David L. Mobley

dmobley@uci.edu

Department of Pharmaceutical Sciences
University of California, Irvine
Irvine, CA 92697
Ph. (949) 385-2436
Fax (949) 824-2949
http://www.mobleylab.org

EDUCATION

Ph.D. **University of California at Davis**, Physics, June, 2004. Advisers: Daniel L. Cox, Rajiv Singh.
M.S. **University of California at Davis,** Physics, 2001
B.S. **University of California at Davis,** Physics, 2000, with highest honors

PROFESSIONAL AND RESEARCH EXPERIENCE

July 2018-present: Professor, Depts. of Pharmaceutical Sciences and Chemistry, University of California, Irvine
July 2014-June 2018: Associate Professor, Depts. of Pharmaceutical Sciences and Chemistry, University of California, Irvine

January 2013-June 2014: Assistant Professor, Department of Chemistry, University of California Irvine

July 2012-June 2014: Assistant Professor, Department of Pharmaceutical Sciences, University of California, Irvine

July 2012-June 2015: Adjunct Professor, Department of Chemistry, University of New Orleans

July 2008- June 2012: Assistant Professor, Department of Chemistry, University of New Orleans.

June 2008-July 2008: Specialist, UC San Francisco, Adviser: Ken Dill

December 2007-June 2008: Chief Science Officer, Simprota Corporation

July 2004-December 2007: Postdoctoral Researcher, UC San Francisco, adviser: Ken Dill

June 2003-June 2004: Research Assistant, UC Davis, advisers: Daniel L. Cox and Rajiv R. P. Singh

Aug 2003-Dec. 2003: Graduate Fellow, Kavli Institute of Theoretical Physics, Santa Barbara, attending "Pattern Formation in Physics and Biology" program

2001-2003: National Science Foundation NEAT-IGERT Fellow, UC Davis, advisers: Daniel L. Cox, Rajiv R. P. Singh and Marjorie L. Longo

1999-2000: Undergraduate Research Assistant, UC Davis, adviser: Winston Ko

HONORS, AWARDS AND FELLOWSHIPS

- NSF CAREER Award, July 2014.
- Hewlett-Packard Outstanding Junior Faculty Award in Computational Chemistry, American Chemical Society, Fall, 2009.
- Graduate Fellowship, Kavli Institute for Theoretical Physics, Aug.-Dec. 2003.
- National Science Foundation NEAT-IGERT Fellowship, UC Davis, 2001-2003.
- UC Davis Physics Department Award, 2000-2001.
- Saxon-Patten Prize, University of California, Davis, 2000.
- Departmental Citation in Physics, University of California, Davis, 2000.
- Howard Hughes Medical Institute Science Teaching Internship, Spring 2000.

PUBLICATIONS (NUMBERED CHRONOLOGICALLY)
#- contributed equally, * - corresponding author

AS A FACULTY MEMBER (UNO AND UCI):

70. M. Riquelme, A. Lara, **D. L. Mobley**, T. Verstraelen, A. R. Matamala, and E. Vöhringer-Martinez, "Hydration Free Energies of Organic Molecules in the FreeSolv Database Calculated with Polarized Atom In Molecules Atomic Charges and the GAFF Force Field", *J. Chem. Inf. Model.* **58** (9): 1779-1797. PMCID PMC6195221.
69. S. Gill, N. M. Lim, P. Grinaway, A. S. Rustenburg, J. Fass, J. D. Chodera, **D. L. Mobley**, "Binding Modes of Ligands Using Enhanced Sampling (BLUES): Rapid Decorrelation of Ligand Binding Modes Using Nonequilibrium Candidate Monte Carlo," *J. Phys. Chem. B.* 122(21):5579-5598 (2018). PMCID PMC5980761.
68. G. Duarte Ramos Matos and D. L. Mobley, "Challenges of the use of atomistic simulations to predict solubilities of drug-like molecules", *F1000 Research*, May 2018 (DOI).
67. A. Kyrychenko, N. M. Lim, V. Vasquez-Montes, M. V. Rodnin, J. Alfredo Freites, L. P. Nguyen, D. J. Tobias, **D. L. Mobley**, A. S. Ladokhin, "Refining Protein Penetration into the Lipid Bilayer Using Fluorescence Quenching and Molecular Dynamics Simulations: The Case of Diphtheria Toxin Translocation Domain," *J. Membrane Biology*. (DOI)
66. P. S. Cremer, A. H. Flood, B. C. Gibb, and **D. L. Mobley**, "Collaborative routes to clarifying the murky waters of aqueous supramolecular chemistry", *Nature Chemistry* 10:8-16 (2018).
65. X. Yang, H. Lei, P. Gao, D. G. Thomas**, D. L. Mobley**, and N. A. Baker, "Atomic radius and charge parameter uncertainty in biomolecular solvation free energy calculations," *J. Chem. Theory Comput.* 14(2):759-767 (2018).
64. R. Abel, L. Wang, **D. L. Mobley** and R. A. Friesner, "A Critical Review of Validation, Blind Testing, and Real-World Use of Alchemical Protein-Ligand Binding Free Energy Calculations," *Cur. Top. Med. Chem.* **17**(23):2577-2585 (2017)**.**
63. Z. A. Könst, A. R. Szklarski, S. Pellegrino, S. E. Michalak, M. Meyer, C. Zanette, R. Cencic, Sangkil Nam, V. K. Voora, D. A. Horne, J. Pelletier, D. L. Mobley, G. Yusupova, M. Yusupov and C. D. Vanderwal, "Synthesis Facilitates an understanding of the structural basis for translation inhibition by the lissoclimides," Nature Chemistry **9**:1140-1149 (2017).
62. **D. L. Mobley** and M. K. Gilson, "Predicting binding free energies: Frontiers and benchmarks", *Ann. Rev. Biophys.* **46:**531-558 (2017). PMCID PMC5544526.
61. G. D. R. Matos, D. Y. Kyu, H. H. Loeffler, J. D. Chodera, M. R. Shirts and **D. L. Mobley**, "Approaches for calculating solvation free energies and enthalpies demonstrated with an update of the FreeSolv database," *Journal of Chemical and Engineering Data* **62**(5):1559-1569 (2017). PMCID PMC5648357.
60. L. J. Gosink, C. C. Overall, S. M. Reehl, P. D. Whitney, **D. L. Mobley** and N. A. Baker, "Bayesian Model Averaging for Ensemble-Based Estimates of Solvation Free Energies", *J. Phys. Chem. B* **121**(15):3458-3472 (2017).
59. M. R. Shirts, C. Klein, J. M. Swails, J. Yin, M. K. Gilson, **D. L. Mobley**, D. A. Case, E. D. Zhong, "Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset", in *J. Comput.-Aided Mol. Design* **31:**147-161 (2017).
58. J. Yin, N. M. Henriksen, D. R. Slochower, M. R. Shirts, M. W. Chiu, **D. L. Mobley** and M. K. Gilson, "Overview of the SAMPL5 host-guest challenge: Are we doing better?", in *J. Comput. Aided Mol. Design* **31:**1-19 (2017). PMCID PMC5241188.
57. A. S. Rustenburg, J. Dancer, B. Lin, J. A. Feng, D. F. Ortwine, **D. L. Mobley**, and J. D. Chodera, "Measuring experimental cyclohexane-water distribution coefficients for the SAMPL5 challenge", in *J. Comput.-Aided Mol. Design* **30:**945-958 (2016).
56. S. Evoli, D. L. Mobley, R. Guzzi and B. Rizzuti, "Multiple binding modes of ibuprofen in human serum albumin identified by absolute binding free energy calculations," *Physical Chemistry Chemical Physics* **18**:32358-32368 (2016). PMCID PMC5130592
55. C. C. Bannan, K. H. Burley, M. Chiu, M. R. Shirts, M. K. Gilson, and **D. L. Mobley***, "Blind prediction of cyclohexane-water distribution coefficients from the SAMPL5 challenge", *J. Comput. Aided Mol. Design* **30:**927-944 (2016). PMCID PMC5209301
54. N. M. Lim, L. Wang, R. Abel, and **D. L. Mobley***, "Sensitivity in binding free energies due to protein reorganization", *J. Chem. Theory Comput.* **12**(9): 4620-4631 (2016). One of the top 10 most read articles for August, 2016. PMCID PMC5021633.
53. C. C. Bannan, G. Calabro, D. Y. Kyu, **D. L. Mobley***, "Calculating Partition Coefficients of Small Molecules in Octanol/Water and Cyclohexane/Water", *J. Chem. Theory. Comput.* **12**(8): 4015-4024 (2016). One of the top 10 most read articles for August, 2016. PMCID PMC5053177.
52. S. Liu, S. Cao, K. Hoang, K. L. Young, A. S. Paluch and **D. L. Mobley***, "Using MD Simulations To Calculate How Solvents Modulate Solubility", *J. Chem. Theory and Comput.*, **12**(4), 1930–1941 (2016). PMCID PMC4945102.
51. P. V. Klimovich and **D. L. Mobley***, "A Python tool to set up relative free energy calculations in GROMACS,". *J. Comput. Aided Mol. Design*, **29**(11), 1007–1014 (2015). PMCID PMC4749424.
50. S. Liu, L. Wang, and **D. L. Mobley*,** "Is ring breaking feasible in relative binding free energy calculations?", *J.*

