

Mona Minkara, Ph. D.

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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 Associate with J. Ilja Siepmann, Sept 2015 – Present
University of Minnesota, Minneapolis, MN.
Analyzing the effects of 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

Peer-Reviewed Articles

“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

Manuscripts in Preparation

“Gibbs ensemble Monte Carlo Simulations for Additive Loading in Surfactant Bilayers.” **Minkara, M. S.**; Hembree, R.; Venteicher, C.; Koenig, P. H.; Eike, D.; Jamadagni, S. N.; Siepmann, J. I., In preparation

“Monte Carlo Simulations Probing the Liquid/Vapor Interface of Water/Hexane Mixtures.” **Minkara, M. S.**; Stein, D.; Venteicher, C.; Peters, C. J.; Siepmann, J. I., In preparation

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

- Preparing Future Faculty Course (GRAD8101), University of Minnesota, Minneapolis, MN. Fall 2017
- Volunteered for Empowerment Through Integration (ETI) August 2017
Helped write and implement a blind accessible STEM curriculum for blind children, Lebanon.
- Mentored an undergraduate student in research project, University of Minnesota, Minneapolis, MN. January 2017 – Present
- Taught a session of a seminar, “Probing Chemical Systems with Molecular Simulation” (CHEM1905), University of Minnesota, Minneapolis, MN. October 28, 2016
- Mentored a high school student in research project, University of Minnesota, Minneapolis, MN. Summer 2016
- General Chemistry TA (CHM2045), University of Florida, Gainesville, FL. Summer 2014
- Pforzheimer Learning & Teaching Center, Wellesley College, Wellesley, MA. September 2008 – September 2009

AWARDS & HONORS

- 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. 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

“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.

“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 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.

“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)

REFERENCES

J. Ilja Siepmann
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