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Postdoctoral Associate, Department of Chemistry

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EDUCATION

Ph.D. in Chemistry, University of Florida 2015
“Design of a Novel Inhibitor for *Helicobacter pylori*”
Co-advisors: Kenneth M. Merz Jr. and Erik Deumens
B.A. in Chemistry and Middle Eastern Studies, Wellesley College 2009

PROFESSIONAL APPOINTMENTS

Postdoctoral Fellow with J. Ilja Siepmann, Sept 2015 – Present
University of Minnesota, Minneapolis, MN.
Analyzing the effects of *n*-hexane vapor on the surface tension and structure of water films at different temperatures and partial pressures.

Studying the loading of *n*-nonane, ethyl butyrate, and 1-hexanol into oligoether surfactant bilayers.

Elucidating fluid phase equilibria and structure of pentadecanoic acid Langmuir monolayers.

PUBLICATIONS

“Multiple Drugs and Multiple Targets: An Analysis of the Electrostatic Determinants of Binding Between Non-nucleoside HIV-1 Reverse Transcriptase (RT) Inhibitors and Variants of HIV-1 RT.” **Minkara, M. S.**; Davis, P. H.; Radhakrishnan, M. L. *Proteins* **2012**, *80* (2), 573-590. DOI: 10.1002/prot.23221

“Analysis of Fast Boundary-integral Approximations for Modeling Electrostatic Contributions of Molecular Binding.” Kreienkamp, A. B.; Liu, L. Y.; **Minkara, M. S.**; Knepley, M. G.; Bardhan, J. P.; Radhakrishnan, M. L. *Molecular Based Mathematical Biology* **2013**, *1*, 214-150. DOI: 10.2478/mlbmb-2013-0007

“Molecular Dynamics Study of *Helicobacter pylori* Urease.” **Minkara M. S.**; Ucisik, M. N.; Weaver, M. N.; Merz, K. M. Jr. *J. Chem. Theory Comput.* **2014**, *10* (5), 1852-1862. DOI: 10.1021/ct5000023

“Effect of 10.5 M Aqueous Urea and *Helicobacter pylori* Urease: A Molecular Dynamics Study.” **Minkara, M. S.**; Weaver, M. N.; Merz, K. M. Jr. *Biochemistry* **2015**, *54* (26), 4121–4130. DOI: 10.1021/acs.biochem.5b00078

“Implementation of Protocols to Enable Doctoral Training in Physical and Computational Chemistry of a Blind Graduate Student.” **Minkara, M. S.**; Weaver, M. N.; Gorske, J.; Merz, K. M. Jr. *Chem. Educ.* **2015**, *92* (8), 1280-1283. DOI: 10.1021/ed5009552

“Reduction of Urease Activity by Interaction with the Flap Covering the Active Site.” Macomber, L.; **Minkara, M. S.**; Hausinger, R. P.; Merz, K. M. Jr. *Chem. Inf. Model.* **2015**, *55* (2), 354-361. DOI: 10.1021/ci500562t

“Probing Additive Loading in the Lamellar Phase of a Nonionic Surfactant: Gibbs Ensemble Monte Carlo Simulations using the SDK Force Field.” **Minkara, M. S.**; Lindsey, R. K.; Hembree, R. H.; Venteicher, C. L.; Jamadagni, S. N.; Eike, D. M.; Ghobadi, A. F.; Koenig, P. H.; Siepmann, J. I., *Manuscript accepted for publication in Langmuir*

“Monte Carlo Simulations Probing the Liquid/Vapor Interface of Water/Hexane Mixtures.” **Minkara, M. S.**; Josephson, T.; Venteicher, C. L.; Chen, J. L.; Stein, D. J.; Peters, C. J.; Siepmann, J. I., *Manuscript accepted for publication in Molecular Physics*

RESEARCH EXPERIENCE

Ph. D. Graduate Fellow, Aug 2010 – Aug 2015
Co-advised by Kenneth M. Merz Jr. and Erik Deumens,
University of Florida, Gainesville, FL.

Dissertation: “Design of a Novel Inhibitor for *Helicobacter pylori*” **Minkara, M. S., 2015.**

Discovered a new flap state in *Helicobacter pylori* urease (HPU) for the active site-covering flap. Determined possible inhibitors for *Klebsiella aerogenes* urease, using docking study of over 14 million ligands from the ZINC database, and tested them experimentally. Discovered a possible pathway in which urea is shuffled into the active site of HPU. Discovered, in conjunction with an exhaust flap, a possible pathway for the release of ammonium into surrounding environment. Described my experience as a graduate student and delineated some of the methods that were used to conduct my research.

Research Assistant with Mala Radhakrishnan, Sept 2007 – Aug 2010
Wellesley College, Wellesley, MA.