Chem. Inform. Modeling, **55**(4):727-735 (2015). PMCID PMC4489933.
49. P. V. Klimovich, M. R. Shirts and **D. L. Mobley***, "Guidelines for the analysis of free energy calculations", *J. Comput. Aided Mol. Design*. **29**(5):397-411 (2015). PMCID PMC4420631.
48. L. Wang, Y. Wu, Y. Deng, B. Kim, L. Pierce, G. Krilov, D. Lupyan, S. Robinson, M. K. Dahlgren, J. Greenwood, D. L. Romero, C. Masse, J. L. Knight, T. Steinbrecher, T. Beuming, W. Damm, E. Harder, W. Sherman, M. Brewer, R. Wester, M. Murcko, L. Frye, R. Farid, T. Lin, **D. L. Mobley**, W. L. Jorgensen, B. J. Berne, R. A. Friesner, and R. Abel*. "Accurate and reliable prediction of relative ligand binding potency in prospective drug discovery by way of a modern free-energy calculation protocol and force field", *J. Am. Chem. Soc*. 137(7):2695-2703 (2015).
47. A. S. Paluch*, S. Parameswaran, and **D. L. Mobley**, "Predicting the excess solubility of acetanilide, acetaminophen, phenacetin, benzocaine, and caffeine in binary water/ethanol mixtures via molecular simulation", *J. Chem. Phys*. **142**: 044508-1 to 044508-10 (2015). PMCID PMC4312346
46. S. Parameswaran and **D. L. Mobley***, "Box size effects are negligible for solvation free energies of neutral solutes", *J. Comput. Aided Mol. Design*. **28**:825-829 (2014).
45. **D. L. Mobley*** and J. P. Guthrie, "FreeSolv: A database of experimental and calculated hydration free energies, with input files," *J. Comput. Aided Mol. Design* **28**:711-720 (2014). PMCID PMC4113415
44. C. J. Fennell*, K. L. Wymer, and **D. L. Mobley***, "A fixed-charge model for alcohol polarization in the condensed phase, and its role in small molecule hydration", *J. Phys. Chem. B* **118**(24):6438-6446 (2014). Invited article.
43. **D. L. Mobley*,** S. Liu, N. M. Lim, K. L. Wymer, A. L. Perryman, S. Forli, N. Deng, J. Su, K. Branson, and A. J. Olson, "Blind prediction of HIV integrase binding from the SAMPL4 challenge", *J. Comput. Aided Mol. Design* 28(4):327-345 (2014). PMCID PMC4331050.
42. H. S. Muddana, A. T. Fenley, **D. L. Mobley***, and M. K. Gilson*, "The SAMPL4 host-guest blind prediction challenge: an overview", *J. Comput. Aided Mol. Design* 28(4):305-317 (2014). PMCID PMC4053502
41. T. S. Peat*, O. Dolezal, J. Newman, **D. L. Mobley**, J. J. Deadman, "Interrogating HIV integrase for compounds that bind – a SAMPL4 challenge", *J. Comput. Aided Mol. Design* 28:347-362 (2014). PMCID PMC4346355
40. **D. L. Mobley*,** K. L. Wymer, and N. M. Lim, "Blind prediction of solvation free energies from the SAMPL4 challenge", *J. Comput. Aided Mol. Design* **28**:135-150 (2014). PMCID PMC4006301
39. Y-C. Zheng, Y-C. Duan, J.-L. Ma, R.-M. Xu, X. Zi, W.-L. Lv, M.-M. Wang, X.-W. Ye, S. Zhu, **D. L. Mobley**, Y. Zhu, J.-W. Wang, J.-F. Li, Z.-R. Wang, W. Zhao, H.-M. Zhao, "Triazole-dithiocarbamate based, selective LSD1 inactivators inhibit gastric cancer cell growth, invasion, and migration," *J. Med. Chem*. **56**(21):8543-8560 (2013).
38. G. J. Rocklin, **D. L. Mobley**, K. A. Dill, and P. H. Hünenberger*, "Calculating the binding free energies of charged species based on explicit-solvent simulations employing lattice-sum methods: An accurate correction scheme for finite-size effects", *J. Chem. Phys*. **139**(18):184103 (2013). PMCID PMC3838431. Selected as cover article, and highlighted article, for *J. Chem. Phys*.
37. S. Liu, Y. Wu, T. Lin, R. Abel, J. Redmann, C. M. Summa, V. R. Jaber, N. M. Lim, and **D. L. Mobley***, "Lead Optimization Mapper: Automating free energy calculations for lead optimization", *J. Comput. Aided Mol. Design* **27**(9):755-770 (2013). PMCID PMC3837551.
36. G. J. Rocklin, S. E. Boyce, M. Fisher, I. Fish, **D. L. Mobley**, B. K. Shoichet*, and K. A. Dill*. "Blind prediction of charged ligand binding affinities in a model binding site", *J. Mol. Biol*. **425**(22):4569-4583 (2013). PMID 23896298. Highlighted by Faculty of 1000.
35. G. J. Rocklin, **D. L. Mobley**, and K. A. Dill*, "Calculating the sensitivity and robustness of binding free energy calculations to force field parameters", *J. Chem. Theory Comput*. **9:** 3072-3083 (2013). PMCID PMC3763860.
34. A. Thaxton, S. Izenwasser, D. Wade, E. D. Stevens, **D. L. Mobley**, V. Jaber, S. A. Lomenzo, M. L. Trudell*, "3-aryl-3-arylmethoxyazetidines. A new class of high affinity ligands for monoamine transporters," *Bioorg. Med. Chem. Lett*. **23:** 4404-4407 (2013).
33. J. D. Chodera* and **D. L. Mobley**, "Entropy-enthalpy compensation: Role and ramifications in biomolecular ligand recognition and design", *Annual Reviews in Biophysics* 42:121-142 (2013).
32. G. J. Rocklin, **D. L. Mobley**, and K. A. Dill, "Separated Topologies: A method for relative binding free energy calculations using orientational restraints", *J. Chem. Phys*. 138:085104 (2013). PMCID PMC3598757.
31. **D. L. Mobley*** and P. V. Klimovich, "Perspective: Alchemical free energy calculations for drug discovery", invited perspective, *J. Chem. Phys*. 137:230901 (2012). PMCID PMC3537745. A top ten "most read" article in *J. Chem. Phys*. for December 2012 and January 2013. Second "most accessed" article, *J. Chem. Phys*., Q1 2013. A "most accessed" article, Q2, 2013.
29. **D. L. Mobley*,** S. Liu, D. Cerutti, W. C. Swope, and J. Rice, "Alchemical prediction of hydration free energies for SAMPL", special issue, *J. Comput. Aided Mol. Design* **26**(5):551-562 (2012).
30. C. D. Savoie and **D. L. Mobley***, "Understanding the structural and functional effects of mutations in HIV-1 protease mutants using 100 ns molecular dynamics simulations", *Journal of Computational Science Education* 2(1): 28-34 (2011).
28. **D. L. Mobley***, "Let's get honest about sampling", invited perspective, *J. Comput. Aided Mol. Design Design* **26**(1):93-95 (2012).

