



Arneh Babakhani

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Academic Experience

- 08/2005 – 05/2009: **Doctor of Philosophy, University of California at San Diego**
(expected) Chemistry, with an emphasis in Computational Science
“Computational and Pharmacological Modeling of Membrane Proteins”
Adviser: Prof. J. Andrew McCammon
6 manuscripts (5 published + 1 submitted)
- 03/2007: **Master of Science, Chemistry, University of California at San Diego**

Research Interests:

- 1) Physical & computational chemistry, with applications to biochemistry and pharmacology.
- 2) Cell membrane and transmembrane protein phenomena.
- 3) Virtual screening & drug discovery methodologies.
- 4) Mesoscale biological modeling.
- 5) General techniques in computational science and mathematics.

Selected Skillset:

- 1) Design and implementation of virtual screening protocols
- 2) Lead identification and drug discovery
- 3) Docking methodologies and analysis of protein-ligand interactions
- 4) Molecular dynamics simulations and analysis, using NAMD, GROMACS, VMD
- 5) Protein, membrane, pharmacological modeling and visualization
- 6) Linux/Unix, C++, MATLAB, TCL, Shell programming and scripting

Publications:

- 1) Burke, J; Babakhani, A; Gorfe, A. A.; Kokotos, G.; Li, S.; Woods, V.; McCammon, J. A.; Dennis, E. Inhibitor Binding of Group IVA Phospholipase A2 Probed by Molecular Dynamics and Deuterium Exchange Mass Spectrometry. *J. Am. Chem. Soc.* **2009**, Submitted.
- 2) Babakhani, A.; Talley, T. T.; Taylor, P.; McCammon, J. A. Virtual Screening of the Acetylcholine Binding Protein using a Relaxed Complex Approach. *Computational Biology and Chemistry* **2009**, Accepted.
- 3) Babakhani, A.; Gorfe, A. A.; Kim, J. E.; McCammon, J. A. Thermodynamics of Peptide Insertion and Aggregation in a Lipid Bilayer. *J. Phys. Chem. B* **2008**, In press.
<http://pubs.acs.org/cgi-bin/abstract.cgi/jpcb/k/2008/112/i34/abs/jp804710v.html>
- 4) Gorfe, A. A.; Babakhani, A.; McCammon, J. A. H-ras protein in a bilayer: Interaction and structure perturbation. *J. Am. Chem. Soc.* **2007**, 129, 12280-12286.
<http://pubs.acs.org/cgi-bin/abstract.cgi/jacsat/asap/abs/ja073949v.html>

- 5) Gorfe, A. A.; Babakhani, A.; McCammon, J. A. Free energy profile of H-ras membrane anchor upon membrane insertion. *Angewandte Chemie International Edition* **2007**, 46, 8234-8237.
<http://www3.interscience.wiley.com/journal/116321299/abstract>
- 6) Babakhani, A.; Gorfe, A. A.; Gullingsrud, J.; Kim, J. E.; McCammon, J. A. Peptide insertion, positioning, and stabilization in a membrane: Insight from an all-atom molecular dynamics simulation. *Biopolymers* **2007**, 85, 5-6, 490-497.
<http://www3.interscience.wiley.com/journal/114107490/abstract>
- 7) Gullingsrud, J.; Babakhani, A.; McCammon, J. A. Computational investigation of pressure profiles in lipid bilayers with embedded proteins. *Molecular Simulation* **2006**, 32, 831-838.
<http://www.journalsonline.tandf.co.uk/link.asp?id=157842265v8r04m5>

Conferences presented:

- 1) American Chemical Society Western Regional Meeting, September 2007, San Diego, CA
- 2) National Biomedical Computation Resource, July 2007, La Jolla, CA
- 3) Johnson & Johnson Drug Discovery Symposium, June 2007, La Jolla, CA
- 4) American Chemical Society, September 2006, San Francisco, CA
- 5) National Biomedical Computation Resource, August 2006, La Jolla, CA

Hosted (planned & organized) the following events:

