

# Caitlin C. Bannan

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## Education

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### University of California Irvine (UCI)

*Ph.D. Candidate, Theoretical and Computational Chemistry*

Advisor: Professor David L. Mobley

Irvine, CA

2014–Present

### University of Washington (UW)

*B.S. with Departmental Honors, Chemistry*

Advisor: Professor Munira Khalil

Seattle, WA

2008–2012

## Professional Experience

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### Graduate Student Researcher

*Mobley Group, UCI Chemistry Department*

Irvine, CA

January 2015–Present

- As a part of the Open Force Field Initiative, I helped create smirnoff99Frosst, the first force field in the new SMIRNOFF format. I designed and developed a cheminformatics tools, open source with Python, for learning chemical perception or the way a force field assigns parameters to a molecule based on the atoms environment.
- I created an automated pipeline to compute partition coefficients from alchemical free energy calculations and compare the results to experiment.
- I used a variety of statistical methods to evaluate participant results and reference calculations for predicted distribution coefficients during SAMPL5 challenge.

### Scientific Developer Intern

*OpenEye Scientific Software, Inc.*

Santa Fe, NM

June 2017–September 2017

- I built a machine learning model to predict the microscopic and macroscopic pKa of small molecules using a set of physically calculated features.
- I compared the accuracy of two models, Gaussian Process and Random Forrest, using a 3-fold cross validation scheme and evaluated the final model with an independent test set.
- After the completion of this internship, I used this model to predict the pKa of 24 drug-like molecules for the SAMPL6 blind challenge.

### Chemist I

*Radiation Group, Washington State Department of Health*

Shoreline, WA

September 2012–August 2014

- I prepared environmental samples of various matrices and used analytical radiochemistry techniques to isolate isotopes of interest.
- I operated and maintained quality control records for a variety of instrumentation, primarily gas flow proportional counters and high purity germanium gamma spectrometers.
- My responsibilities included keeping inventory of chemical solutions and radioactive standards and testing safety equipment regularly.

### Undergraduate Research Assistant

*Khalil Lab, UW Chemistry Department*

Seattle, WA

September 2010–June 2012

- I synthesized multivalent metal complexes of platinum, ruthenium, and iron, purified using ion exchange and size exclusion chromatography and then verified purity of these complexes using IR and UV/Vis spectroscopy
- Developed curriculum around scientific literature for University of Washington undergraduate course, Physical Chemistry for Biochemists (2011-2012 school year).

## Teaching Experience

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### Lead Chemistry Tutor

*UW Center for Learning and Undergraduate Enrichment*

**Seattle, WA**

*January 2010–June 2013*

- I led a team of tutors, organized schedules, planned training events, and coordinated with the Chemistry department to provide drop-in tutoring and exam review sessions for undergraduate courses in general, organic, inorganic, and physical chemistry.

### Developmental Teaching Assistant

*Dr. Amanda Brindley, UCI Chemistry Department*

**Irvine, CA**

*Spring 2015, Winter 2016, and Spring 2017*

- I helped convert the UCI general chemistry lecture series to an online course accessible to more students. I separated lecture videos by topic and then wrote worksheets, study guides, and quizzes for each topic.

### Laboratory and Lecture Teaching Assistant

*UCI Chemistry Department*

*Fall 2014, Winter 2015, Fall 2015*

*UW Chemistry Department*

*Fall 2011, Spring 2012*

- As a lecture TA, I led discussion sections to help students review material from class and prepare for exams. In lab, students completed general chemistry experiments while I enforced safety procedures were followed and helped them understand the chemistry concepts being demonstrated.

## Volunteer Experience

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### Iota Sigma Pi - Calcium Chapter

**Irvine, CA**

*May 2015–present*

- Iota Sigma Pi is a national honors society for women in chemistry with a heavy emphasis on outreach and professional development. I served as the Calcium Chapter president from 2016-2018 and am currently the chair of the national website and database modernization committee.

### Mobley Lab Outreach

**Irvine, CA**

*July 2016 – present*

- UCI LEAPS and AAUW Tech Trek programs bring middle school girls and underrepresented minorities to college campuses to encourage them to pursue careers in STEM. For these and other programs, I help plan and lead hands on activities to teach students about computer aided drug design.

## Skills

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- **Programming Languages:** Proficient at Python ([github.com/bannanc](https://github.com/bannanc)), familiar with Java and Bash
- **Python packages:** OpenEye Toolkits, RDKit, OpenMM, MDTraj, NumPy, Matplotlib, Pandas, SciPy, Scikit-learn, NetworkX, PyTest
- **Development tools:** Git, GitHub, Travis Continuous Integration, ReadTheDocs, Code Coverage
- **Software:** GROMACS, Maestro, PyMOL, VMD, Jupyter Notebooks, Mathematica, MatLab

## Awards

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- *Phase I and Phase II Software Fellow* Molecular Sciences Software Institute January 2018 and June 2018
- *Penny J. Gilmer Grant for Women Graduate Students and Post-docs* OpenEye Scientific, Santa Fe, CUP XVII March 2017 and CUP XVIII March 2018
- *WCC Merck Research Award* American Chemical Society National Meeting August 2017
- *Poster Session Third Place* Ewha-UCI Pharmaceutical Sciences Annual Symposium January 2016
- *Outstanding Contributions to the Chemistry Department Teaching Program by a First Year TA* University of California Irvine 2014-2015