27. A. S. Paluch, **D. L. Mobley**, and E. J. Maginn*, "Small Molecule Solvation Free Energy: Enhanced Conformational Sampling Using Expanded Ensemble Molecular Dynamics Simulation", *Journal of Chemical Theory and Computation* 7:2910-2918 (2011).
26. **D. L. Mobley** and M. R. Shirts*, "An introduction to best practices in free energy calculations", in "Biomolecular Simulations: Methods and Protocols", Methods in Molecular Biology 924:271-311 (2013).
25. J. D. Chodera*, **D. L. Mobley**, M. R. Shirts, R. W. Dixon, K. Branson, V. S. Pande, "Alchemical free energy methods for drug discovery: Progress and challenges," *Current Opinion in Structural Biology* 21:150-160 (2011).
24. X. Gu, S. Izenwasser, D. Wade, A. Housman, G. Gulasey, J. B. Rhoden, C. D. Savoie, **D. L. Mobley**, S. A. Lomenzo, and M. D. Trudell*. "Synthesis and Structure-Activity Studies of Benzyl Ester Meperidine and Normeperidine Derivatives as Selective Serotonin Transporter Ligands", *Bioorg. Med. Chem. Lett.* **18**: 8356-8364, 2010.
23. P. V. Klimovich and **D. L. Mobley***, "Predicting hydration free energies using all-atom molecular dynamics simulations and multiple starting conformations", J. Computer-Aided Molecular Design **24**: 307-316 (2010).
22. M. R. Shirts*, **D. L. Mobley** and S. P. Brown, "Free energy calculations in structure-based drug design", in "Structure Based Drug Design", Cambridge University Press (2010), edited by Kenneth M. Merz, Dagmar Ringe and Charles H. Reynolds. Invited chapter.
21. J. Ponder*, C. Wu, V. Pande, J. Chodera, M. Schneiders, **D. Mobley**, I. Haque, D. Lambrecht, R. Distasio, Jr., M. Head-Gordon, G. Clark, M. Johnson, T. Head-Gordon. "Current status of the AMOEBA polarizable force field", *J. Phys. Chem. B*. **114:** 2549-2564 (2010). (Cover article).
20. H. Kaur, S. Izenwasser, A. Verma, D. Wade, A. Housman, E. D. Stevens, **D. L. Mobley**, and M. L. Trudell*. "Synthesis and monoamine transporter affinity of 3α-Arylmethoxy-3β-arylnortropanes", *Bioorg. Med. Chem. Lett.* **10**:6865-6868 (2009).
19. S. E. Boyce#, **D. L. Mobley**#, G. Rocklin, A. P. Graves, K. A. Dill*, B. K. Shoichet*. "Predicting ligand binding affinity with alchemical free energy methods in a polar model binding site", *J. Mol. Biol.* **394:** 747-763 (2009).
17. **D. L. Mobley*** and K. A. Dill, "The binding of small-molecule ligands to proteins: 'What you see' is not always 'what you get'", *Structure* **17**(4): 489-498 (2009).
16. **D. L. Mobley*,** C. I. Bayly, M. D. Cooper, and K. A. Dill, "Predictions of hydration free energies from all-atom molecular dynamics simulations", J. Phys. Chem. B **113:** 4533-4537 (2009). Invited article, special issue on "Calculation of Aqueous Solvation Energies of Drug-Like Molecules: A Blind Challenge".
15. **D. L. Mobley***, C. I. Bayly, M. D. Cooper, M. R. Shirts, and K. A. Dill. "Small molecule hydration free energies in explicit solvent: An extensive test of fixed-charge force fields", *J. Chem. Theory Comput.* **5:** 350-358 (2009). One of the top 10 most downloaded articles from March 2008 to March 2009. One of the top 20 most downloaded articles in 2009.

GRADUATE AND POSTDOCTORAL:

