

# Curriculum Vitae

## Alexander S. Bayden

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### OBJECTIVE

A molecular modeling or scientific programming position

### EDUCATION

Degree	University	Years Attended	Major	GPA
Ph.D.	University of Pittsburgh	2000-2005	Chemistry (Physical)	3.84
B.S.	Virginia Polytechnic Institute & State University	1996-2000	Chemistry	3.83

### RESEARCH

#### Postdoctoral Research at AstraZeneca / Randstad

- Investigating the role of water in protein-ligand interactions
- Creating and testing computational chemistry workflows
- Running water-related calculations for computational chemists

#### Postdoctoral Research at Virginia Commonwealth University)

- Molecular Modeling
  - Docking / 3D Database Searching
    - Design of pentapeptide inhibitors for *O*-acetylserine sulfhydrylase, a potential antibiotic drug target
    - In-silico screening for inhibitors of parainfluenza fusion protein
    - Docking of small-molecule probes to TrmD, a promising antibiotic target
    - Computational hydrophobic analysis of polysubstituted pyrroles as potential tubulin inhibitors
  - Searching for molecular basis of selectivity in nitration of tyrosines
  - Studying the mechanism of p53 tetramerization
  - Modeling interactions between SHP2 and EGFR proteins with respect to radiation sensitivity
- Python Programming / Automation
  - Automation of analysis for docking results and molecular dynamics trajectories
  - Development of a web application that finds the best proton configuration for a protein-ligand complex as well as predicts how  $\Delta G_{\text{binding}}$  changes with pH
  - Development of an intuitive GUI for the HINT program
  - Development of a web application that finds how easy it is to displace waters from protein active sites
  - Development of an improved, more intuitive way to visualize molecular dynamics trajectories
  - Development of CoMBASA, a tool for pharmacophore analysis and visualization

#### Graduate and Undergraduate Research at the University of Pittsburgh

- Providing computational support for a synthetic group by modeling organometallic catalysis in the synthesis of a promising antibacterial agent Guanacastepene A
  - Dissertation: "Modeling Organorhodium Catalysis"
- Investigation of adsorption of hydrogen on the Si[100] surface
- Development of global optimization algorithms (C++)
- Reimplementing a program for analysis of photoacoustic calorimetry signals (Visual Basic)

**Citizenship: U.S. Citizen**

## MOLECULAR MODELING SKILLS

- Experience with molecular modeling
  - Skills in both QM and MM methods
  - Docking / Virtual screening / 3D pharmacophore searching
  - QSAR / QSPR
  - Estimation of Gibbs free energies of non-covalent interactions
- Experience with modeling and visualization packages
  - Schrödinger
    - Maestro, Glide, Prime
  - OpenEye
    - VIDA, SZMAP
  - Other
    - Sybyl, MOE, GOLD, HINT, Gaussian, VASP, CAChe, Hyperchem, GAMESS, Cerius2, OpenBabel, gOpenMol, XMakeMol, kmovisto

## COMPUTER ENVIRONMENT

- Programming
  - Python, C/C++ with MPI, SQL, Basic/Visual Basic, MatLab, Pascal, ASP.#, HTML, JavaScript
- Algorithms skills
  - Non-stochastic optimization algorithms
  - Global optimization algorithms
  - Algorithms for matrix manipulation
  - Sorting algorithms
  - Strong skills in algorithm analysis
- Computer administration skills
  - UNIX (Linux and OS X as an administrator, IRIX / AIX / Solaris / BSD as a user)
    - Security has never been breached on a single Linux machine under my administration
  - Windows 7 / Vista / XP / 2000 / ME / 9X / 3.1 / CE, DOS
    - Administered a Windows 2000-based web server with over forty user accounts for years without a single security breach
  - Solved network problems arising from malicious attacks
- Hardware
  - Participated in building and maintaining clusters for high-performance computing
  - Repaired , built and upgraded PCs, Macintoshes, PDAs, GPS devices and cell phones
  - Recovered data from damaged drives

## CHEMISTRY UNIQUE SYSTEMS

- Understanding of the drug development process
- Basic organic and inorganic synthetic techniques
- Taught analytical chemistry lab and physical chemistry lab
  - Did it all and taught it all, from casting ion-selective membranes to operating an STM

## SPECIAL RECOGNITION

2000 Graduate Excellence Fellowship  
2000 Hypercube Scholar Award  
2000 Virginia Polytechnic Institute and State University Academic Excellence Award  
1996 National Honor Society

2000 Chair's Scholar Grant  
1997-2000 Bilisoly Scholarship

## GRE SCORES

Verbal 500    Quantitative **800** (perfect)    Analytical 720    Chemistry 820

## EMPLOYMENT

### **2011-Present Postdoctoral Fellow at AstraZeneca/Randstad**

- Investigating the role of water in protein-ligand interactions
- Running water-related calculations for computational chemists
- Creating and testing computational chemistry workflows

### **2006-2010 Postdoctoral Fellow / Lab & Research Specialist II at the Virginia Commonwealth University Medicinal Chemistry Department**

- Computational medicinal chemistry research and scientific application development (See pg 1)
- Some server administration
- Training collaborators at the University of Parma, Italy to use software developed at Virginia Commonwealth University

