J. *et al.* Predicting octanol/water partition coefficients and p*K*a for the SAMPL7 challenge using the SM12, SM8 and SMD solvation models. *J Comput Aided Mol Des* **36**, 687–705 (2022). https://doi.org/10.1007/s10822-022-00474-1
- Ollier, R.C.; Nguyen, T.; Agarwal, H.; Phifer, J.R.; Ferreira da Silva, L.; Gonçalves Nogueira, G.; Pereira Barbosa, A.K.; Ley, R.T.; O'Loughlin, E.J.; Rygelski, B.T.; Sabatino, S.J.; Paluch, A.S. Predicting the Solubility of Nonelectrolyte Solids Using a Combination of Molecular Simulation with the Solubility Parameter Method MOSCED: Application to the Wastewater Contaminants Monuron, Diuron, Atrazine, and Atenolol *Processes* **2022**, *10*, 538. https://doi.org/10.3390/pr10030538
- Sabatino, S.J., Paluch, A.S. Predicting octanol/water partition coefficients using molecular simulation for the SAMPL7 challenge: comparing the use of neat and water saturated 1-octanol. J Comput Aided Mol Des 35, 1009–1024 (2021). https://doi.org/10.1007/s10822-021-00415-4
- Roese, S.N.; Heintz, J.D.; Uzat, C.B.; Schmidt, A.J.; Margulis, G.V.; Sabatino, S.J.; Paluch, A.S. Assessment of the SM12, SM8, and SMD Solvation Models for Predicting Limiting Activity Coefficients at 298.15 K. Processes 2020, 8, 623. https://doi.org/10.3390/pr8050623