18. C. L. McClendon, G. Friedman, **D. L. Mobley**, H. Amirkhani, and M. P. Jacobson*, "Quantifying correlations between allosteric sites in thermodynamic ensembles", *J. Chem. Theory Comput.* **5** (9): 2486-2502 (2009).
14. **D. L. Mobley,** A. Barber II, C. Fennell, and K. A. Dill*, "Charge asymmetries in hydration of polar solutes", *J. Phys. Chem. B*. **112:** 2405-2414 (2008). Erratum: **D. L. Mobley***, J. R. Baker, A. E. Barber II, C. J. Fennell, and K. A. Dill, "Erratum: Charge Asymmetries in Hydration of Polar Solutes", *J. Phys. Chem. B* (2011) (http://dx.doi.org/10.1021/jp210487k).
13. **D. L. Mobley***, J. D. Chodera and K. A. Dill, "Treating entropy and conformational change in implicit solvent simulations of small molecules", *J. Phys. Chem. B*, **112**: 938-946 (2008).
12. A. Nicholls*#, **D. L. Mobley*#**, J. P. Guthrie, J. D. Chodera, and V. S. Pande. "Predicting small-molecule solvation free energies: A blind challenge test for computational chemistry," *J. Med. Chem.* **51**:769-779 (2008).
11. T. Steinbrecher, **D. L. Mobley**, and D. A. Case*. "Non-linear scaling schemes for Lennard-Jones interactions in free energy calculations", *J. Chem. Phys.*, **127:** 214108 (2007). Selected for the *Virtual Journal of Biological Physics* 14 (12) (2007).
10. M. R. Shirts#*, **D. L. Mobley**#, J. D. Chodera, and V. S. Pande. "Accurate and efficient corrections for missing dispersion interactions in molecular simulations", *J. Phys. Chem. B*. **111**:13052-13063 (2007).
9. **D. L. Mobley#**, A. P. Graves#, J. D. Chodera, A. C. McReynolds, B. K. Shoichet* and K. A. Dill*, "Predicting absolute ligand binding free energies to a simple model site," *Journal of Molecular Biology* **371**(4): 1118-1134 (2007). One of the top 25 hottest articles, July-September, 2007.
8. M. R. Shirts*, **D. L. Mobley**, and J. D. Chodera, "Alchemical free energy calculations: Ready for prime time?" *Annual Reports in Computational Chemistry* **3**: 41-59 (2007), invited review.
7. **D. L. Mobley**, J. D. Chodera, and K. A. Dill*, "Confine and Release Method: Obtaining Correct Binding Free Energies in the Presence of Protein Conformational Change", *Journal of Chemical Theory and Computation* **3**(4): 1231 (2007). One of the top 25 most accessed articles, July-September, 2007. A most accessed article for 2007.
6. **D. L. Mobley**, E. Dumont, J. D. Chodera, K. A. Dill*, "Comparison of charge models for fixed-charge force fields: Small-molecule hydration free energies in explicit solvent", *J. Phys. Chem. B* **111**(9):2242 (2007). Erratum: DOI 10.1021/jp108173f (2011).

5. A. M. Stein, T. Demuth, **D. Mobley**, M. Berens, and L. Sander*, "A Mathematical Model of Glioblastoma Tumor Spheroid Invasion in a 3-D in vitro Experiment", *Biophysical Journal,* **92**(1):356 (2007).
4. **D. L. Mobley**, J. D. Chodera, K. A. Dill*, "On the use of orientational restraints and symmetry number corrections in alchemical free energy calculations", *J. Chem. Phys.* **125**:084902 (2006). Selected for the *Virtual Journal of Biological Physics Research* 12(5) (2006).
3. **D. L. Mobley**, C. R. Pike, J. E. Davies, D. L. Cox*, R. R. P. Singh, "Hysteresis loops of Co-Pt perpendicular magnetic multilayers". *Journal of Physics: Condensed Matter,* **16**: 5897-5906 (2004).
2. **D. L. Mobley**, D. L. Cox, R. R. P. Singh, M. W. Maddox, M. L. Longo, "Modeling Amyloid Beta Peptide Insertion into Lipid Bilayers". *Biophysical Journal,* **86**(6): 3585-3597 (2004).
1. **D. L. Mobley**, D. L. Cox*, R. R. P. Singh, R. V. Kulkarni and A. Slepoy, "Simulations of Oligomeric Intermediates in Prion Diseases", *Biophysical Journal*, **85**(4):2213-2223 (2003).

PUBLICATIONS UNDER REVIEW OR IN PRESS

- C. C. Bannan, D. L. Mobley and G. Skillman, "SAMPL6 Challenge Results from pKa Predictions Based on a General Gaussian Process Model," in press, JCAMD. https://doi.org/10.26434/chemrxiv.6406505.v1
- H. H. Loeffler, S. Bosisio, G. Duarte Ramos Matos, D. Suh, B. Roux, D. L. Mobley, J. Michel, "Reproducibility of free energy calculations across different molecular simulation software", accepted, *J. Chem. Theory Comput*. DOI: 10.26434/chemrxiv.6402425.v1
- D. L. Mobley, C. C. Bannan, A. Rizzi, C. I. Bayly, J. D. Chodera, V. T. Lim, K. A. Beauchamp, M. R. Shirts, M. K. Gilson, and P. K. Eastman, "Open Force Field Consortium: Escaping atom types using direct chemical perception with SMIRNOFF v0.1", accepted, *J. Chem. Theory Comput*., DOI http://biorxiv.org/cgi/content/short/286542v1.
- C. Zanette, C. C. Bannan, C. I. Bayly, J. Fass, M. K. Gilson, M. R. Shirts, J. D. Chodera and D. L. Mobley, "Towards learned chemical perception of force field typing rules," in review, DOI https://doi.org/10.26434/chemrxiv.6230627.v1 .
- A. Rizzi, S. Murkli, J. N. McNeill, W. Yao, M. Sullivan, M. K. Gilson, M. W. Chiu, L. Isaacs, B. C. Gibb, D. L. Mobley, J. D. Chodera, "Overview of the SAMPL6 host-guest binding affinity prediction challenge", in press, JCAMD. DOI: https://doi.org/10.1101/371724
- M. Isik, D. Levorse, A. S. Rustenburg, I. E. Ndukwe, H. Wang, X. Wang, M. Reibarkh, G. E. Martin, A. Makarov, D. L. Mobley, T. Rhodes, J. D. Chodera, "pKa measurements for the SAMPL6 prediction challenge for a set of kinase inhibitor-like fragments," in press, JCAMD (DOI)
- K. H. Burley, S. C. Gill, N. M. Lim and D. L. Mobley, "Enhancing sidechain sampling using non-equilibrium candidate Monte Carlo", submitted. DOI: 10.26434/chemrxiv.7184876.v1
- E. Braun, J. Gilmer, H. B. Mayes, D. L. Mobley, J. I. Monroe, S. Prasad, D. M. Zuckerman, "Best practices for foundations in molecular simulations", (link), in press, *Living Journal of Computational Molecular Science*
- G. D. R. Matos, G. Calabró and D. L. Mobley, "Infinite Dilution Activity Coefficients as Constraints for Force Field Parameterization and Method Development", (DOI)
- K. H. Burley, S. C. Gill, N. M. Lim and D. L. Mobley, "Enhancing Sidechain Rotamer Sampling Using Non-Equilibrium Candidate Monte Carlo", (DOI)
-

MEETINGS/WORKSHOPS/SESSIONS ORGANIZED

- "Physics-based methods for absolute and relative binding affinities", October 16-17, 2006, Monterey, CA.
- "Free energy methods in drug design", Vertex Pharmaceuticals, Cambridge, MA, May 17-19, 2010 (co-organizer).
- "2012 workshop on free energy methods in drug design," Vertex Pharmaceuticals, Cambridge, MA, May 2012 (lead organizer).
- "Shiny New Things" session, OpenEye Software CUP XIII, Santa Fe, NM, March 5-7, 2012.
- SAMPL4 "Statistical Asssessment of Modeling of Proteins and Ligands" blind prediction challenge and workshop, Sept. 20, 2013.
- "2014 Workshop on Free Energy Methods in Drug Design", Vertex Pharmaceuticals, Cambridge, MA, May 2014 (co-organizer).
- "Biomolecular Recognition", Telluride Workshop, July 2014. Lead organizer.
- "Accelerating our Understanding of Supramolecular Chemistry in Aqueous Solutions", NSF Workshop,

Washington, DC, May 2015. Co-organizer.
- "2016 Workshop on Free Energy Methods in Drug Design", Vertex Pharmaceuticals, Boston, MA, May 2016.
- "Workshop for Best Practices in Molecular Simulation", August 24-25, 2017, National Institutes of Standards and Technology, Gaithersburg, MD. Co-organizer.
- "Workshop on Free Energy Methods, Kinetics and Markov State Models in Drug Design", Cambridge, MA, May 2018. Co-organizer.