### **2006 Prototyped a financial web site for Russia House International, Inc.**

- Project completed successfully under strict time constraints

### **2006 Ran a computer repair / data recovery business**

### **1999-2005 Employment at the University of Pittsburgh**

- 2000-2005 Research Assistant
  - Successfully developed global optimization algorithms and implemented them in C++
  - Provided computational support for the following projects:
    - Rh-based synthesis of combinatorial libraries and antimicrobial agents
    - Modeling adsorption of H<sub>2</sub> on the Si(100) surface
  - Communication
    - Trained new group members in molecular modeling and algorithm development
    - Conducted presentations about the results and recent developments in the field
    - Wrote publications and applications for grants
- 2002-2005 Maintained the Chemistry Department's web site at the University of Pittsburgh
  - Created and updated relational databases
  - Created and updated web interfaces for these databases using ASP.#
  - Conducted maintenance on the web server
  - Interviewed people and wrote news stories
  - Provided training for secretaries and junior web team members
  - Provided recommendations for software purchases
  - Worked with another team of developers to completely redesign the site
- 2003 Temporarily took over the duties of system administrator for the Chemistry Department's Windows computers at the University of Pittsburgh
- 2000-2002 Taught general chemistry recitation, analytical chemistry lab and physical chemistry lab
  - Besides teaching, duties included operating and troubleshooting a lot of instruments
- 1999 University of Pittsburgh REU Program
  - Successfully redesigned and reimplemented a program for analysis of photoacoustic calorimetry signals
    - Interacted with users to determine the requirements and new features for the upgraded program
    - Converted a QuickBasic program into Visual Basic
    - Wrote documentation, performed installations and trained users

## PUBLICATIONS

### Printed in Journals

- Bayden, A. S.; Yakovlev, V. A.; Graves, P. R.; Kellogg, G. E.; Mikkelsen, R. B. Factors Influencing Tyrosine Nitration - Structure-Based Predictive Models. *Free Rad. Biol. & Med.* 2011, 50, 749-62.
- Yakovlev, V. A.; Bayden, A. S.; Graves, P. A.; Kellogg, G. E.; Mikkelsen, R. B. Nitration of the Tumor Suppressor Protein p53 at Tyrosine 327 Promotes p53 Oligomerization and Activation. *Biochemistry*, 2010, 49, 5331-5339.
- Salsi, E.; Bayden, A. S.; Spyraakis, F.; Amadasi, A.; Campanini, B.; Bettati, S.; Dodatko, T.; Cozzini, P.; Kellogg, G. E.; Cook, P. F.; Roderick, S. L.; Mozzarelli, A. Design of *O*-acetylserine sulfhydrylase inhibitors by mimicking Nature. *J. Med. Chem.* 2010, 53, 345-356. (First two authors contributed equally.)
- Bayden, A. S.; Fornabaio, M.; Scarsdale, N. J.; Kellogg, G. E. Web application for studying the free energy of binding and protonation states of protein-ligand complexes based on HINT. *J. Comp. Aid. Mol. Des.*, 2009, 23, 621-632.
- Bayden, A. S.; Brummond, K. M.; Jordan, K. D. Computational Insight Concerning Catalytic Decision Points of the Transition Metal Catalyzed [2 + 2 + 1] Cyclocarbonylation Reaction of Allenes. *Organometallics*, 2006, 25, 5204-5206.
- Bayden, A. S.; Jordan, K. D. Use of extended dimensions in global optimization. *Chem. Phys. Lett.* 2004, 385, 101-104.

### Manuscripts in Preparation

- Tripathi, A.; Mosier, P.; Bayden, A. S.; Da, C.; Kellogg, G. E. CoMBASA: A New Complementary Map-Based Active Site Analysis Tool for Determining Receptor-Based Pharmacophore.

## POSTERS

- Drug Discovery Applications of Solvent Mapping with SZMAP. *242nd ACS National Meeting, Denver, CO*, 2011.
- Bridging radicals and other factors influencing tyrosine nitration.
  - *2<sup>nd</sup> Biennial Chemical Insights into Biological Processes Symposium, Frederick MD*, 2010.
  - *27<sup>th</sup> Annual Daniel T. Watts Research Poster Symposium, Richmond, VA*, 2010.
- Predicting Specificity for Selective Nitration of Tyrosines. *Biotech-After-Hours, Richmond, VA*, 2009.
- Novel Applications of Python in Computational Chemistry Workflows. *CUP X, Santa Fe, NM*, 2009.
- Applying Computational Titration to Selective Nitration of Tyrosines. *236th ACS National Meeting, Philadelphia, PA*, 2008.
- Modeling Interactions of Potential Antibiotic Targets OASS A and OASS B with Inhibitory Peptides. *25<sup>th</sup> Annual Daniel T. Watts Research Poster Symposium, Richmond, VA*, 2008.
- Design and Implementation of the Computational Titration Biomacromolecular Analysis as a Web-enabled Online Modeling Tool.
  - *2<sup>nd</sup> Annual Summit on Systems Biology, Richmond, VA*, 2007.
  - *24<sup>th</sup> Annual Daniel T. Watts Research Poster Symposium, Richmond, VA*, 2007.
- Modeling Organometallic Catalysis. *University of Pittsburgh Department of Chemistry Graduate Student Research Showcase Poster Session, Pittsburgh, PA*, 2004.
- Theoretical Study of the Si(100) Surface.
  - *University of Pittsburgh Department of Chemistry Graduate Student Research Showcase Poster Session, Pittsburgh, PA*, 2003.
  - *University of Pittsburgh Computer Science Day, Pittsburgh, PA*, 2003.
- Dimensional Strategies in Barrier Avoiding Minimization Algorithms. *American Conference on Theoretical Chemistry, Champion, PA*, 2001.

## ORAL PRESENTATIONS.

- Computational Titration *Institute for Structural Biology and Drug Discovery of Virginia Commonwealth University Student Seminar Series, Richmond, VA, 2008.*
- Dimensional strategies in barrier avoiding minimization algorithms. *35<sup>th</sup> Central Regional ACS Meeting, Pittsburgh, PA, 2003.*
- Reimplementing a program for analysis of photoacoustic calorimetry signals. *University of Pittsburgh Chemistry REU Symposium, Pittsburgh, PA, 1999.*