

Seth A. Hayik
499 W. Lancaster Ave
Apt A3
Downingtown PA 19335
(610)207-6094
hayik@ufl.edu

Education:

- **Fox Chase Cancer Center**
January 2007-Present
Expected Graduation: March 2009
Supervisor: Dr. Roland Dunbrack

- **University of Florida, Quantum Theory Project**
August 2005-Present
Expected Graduation: March 2009
Supervisor: Dr. Kenneth M. Merz

- **Pennsylvania State University, Dept. of Chemistry**
September 2003-August 2005
Supervisor: Dr. Kenneth M. Merz

- **Philadelphia University, Dept. of Chemistry**
B.S. Biochemistry, May 2003
Supervisor: Dr. Charles Bock

Research Experience:

- **Fox Chase Cancer Center**
Graduate Student, January 2007 through present
Ph.D. research focused on drug discovery using DOCK and Autodock. Worked with a small, local pharmaceutical company relaying computational results and predictions to be experimentally tested.

- **University of Florida**
Graduate Student, August 2005 through present
Ph.D. research using mixed, linear scaling QM/MM methods in the AMBER suite to find relative binding free energies. Project included developing, maintaining and debugging Fortran code within AMBER and managing large amounts of data created from calculations.

- **Pennsylvania State University**
Graduate Student, August 2003 through August 2005
Ph.D. research using X-Ray crystallography structure refinement with a linear scaling QM package, as well as updating QM/MM code within AMBER. Projects

involved working with post doc using refinement code and beginning to understand and use AMBER.

- **Locus Pharmaceuticals**

Intern, May 2003 through August 2003

Methodically expanded and examined in-house fragment conformer library using Maestro and Gaussian. Worked closely with full-time employees to visualize conformers and present results to be included in library.

- **Philadelphia University**

Undergraduate Student, August 1999 through May 2003

Research involved mutagenicity of azo and other dyes used in textiles. Projects included use of QSAR methods and QM calculations through Spartan to study mechanisms and develop predictive models.

Presentations:

- “QM/MM Solvation Using the Poisson-Boltzmann Equation”, Seth A. Hayik and Kenneth M. Merz Jr., ACS National Meeting Sci-Mix Session, Philadelphia, PA 2008 *poster*.
- “QM/MM Solvation Using the Poisson-Boltzmann Equation”, Seth A. Hayik and Kenneth M. Merz, Jr., ACS National Meeting COMP Division Session, Philadelphia, PA 2008 *poster*.
- “Calculating Binding Affinities of Zinc Proteins Using QM/MM Methods”, Seth A. Hayik and Kenneth M. Merz, Jr., Univ. Of Penn. CBI Picnic, Swarthmore, PA, 2008 *poster*.
- “A Mixed QM/MM Method to Determine Protein/Ligand Binding Affinity”, Seth A. Hayik and Kenneth M. Merz, Jr., Sanibel Symposium, St. Simon Island, Georgia, 2007 *poster*.
- “QM/MM with DCQTP in AMBER”, Seth A. Hayik and Kenneth M. Merz, Jr., AMBER Developer’s Meeting, Salt Lake City, Utah, 2007 *talk*.
- “A Mixed QM/MM Method to Determine Protein/Ligand Binding Affinity”, Seth A. Hayik and Kenneth M. Merz, Jr., Sanibel Symposium, St. Simon Island, Georgia, 2006 *poster*.
- “Progress of DCQTP in AMBER9”, Seth A. Hayik and Kenneth M. Merz, Jr., Stony Brook, New York, 2006 *talk*.

Work in Progress:

- “A QM/MM Method to Predict Binding Free Energies: Study of Zinc Containing Proteins”, Seth A. Hayik, Roland Dunbrack and Kenneth M. Merz, Jr., 2009.

- “Binding Free Energies of a Large Diverse Set Predicted through QM/MM Methods”, Seth A. Hayik, Roland Dunbrack and Kenneth M. Merz, Jr., 2009
- “Discovery of a Novel Inhibitor for a Ubiquitin-Specific Protease from Virtual Screening”, Seth A. Hayik, Seth Goldenberg, Kenneth M. Merz, Jr. and Roland Dunbrack, 2009.

Publications:

1. Hayik, Seth A.; Liao, N.; Merz, K.M., Jr. **A Combined QM/MM Poisson-Boltzmann Approach.** *J. Chem. Theory and Comput.*, (2008) 4(8), 1200-1207.
2. Yu, Ning; Hayik, Seth; Merz, Kenneth M. **Critical assessment of quantum mechanics based energy restraints in protein crystal structure refinement.** *Protein Sci.*, (2006) 15, 2773-2784.
3. Yu, Ning; Hayik, Seth; Wang, Bing; Liao, Ning; Reynolds, Charles H.; Merz, Kenneth M. **Assigning the Protonation States of the Key Aspartates in β -Secretase Using QM/MM X-ray Structure Refinement.** *J. Chem. Theory Comput.*, (2006) 2(4), 1057-1069.
4. Bhat, Krishna L; Hayik, Seth; Sztandera, Les; Bock, Charles W. **Mutagenicity of aromatic and heteroaromatic amines and related compounds: A QSAR investigation.** *QSAR & Combinatorial Science* (2005), 24(7), 831-843.
5. Bhat, Krishna L; Hayik, Seth; Corvo, Joseph N.; Marycz, Damien M.; Bock, Charles W. **A computational study of the formation of 1,3,2-dioxaborolane from the reaction of dihydroxyborane with 1,2-ethanediol.** *THEOCHEM* (2004), 673(1-3), 145-154.
6. Hayik, Seth; Bhat, Krishna L; Bock, Charles W. **Structure of 4-[4-(Dimethylamino)-Phenylazo]-Benzeneboronic Acid and Its Cyclic Esters with D-Glucose: A Computational Study.** *Structural Chemistry* (2004), 15(2), 133-147.
7. Bhat, Krishna L; Hayik, Seth; Bock, Charles W.; Brendley, William H., Jr. **MTBE and its degradation products: molecular modeling study.** *Contaminated Soils* (2003), 8 101-118
8. Bhat, Krishna L; Hayik, Seth; Bock, Charles W. **A computational study of the formation of a boron-oxygen-carbon linkage. The reaction of monohydroxy borane with methanol.** *THEOCHEM* (2003), 638 107-117.

9. Sztandera, Les; Garg, Ashish; Hayik, Seth; Bhat, Krishna L; Bock, Charles W. **Mutagenicity of aminoazo dyes and their reductive-cleavage metabolites: a QSAR/QPAR investigation.** *Dyes and Pigments* (2003), 59(2), 117-133.

Teaching Experience:

- **Pennsylvania State University – Main Campus**
Teaching Assistant, Fall 2003 and Spring 2005
Lead recitations, laboratory classes and held office hours. Graded quizzes and lab books.
- **Philadelphia University**
Biochemistry Teaching Assistant, Fall 2002 through Spring 2003
Prepared solutions and gels before Biochemistry Lab, answered student questions and monitored progress during lab.
- **Philadelphia University**
Peer Tutor, Fall 2001 through Spring 2003
Tutored peers for general chemistry, physical chemistry and biochemistry undergraduate classes.

Achievements:

- Major AMBER contributor
- Penn State Roberts Graduate Student Fellowship – 2003
- Eagle Scout

References available upon request.