GRANTS AND CONTRACTS RECEIVED (PI UNLESS OTHERWISE INDICATED)

FINANCIAL:

- "Advancing new computational methods for predicting protein-ligand binding", University of New Orleans Summer Research Program SCoRe grant, $12,600. July 1, 2009 through Aug. 15, 2009.
- "Improving drug discovery and biomedical innovation using molecular simulations", Louisiana Board of Regents Research Enhancement Program, June 1, 2010 through May 30, 2011. $121,303. As PI.
- "Advancing new computational methods for predicting protein-ligand binding", Louisiana Board of Regents Research Competitiveness Subprogram, June 1, 2010 through May 30, 2013. $132,375. As PI.
- "Leveraging next generation supercomputing to study complex emergent phenomena in novel materials", NSF EPSCoR grant, PI: Michael Khonsari. $4M (UNO component $1.56 M across 5 investigators; $390k to me). As co-investigator. Oct. 1, 2010 through Sept. 30, 2015. NSF EPS-1003897.
- "Improving alchemical methods for predicting protein-ligand binding", NIH R-15 AREA grant, March 1, 2012 – Feb. 28, 2015. $265,056.
- "CAREER: Computing accurate free energies for solubility, solvation, and transfer," National Science Foundation, $601,354, July 15, 2014 through July 14, 2019. As PI.
- "Accelerating our Understanding of Supramolecular Chemistry in Aqueous Solutions: A Workshop Proposal", NSF Workshop proposal, as co-organizer. $48,784.
- "Alchemical free energy calculations for efficient drug lead optimization", National Institutes of Health, $1,393,256. 9/1/2014 through 8/31/2015. As PI.
- "Developing Community Best Practices for Molecular Simulation Software", a workshop proposal through NSF MolSSI, $15,000, 2/13/2017 through 9/30/2017.
- "Macromolecular movements by simulation and diffuse scatter", University of California Lab Fees through the UC Office of the President, ($1.2M total; $300,000 UCI). 3/1/2017 through 2/29/2020. As co-investigator.
- "Advancing predictive physical modeling through focused development of model systems to drive new modeling innovations", National Institutes of Health, $1,161,791 total (including three subcontracts). 9/10/2018 through 8/31/2022. As PI.

COMPUTER OR STAFF TIME:

- "Predicting protein-ligand binding and solvation", Louisiana Optical Network Initiative computer time allocation, for 500,000 service units. March 30, 2009.
- "Infrastructure for accurate and efficient binding affinity calculations", 6 months of Louisiana Optical Network Initiative staff scientist time. February 27, 2009 through Feb. 26, 2010.
- "Computational methods for protein-ligand binding", PetaShare allocation for 1 TB storage, December, 2008.
- "Computational methods for protein-ligand binding", computer time allocation, Louisiana Optical Network Initiative. 50,000 service units, December 2008 through December 2009.
- "Predicting protein-ligand binding", Louisiana Optical Network Initiative, Jan. 1, 2010, for 300,000 service units.
- "GPU-accelerated calculation of ligand binding affinities to biological macromolecules", NSF Teragrid, 250,000 SUs. As co-PI. Jan. 1, 2010 through Jan. 1, 2011.
- "Equilibration of charges in Cytochrome C Peroxidase free energy calculations", Louisiana Optical Network Initiative, July 1, 2010 through July 1, 2011. 50,000 SUs.
- "Guiding Biotin Carboxylase Lead Development", Louisiana Optical Network Initiative, October 1, 2010 through October 1, 2011. 400,000 SUs.
- "GPU-accelerated calculation of ligand binding affinities to biological macromolecules", NSF Teragrid renewal, 1.2M SUs. March 18, 2011 through March 17, 2012. Co-PI.
- "Next generation GPU-based codes for materials discovery", Louisiana Optical Network Initiative (LONI), 6 months of staff scientist time. March 14, 2011 through October 2011. Co-PI.
- "Improving alchemical methods for predicting protein-ligand binding", NSF XSEDE computer time allocation, October 1, 2011 through Sept. 31, 2012. 1.2 M SUs.
- "Binding affinity prediction for trypsin and DNA gyrase", Louisiana Optical Network Initiative computer time allocation, October 1, 2011 through Sept. 31, 2012. 1.0 M SUs.

- "Testing new approaches to alchemical calculations for protein-ligand binding", NSF XSEDE renewal, 808,000 SUs, Jan. 1, 2013 through Jan. 1, 2014.

INVITED PRESENTATIONS

- "Developing and using free energy calculations to guide pharmaceutical lead optimization", UC Riverside, Oct. 28, 2018.
- "Binding free energy calculations and binding mode sampling", Statistical Physics in Biology workshop, Arizona State University, Oct. 8, 2018
- "Binding free energy calculations and ligand binding mode sampling," Computational Chemistry Gordon Conference, Mount Snow, Vermont, July 23, 2018.
- "Towards accurate, efficient prediction of protein-ligand interactions for lead optimization", Pfizer, Groton, CT, May 18, 2018.
- "Enabling quantitative, predictive biomolecular design", Yale Chemistry seminar, May 18, 2018.
- "SAMPL: Past, present and future", Drug Discovery Data Resource Workshop, San Diego, CA, February 2018.
- "Free energy calculations tutorial", an all-day tutorial at the University of Concepcion, Chile, December 2017.
- "Insights into protein ligand interactions from molecular simulations," Symposium on Molecular Interactions in Chemistry and Biology, University of Concepcion, Chile, December 2017.
- "Towards automating force field development: Force field assignment via direct chemical perception", CECAM Meeting "Designing force fields in an era of cheap computing," Sheffield, England, July 27, 2017.
- "Adapting free energy methods to predict binding modes of ligands," at "Free energy calculations: Three decades of adventure in chemistry and biophysics" Telluride Science Research Center conference, Telluride, CO, July 12, 2017.
- "Adapting free energy methods to predict binding modes of ligands," CECAM "Beyond Kd: New computational methods to address challenges in drug discovery" workshop, EPFL, Lausanne, Switzerland, June 13, 2017.
- "Making alchemical free energy calculations practical for drug discovery", Pfizer, April 12, 2017
- "What happened when Ant let us put MD on Orion: Towards fragment binding mode occupancies with BLUES" and "Automating best practices: Good for users, good for science," OpenEye Scientific Software Customers, Users and Programmers meeting, Santa Fe, NM, March 2017.
- "Using physics-based modeling to improve pharmaceutical drug discovery", CSU Los Angeles, Nov. 10, 2016.
- "Examining how protein sampling impacts the convergence of relative binding free energy calculations," Workshop on Free Energy Methods in Drug Discovery, Boston, MA, May 2016.
- "Applications of alchemical binding calculations to protein conformational change," American Chemical Society Meeting, San Diego, CA, April 2016.
- "SAMPL5: Distribution Coefficients and Host-Guest Binding", D3R/SAMPL5 Workshop, San Diego, CA, April 2016
- "Using free energy calculations to test and improve force fields and guide lead optimization", American Chemical Society National Meeting, Boston, MA, Aug. 17, 2015.
- "Using Free Energy Calculations to Probe Protein-Ligand Interactions and Guide Discovery", Zing Computational Chemical Biology workshop, Cairns, Australia, Aug. 8, 2015.
- "Successes and challenges in calculating binding free energies from molecular simulations", Banff International Research Station workshop on "Free Energy Calculations: A Mathematical Perspective", Oaxaca, Mexico, July 20, 2015.
- "Using molecular simulations to understand and predict biomolecular interactions and solvation", Telluride Workshop on Protein Electrostatics, Telluride, CO., July 10, 2015.
- "Testing force fields and free energy calculations with solvation, solubility and other properties", Snowmass Workshop on Free Energy Calculations, Snowmass, CO., July 7, 2015.
- "Using molecular simulations to understand and predict biomolecular interactions and solvation", Tulane University Chemistry seminar, New Orleans, LA, March 16, 2015.
- "Using modeling and free energy calculations to guide drug lead optimization", 1st Ewha-UCI joint symposium, Ewha University, Seoul, Korea, Sept. 29, 2014.
- "Using computer modeling to guide pharmaceutical drug discovery", Chemistry seminar, CSU Northridge, Northridge, CA, Sept. 17, 2014.
- "Using model systems to improve binding free energy calculations for drug discovery," AAAS Regional Meeting, Riverside, CA, June 2014.

