

Kristina E. Furse

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— HIGHLIGHTS —

- Extensive experience in molecular modeling and classical molecular dynamics simulation of large biomolecular systems
- GPA 4.0/4.0 at Vanderbilt University with minimal previous training in science
- Excellent visual, verbal, and written communication skills and strong problem solving abilities
- Strong artistic abilities and experience with a wide range of different media including digital art

— EDUCATION —

- 2005 **Ph. D.** in Chemistry, Vanderbilt University, Nashville, TN (GPA 4.0/4.0)
Dissertation: "Computational Modeling of Protein-Small-Molecule Interactions"
- 1996 **B.A.** in Liberal Arts, University of Richmond, Richmond, VA (GPA 3.6/4.0)

— RESEARCH EXPERIENCE —

- 2006-present **Postdoctoral Research Associate**, University of Notre Dame, Notre Dame, IN
Research Advisor: Steven A. Corcelli, Ph.D.
- Developed and applied computational methods to model time-dependent fluorescence experiments at the DNA-water interface
 - Collected, organized and analyzed 20+ TB of simulation data
 - Created new trajectory analysis programs using Fortran and Perl
- 2001-2006 **Graduate Student**, Vanderbilt University, Nashville, TN
Research Advisor: Terry P. Lybrand, Ph.D.
- Produced *de novo* theoretical models of G-protein coupled receptors and conducted manual and automated drug docking studies
 - Developed force field parameters for numerous non-standard drug molecules
 - Developed new tools to extract and visualize data from MD simulations

— TEACHING EXPERIENCE —

- 2004 Instructor for Molecular Modeling Flextime, IGP Vanderbilt University
- 2000-2001 Teaching Assistant/Tutor in Physical Chemistry, Vanderbilt University
- 1993 Teaching Assistant in General Chemistry, University of Richmond

— COMPUTATIONAL EXPERIENCE —

Molecular dynamics simulation (AMBER), molecular visualization and modeling (Chimera, VMD, DINO, MDDISPLAY, PSSHOW), multiple sequence alignment (AMPS, AMAS, Alscript), ab initio calculation (Gaussian), automated docking (DOCK, Autodock), programming (Fortran, Perl, basic shell scripting), digital art (Photoshop, Illustrator, Quark), multimedia design (Authorware, MapInfo, SoundEdit, XHTML and CSS).

— HONORS —

- 2009 Cover of *Physical Chemistry Chemical Physics* Issue 37
2006 Cover of *Biochemistry* July-September Issues
2005 Graduate Student Poster Award, Sanibel Symposium
2004 Warren Graduate Research Fellowship, Vanderbilt University
2002-2004 NIH Molecular Biophysics Training Grant Education Committee
2002 Poster Award, Vanderbilt Biomolecular Modeling Symposium
2001-2003 NIH Molecular Biophysics Training Grant Funded Trainee
2000-2001 GAANN Fellowship
1996 Phi Beta Kappa
1992-1996 National Merit Scholarship
1992-1996 University Scholarship, University of Richmond

— OTHER WORK AND EDUCATIONAL EXPERIENCE —

- 1996-present Freelance Artist (drawing, painting and digital art commissions)
1997 Scene Painter, Goodspeed Opera House, East Haddam, CT
1996-1997 Scene Painter, Prop Art, Nashville, TN
1995-1996 Multimedia Project Manager, Duthie Associates, Inc, Nashville, TN
1995 Animation Workshop, New York University, NY
1994 Conversational Japanese, Hamamatsu, Japan
1992 International Conference “Violence in the Cities” Caux, Switzerland
1992 Wilderness Southeast Student Education/Adventure, Belize, Central America
1990 Initiative for Understanding Student Ambassador, Russia and Ukraine

— PUBLICATIONS —

- Lindquist, B. A., Furse, K. E. and Corcelli, S. A. “Nitrile groups as vibrational probes of biomolecular structure and dynamics: an overview,” *Phys. Chem. Chem. Phys.* **2009**, *11*, 8119-8132.
- Furse, K. E. and Corcelli, S. A. “Effects of Long-Range Electrostatics on Time-Dependent Stokes Shift Calculations,” *J. Chem. Theo. Comp.* **2009**, *5*, 1959-1967.
- Furse, K. E. and Corcelli, S. A. “The Dynamics of Water at DNA Interfaces: Computational Studies of Hoechst 33258 bound to DNA,” *J. Am. Chem. Soc.* **2008**, *130*, 13103-13109.
- Furse, K. E., Lindquist, B. A. and Corcelli, S. A. “Solvation Dynamics of Hoechst 33258 in Water: An Equilibrium and Nonequilibrium Molecular Dynamics Study,” *J. Phys. Chem. B* **2008**, *112*, 3231-3239.
- Furse, K. E., Pratt, D. A., Schneider, C., Brash, A. R., Porter, N. A. and Lybrand, T. P. “Molecular Dynamics Simulations of Arachidonic Acid-Derived Pentadienyl Radical Intermediate Complexes with COX-1 and COX-2: Insights into Oxygenation Regio- and Stereoselectivity,” *Biochemistry* **2006**, *45*, 3206-3218.
- Furse, K. E., Pratt, D. A., Porter, N. A. and Lybrand, T. P. “Molecular Dynamics Simulations of Arachidonic Acid Complexes with COX-1 and COX-2: Insights into Equilibrium Behavior,” *Biochemistry* **2006**, *45*, 3189-3205.
- Furse, K. E. and Lybrand, T. P. “Three-Dimensional Models for β -Adrenergic Receptor Complexes with Agonists and Antagonists,” *J. Med. Chem.* **2003**, *46*, 4450-4462.

Ding, X-Q., Pinon, D. I., Furse, K. E., Lybrand, T. P. and Miller, L. J. "Refinement of the Conformation of a Critical Region of Charge-Charge Interaction between Cholecystokinin and Its Receptor," *Mol. Pharmacol.* **2002**, *61*, 1041-1052.

— PRESENTATIONS —

Furse, K. E. and Corcelli, S. A. *Visualizing Biomolecular Structure and Dynamics*, Visualization in Science and Education Gordon Research Conference, July 26-31, 2009, Oxford, UK.

Furse, K. E. and Corcelli, S. A. *Dynamics of water at the DNA interface*, Center for Research Computing Workshop on Scientific Computing, April 30, 2009, University of Notre Dame, IN.

Furse, K. E. and Corcelli, S. A. *Molecular dynamics simulations of solvation dynamics at biological interfaces*, 236th ACS National Meeting, August 17-21, 2008, Philadelphia, PA.

Furse, K. E., Pratt, D. A., Schneider, C., Brash, A. R., Porter, N. A. and Lybrand, T. P. *Origin of Regio- and Stereoselectivity in Cyclooxygenase Reactions*, 45th Sanibel Symposium (U of Florida), March 5-11, 2005, St. Simons Island, GA.

Furse, K. E., Pratt, D. P., Porter, N. A. and Lybrand, T. P. *Dynamic Insight into the Equilibrium Behavior of COX-1 and COX-2 with Arachidonate Bound*, Computational Chemistry Gordon Research Conference, July 4-9, 2004, Plymouth, NH.

Pratt, D. A., Furse, K. E., Schneider, C., Lybrand, T. P., Brash, A. R. and Porter, N. A. *Investigating the Origin of Regio- and Stereoselectivity in the Cyclooxygenase-Mediated Oxygenation of Arachidonic Acid*, Vanderbilt Biomolecular Modeling Symposium, September 20-21, 2002, Nashville, TN.