Curriculum Vitae

Alexander S. Bayden

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OBJECTIVE

Computer aided drug design 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

2021-2022 Senior Research Scientist
2022-2023 Principal Investigator at Biohaven Pharmaceuticals, Inc.

- Computer-aided drug design
  - Worked on many diverse projects requiring many computational approaches
    - Docking / virtual screening, building 1D and 3D QSAR models, core replacement, scaffold morphing, homology modeling, design of covalent inhibitors, molecular dynamics, humanization of antibodies, evaluating druggability of binding sites, *etc*.
  - Worked with contractors and software vendors
  - Used CCG MOE, YASARA, Schrödinger Maestro, DataWarrior, KNIME, CDDVault
  - Machine learning, Python programming

2019-2020 Senior Research Scientist, Computational Chemistry at Kleo Pharmaceuticals Inc.

- Computer-aided drug design

2019 Contractor at NLS Life Science and Therapeutics Discovery, LLC

- Computer-aided design of peptide-based therapeutics

2016-2018 Senior Research Scientist, Computational Chemistry at IDEAYA Biosciences

- Set up a computational chemistry program from scratch
  - Set up computational chemistry software
  - Provided training, installation, troubleshooting and support of molecular modeling software
- Computer-aided small molecule drug design on a diverse set of projects using many different techniques
  - Building QSAR models, docking, tautomer prediction and conformational searching using QM, core replacement, scaffold morphing, virtual screening, homology modeling, design of covalent inhibitors, predicting sites of metabolism, evaluating druggability of binding sites, *etc*.
- Scientific programming in Python

2013-2016 Computational Chemist at CMDBioscience

- Computer-aided design of peptide-based therapeutics
- Making virtual peptide libraries
- Making models for, membrane permeability of peptides, proteolysis of peptides, immunologic response to peptides, selectivity in water displacement from protein active sites
- Scientific programming (Python, Java)
  - Making and improving 3D modeling and informatics applications.
  - Routinely worked with a Linux cluster and a queueing system

2011-2013 Postdoctoral Fellow at Randstad / AstraZeneca R&D Boston (Mentor – Dr. Michelle L. Lamb)

- Developing methods and implementing computational chemistry workflows for investigating the role of water in protein-ligand interactions using Python and SVL programming
- Developing a web application for running water-related calculations on a Linux cluster (Python / Django)
- Running water-related calculations for computational chemists
- Used CCG MOE, Schrödinger Maestro, Glide and Prime, OpenEye VIDA and SZMAP, Tibco Spotfire

2006-2010 Postdoctoral Fellow / Lab & Research Specialist II
at the Virginia Commonwealth University Medicinal Chemistry Department
(Mentor – Prof. Glen E. Kellogg)

- Modeling of Biological Systems
  - Docking / 3D Database Searching
    - 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
    - Design of pentapeptide inhibitors for *O*-acetylserine sulfhydrylase
    - Used Sybyl, GOLD
  - Studying the mechanism of p53 tetramerization
  - Modeling interactions between SHP2 and EGFR proteins with respect to radiation sensitivity
- Scientific Programming (mostly in Python)
  - 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
    - A QSAR-like project for proteins
  - Setting up computational workflows
  - Developing a new way to visualize molecular dynamics trajectories

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 (Academic Advisor – Prof. Kenneth D. Jordan)
  - 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
    - Used Gaussian, GAMESS, VASP
  - Successfully developed global optimization algorithms and implemented them in C++
  - 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
  - Provided training for administrative assistants and junior web team members

- 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

Citizenship: U.S. Citizen

MOLECULAR MODELING SKILLS

- Experience with molecular modeling
  - Skills in both QM and MM methods
  - Docking / Virtual screening / 3D pharmacophore searching / Core replacement
  - Modeling water in biological systems
  - QSAR
- Experience with modeling and visualization packages
  - OpenEye
    - VIDA, SZMAP
  - Schrödinger
    - Maestro, Glide, Prime
  - Other
    - CCG MOE, YASARA, Sybyl, CMDInventus, GOLD, HINT, Gaussian, GAMESS, OpenBabel, ToxTree
  - Data analysis/visualization
    - Spotfire, DataWarrior, Vortex, CMDnavigator, nQuery

COMPUTER ENVIRONMENT

- Programming
  - Python chemical toolkits such as RDKit, YASARA and OpenEye, SQL, Basic/Visual Basic, HTML, Knime
- Background in methods for
  - Data visualization
  - Machine learning
- 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 11 / 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
- Understanding of AWS
- 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 the drug development process
- Taught analytical chemistry lab and physical chemistry lab

GRE SCORES

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

PUBLICATIONS

- Diller, D. J.; Swanson, J.; **Bayden, A. S.**; Brown, C. J.; Thean, D.; Lane, D. P.; Partridge, A. W.; Sawyer, T. K.; Audie, J. Rigorous Computational and Experimental Investigations on MDM2/MDMX-Targeted Linear and Macrocyclic Peptides. *Molecules*, **2019**, *24*, 4586.
- Price-Troska, T.; Yang, Z. Z.; Diller, D.; **Bayden, A.**; Jarosinski, M.; Audie, J.; Ansell, S. M. Inhibiting IL-2 signaling and the regulatory T-cell pathway using computationally designed peptides. *Investigat. New Drug.* **2019**, *37*, 9-16.
- Diller, K. I.; **Bayden, A. S.**; Audie, J.; Diller, D. J. PeptideNavigator: An interactive tool for exploring large and complex data sets generated during peptide-based drug design projects. *Comp. in Biol. and Med.*, **2018**, *92*, 176-187.
- Spyrakis, F.; Ahmed, M. H.; **Bayden, A. S.**; Cozzini, P.; Mozzarelli, A.; Kellogg, G. E. The Roles of Water in the Protein Matrix: A Largely Untapped Resource for Drug Discovery. *J. Med. Chem.*, **2017**, *60*, 6781-6827.
- Price-Troska, T.; Diller, D; **Bayden, A.**; Jarosinski, M.; Audies, J.; Yang, Z. Z.; Ansell, S. M. Inhibiting IL-2 Signaling and the Regulatory T-Cell Pathway Using Computationally Designed Novel Peptides. *Blood*, **2016**, *128*, 3875.
- **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.

PATENTS

- **Bayden, A. S.**; Berbasova, T.; Fisher, L. S.; Kazmierski W.; Rastelli L.; Sawyer T. K.; Spiegel D. A.; Widdison W. C.; Technologies for preventing or treating infections. U.S. Patent WO 2021195401A1, March 25, 2020.

POSTERS

- Software for conformational searching at IDEAYA Biosciences, Inc. *256th ACS National Meeting, Boston, MA*, 2018.
- Python program for solving problems in computer-aided peptide design. *253rd ACS National Meeting, San Francisco, CA*, 2017.
- CoMBASA: A hydropathy-based tool for mapping out receptor-based pharmacophores.
    - *253rd ACS National Meeting, San Francisco, CA*, 2017.
    - *2016 ACS Northeast Regional Meeting, Binghamton, NY*, 2016.
- CMDscaffold: A virtual peptide library for *de novo* rational drug design. *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

- Teaching chemistry to an elementary school student, what works and what does not. *256th ACS National Meeting, Boston, MA,* 2018.
- Structure-based peptide-modeling software for rational drug design. *2016 ACS Northeast Regional Meeting, Binghamton, NY,* 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.
    - *252nd ACS National Meeting, Philadelphia, PA,* 2016.
    - *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 / CERTIFICATIONS

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