- "Making alchemical free energy calculations practical for drug discovery: What will it take and where do we stand?", JCUP Meeting, Tokyo, Japan, June 6, 2014.
- "Using solution-phase free energy calculations to improve binding free energies", 2014 Workshop on Free Energy Methods in Drug Discovery, Boston, MA, May 2014.
- "Making binding free energy calculations practical for drug discovery," Genentech, April 8, 2014.
- "Predicting charged-ligand binding from molecular simulations," Biophysical Society Meeting, San Francisco, CA, Feb. 2014.
- "Predicting binding affinities and transfer free energies from molecular simulations," Arizona State University, Tempe, AZ, Nov. 13, 2013.
- "Developing computer tools to guide pharmaceutical drug discovery," W. M. Keck Center, Claremont Colleges, CA, Oct. 10, 2013.
- "SAMPL4: An overview", workshop on Statistical Assessment of Modeling of Proteins and Ligands (SAMPL) 4, Stanford, CA, Sept. 20, 2013.
- "Free energy calculations: blind predictions, model binding sites, and automated planning," California State University Long Beach Chemistry seminar, September 25, 2013.
- "Free energy calculations: blind predictions, model binding sites, and automated planning," for "Free Energy Calculations: Three Decades of Adventure in Chemistry and Biophysics", Snowmass, CO, July 16, 2013.
- "Small molecule hydration free energy calculations", Chemistry Seminar, University of California, Riverside, CA, May 13, 2013.
- "Alchemical calculations of binding free energies from MD simulations," American Chemical Society meeting, New Orleans, LA, April 8, 2013.
- "Free energy calculations: blind predictions, model binding sites, and automated planning," Stony Brook University, Stony Brook, NY, February 12, 2013.
- "Alchemical free energy calculations provide new insights into protein-ligand binding and solvation", University of Delaware, February 11, 2013.
- "Small molecule hydration free energy calculations," ETH Zurich, Zurich, Switzerland, January 21, 2013.
- "Free energy calculations: blind predictions, model binding sites, and automated planning," Boku University, Vienna, Austria, January 17, 2013.
- "Free energy calculations: blind predictions, model binding sites, and automated planning," Vrije University, Amsterdam, the Netherlands, January 14, 2013.
- "Free energy calculations: model binding sites, multiple binding modes, and automated planning", Schrödinger Software, New York, NY, Sept. 6, 2012.
- "Calculations of binding free energies with molecular simulations: Progress and challenges", American Institute of Mathematical Sciences meeting on Dynamical Systems, Orlando, FL, July 1, 2012.
- "Planning and conducting relative free energy calculations:Automation and issues", Workshop on Free Energy Calculations in Drug Discovery, Cambridge, MA, May 2012.
- "Insights into protein-ligand binding and solvation from atomistic free energy calculations", Chemistry seminar, University of Southern Mississippi, May 2012.
- "Free energy calculations using MD: Is that like 'free lunch'?", OpenEye CUP Meeting, Santa Fe, NM, March 7, 2012.
- "Insights from Predicting Binding Free Energies Using Molecular Simulations", American Chemical Society Southeast Regional Meeting, Richmond, VA, October 28, 2011.
- "Insights into Solvent Effects from Free Energy Calculations", Statistical Assessment of Modeling of Proteins and Ligands (SAMPL) workshop, Stanford, CA, Aug. 1, 2011.
- "Challenges in Predicting Absolute Binding Free Energies from Molecular Dynamics Simulations", July 5, 2011, Telluride Workshop on "Free Energy Simulations: From Academic Research to Industrial Application", Telluride, CO.
- "Challenges in Predicting Absolute Binding Free Energies from Molecular Dynamics Simulations", May 5, 2011, at CECAM meeting on "Dynamics and Thermodynamics of Biomolecular Recognition", Ecole Polytechnique, Palaiseau, France.
- "Predicting binding free energies from molecular simulations", 4th LBRN Workshop on Computational Biology, March 18, 2011, Louisiana State University, Baton Rouge.
- "Insights into solvent effects from free energy calculations", joint Southwest/Southeast Meeting of the American Chemical Society, New Orleans, LA, Dec. 1, 2010.
- "Predicting Protein-ligand Binding Affinities from Molecular Simulations", BioMaPS Institute, Rutgers University, October 5, 2010.

- "Predicting biomolecular binding interactions from thermodynamics," University of New Orleans Department of Physics, March 10, 2010.
- "Predictive calculations of protein-ligand binding", Louisiana State University Department of Biological Sciences, Oct. 5, 2009.
- "Insights from calculations of hydration and binding free energies", University of New Orleans Math Colloquium, Sept. 9, 2009.
- "Computational predictions of protein-ligand binding affinities", Hewlett Packard Outstanding Junior Faculty Award, American Chemical Society Meeting, Washington, D.C., Aug. 18, 2009.
- "Predictive calculations of absolute binding free energies", American Chemical Society Meeting, August 2008, Philadelphia, PA.
- "Predicting binding and solvation free energies with alchemical methods", Telluride Meeting on Algorithmic Development for Enhanced Sampling, Telluride, CO, July 16, 2008.