- 1) UCSD Physical Chemistry Seminar 01/08/2008, Prof. Emily Carter, Princeton University
- 2) UCSD Physical Chemistry Seminar 10/30/2007, Prof. Klaus Schulten, UIUC
- 3) UCSD Physical Chemistry Seminar 10/16/2007, Prof. Ken Dill, UCSF

Teaching Experience in:

- 1) Physical Chemistry (Thermodynamics, CHEM131), UCSD Chemistry & Biochemistry
 - 2) Physical Chemistry (Pharmacology, SPPS 222), UCSD Skaggs School of Pharmacy
 - 3) Physical Chemistry (Laboratory, CHEM105), UCSD Chemistry & Biochemistry
 - 4) Computational Chemistry (Modeling, CHEM215), UCSD Chemistry & Biochemistry
- See <http://mccammon.ucsd.edu/~ababakha/Teaching.html> for evaluations.

Graduate Coursework Completed in:

- Quantum Mechanics • Macromolecular Recognition • Scientific Computation
- Statistical Mechanics • Enzymology • Partial Differential Equations • Parallel Computing

08/1996 – 12/2000: ***Bachelor of Science, Chemistry, University of California at Berkeley***

08/1998 – 06/2001: ***Lawrence Berkeley National Laboratory, Center for Functional Imaging***
Student researcher, projects: Synthesis of Atipamezole and Rotenone derivatives, ran organic reactions, performed chromatography, analyzed spectral data, under Prof. Henry F. VanBrocklin

01/2000 – 12/2000: ***University of California at Berkeley, Department of Chemistry***
Student researcher, project: Expression of the Glycosyl Sulfotransferases. Conducted molecular biology protocols, maintained cell culture, under Prof. Carolyn Bertozzi

08/1999 – 12/1999: ***Teaching Assistant, Organic Chemistry 3B***
Personally instructed 25 students, ran experiments, conducted office hours.



Military Experience United States Navy



- 02/2007 – Present: ***Executive Officer (XO), NMORA 1994 Unit, San Diego, CA***
#2 in Command, Manage a division of 24 sailors, chiefs and junior officers, coordinate administrative paperwork & logistics for monthly drills and annual training activities.
- 08/2005 – Present: ***Lieutenant (O-3), United States Naval Reserve, San Diego, CA***
Drilling Reservist (SELRES), Naval METOC Reserve Activity 1994
Directorate of Intelligence Surveillance and Reconnaissance (ISR)
Special Duty Oceanography (METOC) Community
Train in the usage of imagery for environmental analysis and mission planning, develop and maintain curriculum in ISR analysis.
- 02/2004 – 08/2005: ***Lieutenant Junior Grade (O-2), Mobile Environmental Team San Diego, CA***
Division Officer, managed a division of 16 enlisted personnel and their deployments throughout the world, provided tactical oceanographic products and support to U.S. Naval assets.
- 04/2002 – 01/2004: ***Ensign (O-1), Naval Pacific Meteorology Oceanography Center San Diego, CA***
Command Duty Officer, supervised a division of 10 enlisted personnel, managed watchfloor operations, forecasted for U.S. Third Fleet assets.
- 01/2002 – 03/2002: Basic Officer Accession Training Course, Gulfport, MS.
09/2001 – 12/2001: U.S. Naval Ice Center, Suitland, MD.
06/2001 – 08/2001: U.S. Naval Officer Indoctrination School, Newport, RI.
06/11/2001: Commissioned, Ensign, United States Navy

Awards & Qualifications:

- 07/2005: ***Navy and Marine Corp Achievement Medal***
02/2004: ***Navy and Marine Corp Achievement Medal***
02/2003: ***Command Duty Officer Qualification***
11/2002: ***Optimum Track Ship Router Qualification***
08/2002: ***Forecast Duty Officer Qualification***
09/2002: ***Expert Pistol Marksmanship Medal***
04/2002: ***National Defense Medal***

Details regarding military assignments, missions, and security clearances are available upon request.