Curriculum Vitae

Alexander S. Bayden

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OBJECTIVE

Molecular modeling / scientific programming position in industry

EDUCATION

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

RESEARCH

CMDBioscience

- Computer-aided design of peptide-based therapeutics
- Making virtual libraries
- Scientific programming
    - Developing methods to for predicting ADME/Tox properties of peptides
    - Developing software for stabilizing 3D structure of peptides
    - Developing software for determining which water molecules should be displaced from protein active sites
    - Developing scripts that make structure-based methods easier to use

Postdoctoral Research at AstraZeneca / Randstad (Mentor – Dr. Michelle L. Lamb)

- Developing methods and implementing Python and SVL-based computational chemistry workflows for investigating the role of water in protein-ligand interactions
- Developing a web application for running water-related calculations on a Linux cluster
- Running water-related calculations for computational chemists

Postdoctoral Research at Virginia Commonwealth University (Mentor – Prof. Glen E. Kellogg)

- Modeling of Biological Systems
    - Docking / 3D Database Searching
        - Design of pentapeptide inhibitors for *O*-acetylserine sulfhydrylase
        - *In-silico* screening for inhibitors of parainfluenza fusion protein
        - Docking of small-molecule probes to TrmD, a promising antibiotic target
        - Computational hydropathic analysis of polysubstituted pyrroles as potential tubulin inhibitors
    - Studying the mechanism of p53 tetramerization
    - Modeling interactions between SHP2 and EGFR proteins with respect to radiation sensitivity
- Scientific Programming
    - Automation of analysis for docking results and molecular dynamics trajectories
    - Developing web applications for studying various aspects of energetics of binding in protein-ligand complexes
    - Developing of an intuitive GUI for the HINT program
    - Developing CoMBASA, a tool for pharmacophore analysis and visualization
    - Developing a method for predicting selectivity in nitration of tyrosines
    - Setting up computational workflows

Graduate and Undergraduate Research at the University of Pittsburgh
(Graduate Academic Advisor – Prof. Kenneth D. Jordan)

- Providing computational support for a synthetic group by modeling organometallic catalysis in the synthesis of a promising antibacterial agent, Guanacastepene A
- Development of global optimization algorithms
- Reimplementing a program for analysis of photoacoustic calorimetry signals to run on Windows

Citizenship: U.S. Citizen

MOLECULAR MODELING SKILLS

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

COMPUTER ENVIRONMENT

- Programming
  - Python, Java, C/C++ with MPI, SQL, Basic/Visual Basic, Matlab, ASP.#, HTML, JavaScript
- Data analysis
  - Spotfire, DataWarrior, Vortex, CMDnavigator, nQuery
- Algorithm 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 or OS X machine under my administration
  - Windows 10 / 8.1 / 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-RELATED

- Understanding of crystallography and the drug development process
- Taught analytical chemistry lab and physical chemistry lab

SPECIAL RECOGNITION

2000 Graduate Excellence Fellowship
2000 Chair's Scholar Grant
2000 Hypercube Scholar Award
1997-2000 Bilisoly Scholarship
2000 Virginia Polytechnic Institute and State University Academic Excellence Award
1996 National Honor Society

GRE SCORES

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

EMPLOYMENT

2013-2016 Computational Chemist at CMDBioscience

- Molecular modeling of peptides / scientific programming (See pg. 1)

2011-2013 Postdoctoral Fellow at Randstad / AstraZeneca R&D Boston

- Molecular modeling / scientific programming (See pg. 1)

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_2 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 administrative assistants 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 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

- Bayden, A. S.; Gomez, E. F.; Audie, J.; Chakravorty, D. K; Diller, D. J. A combined cheminformatic and bioinformatic approach to address the proteolytic stability challenge in peptide-based drug discovery. *Pept. Sci.* **2015**, *104*, 775-789.

- Diller, D. J.; Swanson, J.; Bayden A. S.; Jarosinski, M.; Audie, J. Rational, computer-enabled peptide drug design: principles, methods, applications and future directions. *Fut. Med. Chem.* **2015**, *7*, 2173-2193.

- Ahmed, M. H.; Amadasi, A.; Bayden, A. S.; Cashman, D. J.; Cozzini, P.; Da, C.; Chen, D. L.; Fornabaio, M.; Koparde, V. N.; Mozzarelli, A.; Parikh, H. I.; Sarkar, A.; Scarsdale, J. N.; Spyrakis, F.; Surface, J. A.; Tripathi, A.; Zaidi, S. A.; Kellogg, G. E. Understanding water and its many roles in biological structure: some ways to exploit a resource for drug discovery. Chapter in *Computer-Aided Drug Discovery*, Springer, New York, **2015**.

- Bayden, A. S.; Moustakas, D. T.; Joseph-McCarthy, D.; Lamb, M. L. Evaluating free energies of binding and conservation of crystallographic waters using SZMAP. *J. Chem. Inf. and Mod*. **2015**, *55*, 1552-1565.