## Publications

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- [1] **Caitlin C. Bannan**, David L. Mobley, and Skillman A. Geoff. Sampl6 challenge results from pka predictions based on a general gaussian process model. *ChemRxiv*, June 2018. doi: 10.26434/chemrxiv.6406505.v1.
- [2] Camila Zanette, **Caitlin C. Bannan**, Christopher I. Bayly, Josh Fass, Michael K. Gilson, Michael R. Shirts, John D. Chodera, and David L. Mobley. Toward learned chemical perception of force field typing rules. *ChemRxiv*, May 2018. doi: 10.26434/chemrxiv.6230627.v1.
- [3] David Mobley, **Caitlin C. Bannan**, Andrea Rizzi, Christopher I. Bayly, John D. Chodera, Victoria T Lim, Nathan M. Lim, Kyle A. Beauchamp, Michael R. Shirts, Michael K. Gilson, and Peter K. Eastman. Open force field consortium: Escaping atom types using direct chemical perception with smirnoff v0.1. *bioRxiv*, March 2018. doi: 10.1101/286542.
- [4] **Caitlin C. Bannan**, Kalistyn H. Burley, Michael Chiu, Michael R. Shirts, Michael K. Gilson, and David L. Mobley. Blind prediction of cyclohexane–water distribution coefficients from the SAMPL5 challenge. *J. Comput. Aided. Mol. Des.*, pages 1–18, 2016.
- [5] **Caitlin C. Bannan**, Gaetano Calabró, Daisy Y. Kyu, and David L. Mobley. Calculating Partition Coefficients of Small Molecules in Octanol/Water and Cyclohexane/Water. *J. Chem. Theory Comput.*, 12(8):4015–4024, 2016.
- [6] Karla M. Slenkamp, Michael S. Lynch, Jennifer F. Brookes, **Caitlin C. Bannan**, Stephanie L. Daifuku, and Munira Khalil. Investigating vibrational relaxation in cyanide-bridged transition metal mixed-valence complexes using two-dimensional infrared and infrared pump-probe spectroscopies. *Struct. Dyn.*, 3(2):023609, 2016.
- [7] Karla M. Slenkamp, Michael S. Lynch, Benjamin E. Van Kuiken, Jennifer F. Brookes, **Caitlin C. Bannan**, Stephanie L. Daifuku, and Munira Khalil. Investigating vibrational anharmonic couplings in cyanide-bridged transition metal mixed valence complexes using two-dimensional infrared spectroscopy. *J Chem Phys*, 140(8):084505, 2014.
- [8] Benjamin E. Van Kuiken, Marat Valiev, Stephanie L. Daifuku, **Caitlin C. Bannan**, Matthew L. Strader, Hana Cho, Nils Huse, Robert W. Schoenlein, Niranjana Govind, and Munira Khalil. Simulating Ru L3-edge X-ray absorption spectroscopy with time-dependent density functional theory: Model complexes and electron localization in mixed-valence metal dimers. *J Phys Chem A*, 117(21):4444–4454, 2013.

## Invited Presentations

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- [9] **Caitlin C. Bannan**, David L. Mobley, and A. Geoff Skillman. Machine learning and pka predictions in sampl6. Santa Fe, NM, March 2018. Oral presentation at *CUP XVIII OpenEye Scientific Software*, Santa Fe, NM. doi: 10.13140/RG.2.2.20127.25764.
- [10] **Caitlin C. Bannan**, Camila Zanette, Christopher I. Bayly, Joshua Fass, Michael K. Gilson, Michael R. Shirts, John D. Chodera, and David L. Mobley. Automating chemical perception to improve force field parameterization. Washington, D.C., August 2017. Oral presentation at the *254th ACS National Meeting* Washington, D.C. doi: 10.13140/RG.2.2.20127.25764.

## Contributed Presentations

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- [11] **Caitlin C. Bannan**, Camila Zanette, Christopher I. Bayly, Josh Fass, Michael K. Gilson, Lee-Ping Wang, Michael R. Shirts, John D. Chodera, and David L. Mobley. Automated chemical perception for force field parameterization. Poster presentation at the *256th ACS National Meeting* Boston, MA, August 2018. doi: 10.13140/RG.2.2.33881.36969.

- [12] **Caitlin C. Bannan**, Camila Zanette, Christopher I. Bayly, Joshua Fass, Michael K. Gilson, Michael R. Shirts, John D. Chodera, and David L. Mobley. Automating force field parameterization with bayesian inference for chemical perception. Oral presentation at the *Graduate Women in Science Student Research Conference*, Chapman University, Orange, CA.
- [13] **Caitlin C. Bannan**, Camila Zanette, Christopher I. Bayly, Joshua Fass, Michael K. Gilson, Michael R. Shirts, John D. Chodera, and David L. Mobley. Improving Force Field Parameterization with Bayesian Inference for Chemical Perception. Poster presentation at *CUP XVII and XVIII OpenEye Scientific Software*, Santa Fe, NM and *SoCal TheoChem 2.0* Irvine, CA, March 2017, March 2018. doi: 10.13140/RG.2.2.17338.59848.
- [14] **Caitlin C. Bannan**, Daisy Y. Kyu, and David L. Mobley. Computing Partition Coefficients using Alchemical Free Energy Calculations. Irvine, CA, 2016. Poster presentation at the *251st ACS National Meeting* San Diego, CA and the *Ewha-UCI Pharmaceutical Sciences Annual Symposium* Irvine, CA. doi: 10.13140/RG.2.2.29469.31200.