CONTRIBUTED PRESENTATIONS AND CONFERENCES

- "Toward more accurate force fields through direct chemical perception: How to get rid of wizards", CECAM "Beyond Kd: New computational methods to address challenges in drug discovery" workshop, EPFL, Lausanne, Switzerland, June 13, 2017.
- "Toward more accurate force fields through direct chemical perception: How to get rid of wizards", American Chemical Society Meeting talk, April, 2017, San Francisco, CA.
- Attendee at the "Accelerating our Understanding of Supramolecular Chemistry in Aqueous Solutions" NSF Workshop, Washington, DC, May 2015.
- "Automated planning of relative free energy calculations," talk at the American Chemical Society Meeting, New Orleans, LA, April 8, 2013.
- "Absolute binding free energy calculations: Progress towards biological binding sites," talk at the American Chemical Society Meeting, San Diego, CA, April 2012.
- "Small molecule hydration free energy calculations", talk at the American Chemical Society Meeting, San Diego, CA, April 2012.
- "Insights and innovations in alchemical calculations of binding free energies", talk at the American Chemical Society Meeting, San Francisco, CA, March 21, 2010.
- "Alchemical predictions of free energies, from hydration to binding", talk at the American Chemical Society Meeting, Washington, D.C., Aug. 19, 2009.
- "Explicit solvent calculations of transfer free energies", talk at the OpenEye SAMPL meeting, Montreal, Canada, June 18, 2009.
- "Lessons learned from predicting binding free energies in model binding sites" and "Quantitative predictions of protein-ligand binding affinities", talks at the American Chemical Society Meeting, Salt Lake City, UT, March 2009.
- "Predictive calculations of absolute binding free energies", talk at the American Chemical Society Meeting, Aug. 20, 2008, Philadelphia, PA.
- "Predicting absolute binding free energies with physics-based methods", talk at the American Chemical Society Meeting, New Orleans, March, 2008.

GRADUATE AND POSTDOCTORAL PRESENTATIONS

- "Charge asymmetries in hydration of polar solutes," talk at the American Chemical Society meeting, New Orleans, March, 2008.
- "Predicting protein-ligand binding free energies", platform presentation at the Biophysical Society Meeting, February, 2008, Long Beach, CA.
- "There's no success like failure: Insights from hydration free energy calculations", March 2008, OpenEye CUP meeting, Santa Fe, NM.
- "New insights into small molecule solvation and protein-ligand binding from atomistic simulations", September, 2007, Computational Science seminar, Florida State University.
- "Predicting ligand binding free energies in a model binding site," SGX Pharmaceuticals, San Diego, April 2007.
- "Challenges in predicting binding free energies to a simple model binding site", poster presentation, American Chemical Society Meeting, Boston, MA, August, 2007.
- "Insights on aqueous solvation from alchemical free energy calculations", poster presentation, American Chemical

Society Meeting, Boston, MA, August, 2007.

- "Predicting protein-ligand binding affinities in model binding sites", short talk and poster presentation, Computer Aided Drug Design Gordon Conference, July 2007, New Hampshire.
- "Predictive absolute binding free energy calculations for an engineered binding site in T4 Lysozyme", platform presentation at the Biophysical Society Meeting, March, 2007, Baltimore.
- "A top-down, physics-based approach to protein-ligand binding", poster presentation, OpenEye Software CUP VIII meeting, Santa Fe, N.M., February, 2007.
- "It's harder than it looks: Predicting absolute binding free energies for the 'hydrogen atom' of binding sites", poster at the Computational Chemistry Gordon Conference, October, 2006, Les Diablerets, Switzerland.
- "On avoiding sampling and convergence problems in alchemical binding free energy calculations," Sept. 14, 2006 talk at American Chemical Society Meeting, San Francisco, CA.
- "Binding Free Energy Calculations for a Designed Binding Pocket in T4 Lysozyme", February 21, 2006, poster at the Biophysical Society Meeting, Salt Lake City, Utah.
- "Molecular Dynamics Studies of a Designed Binding Pocket in T4 Lysozyme", August 2, 2005, poster at Protein Society meeting, Boston, MA.
- "Calculating Absolute Ligand Binding Free Energies with Thermodynamic Integration (TI)", June 22, 2005, poster at Gordon Research Conference on Proteins, June 19-24, 2005, Holderness, NH.
- "Calculating absolute ligand binding free energies with thermodynamic integration (TI)", April 2005, poster at Flexibility in Biomolecules workshop, Tempe, AZ.
- "Replica Exchange Molecular Dynamics Studies of a Designed Binding Pocket in T4 Lysozyme", February 2005 poster at Biophysical Society meeting, Long Beach, CA.
- "Free Energy Calculations: Methodology and Application to Computational Drug Design", January, 2006, Condensed Matter Physics Seminar, UC Davis.
- "Oligomerization and Aggregation in Amyloid Diseases", April 2, 2004, ICAM workshop on "Lifelike Matter", Santa Fe, NM.
- "The Hunt for the Cause of Cell Death in Alzheimer's Disease", March 19, 2004, science colloquium, Shasta College, Redding, CA.
- "Modeling Alzheimer's A-Beta Peptide Insertion into Lipid Bilayers", Feb. 27, 2004, Biophysics seminar, UC Davis.
- "Modeling Alzheimer's A-Beta Peptide Insertion into Lipid Bilayers", Feb. 10, 2004, short talk at Protein Misaggregation: from Biomolecules to Neurodegeneration workshop, Boston, MA, Feb. 9-11, 2004.
- "Modeling Alzheimer's A-Beta Peptide Insertion into Lipid Bilayers", Feb. 17, 2004, poster at Biophysical Society meeting, Baltimore, MD, Feb. 13-18, 2004.
- "Insights on Hysteresis from a Simple Computer Model", UC Davis Physics Department Colloquium, March, 2003.
- "Evidence for Oligomeric Intermediates in Prion Diseases," poster presentation at Nano and Bio-Nanoscience Research Meeting, June 27, 2002, Stanford University, California.

EDITORIAL AND ADVISORY BOARDS

- Managing Editor and Lead Editor for Perpetual Reviews for the *Living Journal of Computational Molecular Science* (2017-present)
- Editorial board for *Journal of Computer-Aided Molecular Design* (2012-present).
- Editorial board for *Journal of Molecular Recognition* (2017-present).
- Scientific Advisory Board, Schrödinger, LLC (2013-2016).
- Scientific Advisory Board, OpenEye Scientific Software (2016-present)
- Advisory Board, Drug Discovery Data Resource (2015-present)

RESEARCH INTERESTS

- Computational drug design
- Protein-ligand interactions
- Solvation of small molecules and biomolecules
- Free-energy calculations – application and methodology
- Allostery and allosteric regulation
- Molecular biology of disease

- Noise in biological systems
- Force fields and simulation methodology
- Open science/open access/reproducibility in research

JOURNAL PEER REVIEW

Journal of the American Chemical Society; Biochemistry; Biophysical Journal; Biochimica et Biophysica Acta: Membranes; Journal of Medicinal Chemistry; Journal of Computational Chemistry; Springer Lecture Notes in Computer Science; Journal of Physical Chemistry; Journal of Chemical Physics; Biopolymers; Proteins: Structure, Function, and Bioinformatics, PLoS Computational Biology, Journal of Chemical Information and Modelling, Journal of Physics: Condensed Matter, Current Medicinal Chemistry; Proceedings of the National Academy of Science; International Reviews in Physical Chemistry; ACS Omega; Chemical Biology and Drug Design, Supramolecular Chemistry, Physical Review X; book proposal for *Cambridge University Press;* book review for *Garland Science*.

GRANT REVIEWS

Centers for Disease Control (National Institute of Occupational Safety and Health), Innovation and Technology Commission of the Government of Hong Kong, National Academy of Science (2011, 2012), Oak Ridge Institute for Science and Education (2013), National Science Foundation (2013, 2014, 2015), American Association for the Advancement of Science (2014), ACS Chemical Computing Group Travel Award reviews (2014-present), Ausrian Science Fund.