- Spyrakis, F.; Felici, P.; Bayden, A. S.; Salsi, E.; Miggiano, R.; Kellogg, G. E.; Cozzini, P.; Cook, P. F.; Mozzarelli, A. Fine tuning of the active site modulates specificity in the interaction of *O*-acetylserine sulfhydrylase isozymes with serine acetyltransferase. *Biochim. Biophys. Acta, Proteins Proteomics*, **2013**, *1*, 169-181.

- 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*, 749-762.

- 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.; Spyrakis, 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. Comput. Aided. 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

- Bayden, A. S. CMDwater: An entropy-based tool for assessing the displaceability of crystallographic waters in crystal structures of protein-ligand complexes.

- Ahmed, M. H.; Spyrakis, F.; Cozzini, P.; Bayden, A. S.; Mozzarelli A.; Kellogg G. E. The Biochemical, Structural and Energetic Roles of Water: A Largely Untapped Resource for Drug Discovery? invited Perspective for *J. Med. Chem*.

POSTERS

- CMDscaffold: A virtual peptide library for *de novo* rational drug design. *2016 ACS Northeast Regional Meeting, Binghamton, NY*, 2016.
- CoMBASA: A hydropathy-based tool for mapping out receptor-based pharmacophores. *2016 ACS Northeast Regional Meeting, Binghamton, NY*, 2016.
- Relative importance of energy components in CMDwater – a computational tool for making decisions about displacing crystallographic waters during lead optimization. *252nd ACS National Meeting, Philadelphia, PA*, 2016.
- Three-ring scaffold with rich biological activity but no commercial availability. *252nd ACS National Meeting, Philadelphia, PA*, 2016.
- CMDwater: A tool for ranking crystallographic waters for displacement during ligand design. *2016 Mid-Atlantic ACS Regional Meeting, Riverdale, NY*, 2016.
- Solving ADME/Tox Problems in peptide-based drug discovery using descriptor-based technologies. *PepTalks 10, Boston, MA*, 2016.
- Using a combined cheminformatic and bioinformatic approach to address proteolytic stability challenges in peptide-based drug discovery. *250th ACS National Meeting, Boston, MA*, 2015.
- Using CMDInventus for understanding and solving ADME/Tox issues in peptide-based drug discovery. *2015 ACS Northeast Regional Meeting, Ithaca, NY*, 2015.
- The development, validation and application of CMDInventus to enable structure-based peptide drug design and discovery. *2015 ACS Northeast Regional Meeting, Ithaca, NY*, 2015.
- Development, validation and application of various biophysical modules in CMDInventus to enable structure-based peptide drug design and discovery. *2014 ACS Central Regional Meeting, Pittsburgh, PA*, 2014.
- Towards the implementation of novel computation tools in CMDInventus for understanding and solving ADME/Tox issues in peptide-based drug discovery. *TIDES 2014, Providence, RI*, 2014.
- Crystallographic Waters: to Displace or Not to Displace? *245th ACS National Meeting, New Orleans, LA*, 2013.
- Drug Discovery Applications of Solvent Mapping with SZMAP. *242nd ACS National Meeting, Denver, CO*, 2011.
- Bridging radicals and other factors influencing tyrosine nitration.
    - *2nd Biennial Chemical Insights into Biological Processes Symposium, Frederick MD*, 2010.
    - *27th 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. *25th 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.
    - *2nd Annual Summit on Systems Biology, Richmond, VA*, 2007.
    - *24th 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

- Structure-based peptide-modeling software for rational drug design. *2016 ACS Northeast Regional Meeting, Binghamton, NY*, 2016.
- Understanding and solving ADME/Tox issues in peptide-based drug discovery using novel computation tools in CMDInventus. *252nd ACS National Meeting, Philadelphia, PA*, 2016.
- Modeling cell permeation and proteolytic cleavage of peptides. *2016 Mid-Atlantic ACS Regional Meeting, Riverdale, NY,* 2016.
- Understanding and solving ADME/Tox issues in peptide-based drug discovery using novel computation tools in CMDInventus. *250th ACS National Meeting, Boston, MA*, 2015.
- Natural products with the 6-7-5 ring scaffold. *250th ACS National Meeting, Boston, MA*, 2015.
- Addressing proteolytic stability challenges in peptide-based drug discovery using a combined cheminformatic and bioinformatic approach. *2015 ACS Northeast Regional Meeting, Ithaca, NY*, 2015.
- Factors influencing selective nitration of tyrosines in proteins. *2015 ACS Northeast Regional Meeting, Ithaca, NY*, 2015.
- CMDdescriptor – 1D and 3D descriptors for addressing ADME/Tox challenges in peptide-based drug discovery. *2014 ACS Central Regional Meeting, Pittsburgh, PA*, 2014.
- A scaffold with rich biological activity but no commercial availability. *2014 ACS Central Regional Meeting, Pittsburgh, PA*, 2014.
- Using modeling to make decisions about displacing crystallographic waters. *2013 ACS Northeast Regional Meeting, New Haven, CT*, 2013.
- 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. *35th 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.

ADDITIONAL COURSES

- Creating Applications with Python-OEChem Workshop, *Cambridge, MA*, 2011.