Dissertation: “Analyzing the Binding of Nevirapine and Rilpivirine to HIV-1 Reverse Transcriptase through Computationally Derived Charge Optimization.” **Minkara, M. S., 2009.**

Determined that rilpivirine’s charge distribution was closest to optimal, resulting in a more effective drug. Improved upon an electrostatics continuum model, BIBEE/I (boundary-integral based electrostatics estimation with interpolation), which was tested on 600 proteins to predict the energy of solvation to within a mean unsigned error of 4%.

TEACHING EXPERIENCE

Mentorship Program for Aspiring Chemistry Teachers, Spring 2018
Mentor: Professor Jason Goodpaster
University of Minnesota, Minneapolis, MN.

Preparing Future Faculty Course (GRAD8101), Fall 2017
University of Minnesota, Minneapolis, MN.

Volunteered for Empowerment Through Integration (ETI) August 2017
Helped write and implement a blind accessible STEM curriculum for blind children,
Lebanon.

Mentoring an undergraduate student in research project, January 2017 – Present
University of Minnesota, Minneapolis, MN.

Taught a seminar session, October 28, 2016
“Probing Chemical Systems with Molecular Simulation” (CHEM1905),
University of Minnesota, Minneapolis, MN.

Mentored a high school student in research project, Summer 2016
University of Minnesota, Minneapolis, MN.

General Chemistry TA (CHM2045), Summer 2014
University of Florida, Gainesville, FL.

Pforzheimer Learning & Teaching Center, September 2008 – September 2009
Wellesley College, Wellesley, MA.

AWARDS & HONORS

Postdoctoral Scholar Travel Grant from MN section of the American Chemical Society (2018)
Holman Prize Committee Member (2017)
Penn Conference in Theoretical Chemistry (PCTC) Postdoctoral Fellow Awards (2017)
National Academy of Sciences Ford Foundation Postdoctoral Fellowship (2016)
National Federation of the Blind Scholarship (2013)
National Science Foundation Graduate Research Fellowship (2012 – 2015)
University of Florida Grinter Award (2010 – 2012)
University of Florida Alumni Fellowship (2010 – 2012)
Howard Hughes Medical Institute research grant (2009 – 2010)

CONFERENCE PRESENTATIONS

“Gibbs ensemble Monte Carlo Simulations for Additive Loading in Surfactant Bilayers.”
Minkara, M. S. 255th National Meeting of the American Chemical Society, New Orleans, LA.
March 22, 2018.

“Gibbs ensemble Monte Carlo Simulations for Additive Loading in Surfactant Bilayers.”
Minkara, M. S. 2017 Penn Conference in Theoretical Chemistry, Philadelphia, PA. August
17, 2017.

“Tools of a Blind Chemist.” **Minkara, M. S.** 253rd National Meeting of the American Chemical
Society, San Francisco, CA. April 5, 2017.

“Monte Carlo Simulations Probing the Liquid/Vapor Interface of Water/Hexane Mixtures.” **Minkara, M. S.** 253rd National Meeting of the American Chemical Society, San Francisco, CA. April 3, 2017.

“Chemistry Through Blind Eyes.” **Minkara, M. S.** Plenary lecture at the International Symposium on the Teaching of Sciences to Visually Impaired People, at the Normal School for Teachers: Moisés Sáenz, Monterrey, Mexico. September 29, 2016.

“Probing Vapor-liquid Equilibria of Pentadecanoic Acid Langmuir Monolayers.” **Minkara, M. S.** Annual IPRIME meeting at the University of Minnesota, Minneapolis, MN. June 2, 2016.

“Probing Vapor-liquid Equilibria of Pentadecanoic Acid Langmuir Monolayers.” **Minkara, M. S.** Midwest Thermodynamics and Statistical Mechanics Conference at Miami University, Oxford, OH. May 26, 2016.

“Using Access Technologies in the Chemistry and Science Laboratory Classrooms for Multi-Sensory Data Acquisition.” **Minkara, M. S.** 247th National Meeting of the American Chemical Society, Dallas, TX. March 17, 2014.

Posters

“Liquid-Liquid and Liquid-Vapor Interfacial Tension and Preferential Adsorption for Water/Oil Mixtures.” **Minkara, M. S.**; Chen, J. L.; Siepmann, J. I. IPRIME 2017 Annual Meeting, Minneapolis, MN. May 30 – June 1, 2017.

“Vapor-Liquid and Liquid-Liquid Equilibria for a Langmuir Monolayer of Pentadecanoic Acid: A Monte Carlo Study.” **Minkara, M. S.** 253rd National Meeting of the American Chemical Society, San Francisco, CA. April 5, 2017.

“Monte Carlo Studies of Vapor-Liquid Equilibria for a Langmuir Monolayer of Pentadecanoic Acid.” **Minkara, M. S.**; Lindsey, R. K.; Siepmann, J. I. Presented at the 251st National Meeting of the American Chemical Society, San Diego, CA. March, 2016.

“Probing Electrostatic Interactions between Amino Acids and Urea using *ab initio* Calculations.” **Minkara, M. S.**; Urul, D. A.; Weaver, M. N.; Merz, K. M. Jr. Presented at the 251st National Meeting of the American Chemical Society, San Diego, CA. March, 2016.