TEACHING

Winter 2018:	PharmSci 175/275, Computing Techniques in Drug Discovery
Spring 2017:	PharmSci 275, Computing Techniques in Drug Discovery
Spring 2016:	PharmSci 275, Computing Techniques in Drug Discovery
Fall 2015:	PharmSci 223, Biomacromolecules
Spring 2015:	PharmSci 272, Computing Techniques in Drug Discovery
Fall 2014:	PharmSci 171, Physical Biochemistry
Spring 2014:	PharmSci 272, Computing Techniques in Drug Discovery
Winter 2014:	PharmSci/Chem 177, Medicinal Chemistry
Fall 2013:	PharmSci/Chem 223, Biomacromolecules
Winter 2013:	PharmSci/Chem 177, Medicinal Chemistry
Fall 2012:	PharmSci/Chem 223, Biomacromolecules
Spring 2012:	Chem 2310, Computing Techniques in Chemistry and Drug Discovery (new course)
Fall 2011:	Chem 3310, Physical Chemistry; Univ 1001, University Success
Spring 2011:	Chem 1007, General Chemistry Laboratory (3 sections)
Fall 2010:	Chem 3310, Physical Chemistry
Spring 2010:	Chem 1023, General Chemistry Laboratory
Fall 2009:	Chem 6316, Special Topics in Physical Chemistry: Computational Chemistry
Fall 2008:	Chem 1023, General Chemistry Laboratory, sections 1 and 2
2006-present:	Supervising and training graduate students beginning their research
2001:	General Physics Discussion/Laboratory B; UC Davis
2000-2001:	Electronic Instrumentation Laboratory A, B; UC Davis
2000:	General Science, Sacramento High School, with Howard Hughes Medical Institute Science Teaching Internship from UC Davis

COMMITTEE SERVICE

2018-pres.:	UCI RCI Cluster Planning and Oversight Committee, UC Irvine
2017-pres.:	UCI Research Cyberinfrastructure Center Advisory Committee, UC Irvine
2017-pres.:	Vice Chair and Advisor for Graduate Programs, Pharmaceutical Sciences, UC Irvine
2016-2017:	Vice Chair and Co-Advisor for Graduate Programs, Pharmaceutical Sciences, UC Irvine
2015-2017:	Research Cyberinfrastructure Vision Workgroup, UC Irvine
2015-2016:	Graduate Advisor, Pharmacological Sciences, UC Irvine.
2014-pres.:	Public Health Advisory Committee, UC Irvine

2017-pres.: Council on Teaching, Learning and Student Experience, UC Irvine
2014-2017.: Council on Research, Computing, and Libraries, UC Irvine
2013-pres.: Chair, Graduate Admissions, Medicinal Chemistry and Pharmacology Graduate Program and Pharmacological Sciences Program
2011-2012: College of Science Graduate Recruiting Committee
2010: Executive Committee and Chair, Graduate Program, Southeast/Southwest Regional Meeting of the American Chemical Society, New Orleans.
2009-2012: Chair, Graduate Recruiting and Selections Committee, Chemistry Department
2009-2011: Ad hoc web design committee
2008-2009: Graduate Affairs Committee

Ad hoc committee service: Drafting Committee for cases in 2012, 2013, 2014, and 2015. Search committees for Student Affairs Officer and Director of Student Affairs, 2016.

OTHER SERVICE

- Lead PI for the Open Force Field Initiative/Open Force Field Consortium (openforcefield.org)
- Invited participant in MolSSI Workshop, Stanford, CA, April 2017.
- Invited participant in "Workshop for Conceptualization of a Molecular Computation Software Institute", Rice University, Houston, TX, Jan. 22-24, 2015.

STUDENT/POSTDOC SUPERVISION AND DISSERTATION COMMITTEES

- Postdoctorals: Sreeja Parmeswaran (2012-2014), Shun Zhu (2012-2014), Gaetano Calabro (2015-2017), Léa El Khoury (July 2017-present), Sukanya Sasmal (August 2017-present), Jeff Wagner (October 2018-present)
- Graduate students: Camila Zanette (ongoing), Guilherme Matos (ongoing), Nathan Lim (ongoing), Samuel Gill (ongoing), Caitlin Bannan (ongoing), Victoria Lim (ongoing), Kalistyn Burley (ongoing), David Wych (ongoing), Danielle Bergazin (ongoing), Jessica Maat (ongoing), Hannah Baumann (ongoing), Noora Siddiqui (MS, UCI, 2017-2018), Anasuya Kolavennu (M.S., UNO, 2010-2012), Jessica Fuselier (M.S., UNO, 2010-2013), Pavel Klimovich (Ph.D., UCI, 2009-2015), Shuai Liu (Ph.D., UCI, 2010-2015), Hanh Nguyen (MS, UCI, 2015-2016).
- Undergraduate students: Christopher Savoie (2008-2010), Matthew Hellmers (summer 2009), Yu Xuan ("Luna") Liu (Spring 2011), Emily Taylor (Summer 2011), Vivian Jaber (Summer 2011 to Summer 2013), Kimberly Keyes (2012), Karisa Wymer (Fall 2012 to 2015), Nathan Lim (Spring 2013 to Spring 2014), Annie Choi (Fall 2013), Kevin Hoang (Fall 2013-present), Shannon Cao (Fall 2013-June 2015), Nam Thi (Summer 2015-2017), Daisy Kyu (2016-2017), Linh Nguyen (2017-present), Jordan Ehrman (2017-present), Anh Nguyen (2017-present), Meghan Osato (2017-present), James Hariyanto (2018-present).
- High school students: Justin Su (summer 2013).
- Other students: Stefania Evoli (visiting from University of Calabria, Italy; August 2013-February 2014); Maximiliano Riquelme Troncoso (visiting from University of Concepćion, Chile, June-August 2017); Zuzana Jandova (visiting from BOKU University, Vienna, April-June 2018).
- Dissertation committees: Yu Hongtao, Jianxia Zhang, Andrea Forsyth, Gayatri Sahu, Debashish Mohanty, Alexis Lee, Shiva Adireddy, Angela Ellender, Joshua Shraberg (University of New Orleans); Mahua Roy, Scott Hollingsworth, Camila Zanette, (UCI). Also Gerhard König, Universität Wien (external), Anita de Ruiter, BOKU, Vienna (external); Stefania Evoli. University of Calabria, Italy (external).
- Orals/advancement committees: Michelle Fairhurst, Scott Hollingsworth, Saikat Bala, Anupam Chatterjee, Eric Samuels, Calvin Lau, Megan Newcomb, Vy Duong, Megha Unhelkar, Luiz Passalacqua, Saad Muhammad (UCI).

STUDENT AND POSTDOCTORAL FELLOWSHIPS SUPPORTED

- NSF GRFP: Nathan Lim, Victoria Lim
- NSF MolSSI Fellow Phase I: Caitlin Bannan, Nathan Lim
- NSF MolSSI Fellow Phase II: Caitlin Bannan
- DOE Computational Science Graduate Fellowship: Noora Siddiqui
- NIH T32 Recipients: Kalistyn Burley
- Open Force Field: Jessica Maat, Jeff Wagner

PROFESSIONAL MEMBERSHIPS

- American Chemical Society
- Biophysical Society