“Molecular Dynamics Study of *Helicobacter pylori* Urease in 150 Millimolar Aqueous NH₄Cl.” **Minkara, M. S.**; Weaver, M. N.; Merz, K. M. Jr. Presented at the 249th National Meeting of the American Chemical Society, Denver, CO. March, 2015.

“Effect of 10.5 M Aqueous Urea on *Helicobacter pylori* Urease: A Molecular Dynamics Study.” **Minkara, M. S.**; Weaver, M. N.; Merz, K. M. Jr. Presented at the 248th National Meeting of the American Chemical Society, San Francisco, CA. August, 2014.

“Molecular Dynamics Study of *Helicobacter pylori* Urease.” **Minkara, M. S.**; Ucisik, M. N.; Weaver, M. N.; Merz, K. M. Jr. Presented at the 247th National Meeting of the American Chemical Society, Dallas, TX. March, 2014.

“A Computational Analysis of Molecular Recognition in the Trypsin/Bovine Pancreatic Trypsin Inhibitor (BPTI) System Using Multiple Electrostatic Models.” **Minkara, M. S.**; Bardham, J.; Radhakrishnan, M. Presented at The Protein Society 24th Annual Symposium, San Diego, CA. August, 2010.

“Improving the Binding of Nevirapine and Rilpivirine to HIV-1 Reverse Transcriptase through Computationally Derived Charge Optimization.” **Minkara, M. S.** & Radhakrishnan, M. Senior research thesis, Department of Chemistry, Wellesley College, Wellesley, MA. April, 2009.

“Analyzing Electrostatic Determinants of Affinity and Promiscuity in the HIV-1 Reverse Transcriptase.” **Minkara, M. S.** & Radhakrishnan, M. Presented at the 53rd Annual meeting of the Biophysical Society, Boston, MA. March, 2009.

“Improving the Binding of Nevirapine and Rilpivirine to HIV-1 Reverse Transcriptase through Computationally Derived Charge Optimization.” **Minkara, M. S.** & Radhakrishnan, M. Presented at the 237th National meeting of the American Chemical Society, Salt Lake City, UT. March, 2009.

INVITED TALKS

Scientific

“Probing Interfaces and Mesophases with Molecular Simulation.” **Minkara, M. S.** Michigan State University, East Lansing, MI. February 20, 2018.

“A Computational Study of How Solutes Load into a Surfactant Bilayer Using Monte Carlo Techniques.” **Minkara, M. S.** Carleton College, Northfield, MN. February 16, 2018.

“Journey of a Blind Computational Chemist.” **Minkara, M. S.** Muslimas of University of Arkansas, Fayetteville, AR. May 2, 2017.

“Molecular Simulation Studies Aiding Drug Design and Delivery.” **Minkara, M. S.** Vanderbilt University, Nashville, TN. April 25, 2017.

“Molecular Dynamics Study of *Helicobacter pylori* Urease.” **Minkara, M. S.** Wellesley College, Wellesley, MA. February 23, 2015.

“Molecular Dynamics Simulations Investigating *Helicobacter pylori* Urease.” **Minkara, M. S.** University of Minnesota, Minneapolis, MN. January 30, 2015.

Outreach

“Navigating Graduate School with a Disability.” **Minkara, M. S.** University of California, Berkeley, Keynote Speaker at the “Is a Ph.D. for Me?” Conference, Berkeley, CA. April 13, 2018.

“Journey of a Blind Computational Chemist.” **Minkara, M. S.** Washburn High School, Minneapolis, MN. November 7, 2017.

“Journey of a Blind Computational Chemist.” **Minkara, M. S.** Wellstone High School, Minneapolis, MN. May 19, 2017.

“Chemistry Through Blind Eyes.” **Minkara, M. S.** Keynote lecture presented at the 4th Forum on the Teaching of Science to Visually Impaired Students, at Universidad Iberoamericana, Mexico City, Mexico. October 3, 2016.

CAMPUS TALKS

“Molecular Dynamics Simulations Investigating *Helicobacter pylori* Urease.” **Minkara, M. S.** University of Florida, Gainesville, FL. January 21, 2014.

“Design of Novel Inhibitors of *Helicobacter pylori* Urease.” **Minkara, M. S.** University of Florida, Gainesville, FL. March 19, 2013.

“Ligand Docking to *Klebsiella aerogenes* Urease.” **Minkara, M. S.** University of Florida, Gainesville, FL. February 14, 2012.

Undergraduate Defense: “Analyzing Electrostatic Determinants of Affinity and Promiscuity in the HIV-1 Reverse Transcriptase System Using Charge Optimization.” **Minkara, M. S.** Wellesley College, Wellesley, MA. May 18, 2009.

PROFESSIONAL AFFILIATIONS

American Chemical Society (2008 – Present)

National Federation of the Blind (2011 – Present)

Associate for the Chemists with Disabilities Committee of the ACS (2017 – Present)

REFERENCES

J. Ilja Siepmann
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