

Donald Hamelberg, Ph.D.

EDUCATION AND TRAINING

Postgraduate Research Fellow Howard Hughes Medical Institute and University of California at San Diego La Jolla, California Advisor: Prof. J. Andrew McCammon	2003 – 2005
Postdoctoral Research Fellow National Center for Data mining/Laboratory for Advanced Computing University of Illinois, Chicago, Illinois Director: Prof. Robert Grossman	2001 – 2003
Ph.D. and M.S. in Biophysical Chemistry (GPA = 4.0/4.0) Georgia State University, Atlanta, Georgia Advisor: Regent's Prof. David W. Wilson Dissertation title: "Molecular dynamics simulation and free energy perturbation studies of the minor groove of DNA: Structures and cation interactions"	1996 - 2001
B.Sc. with honors in Chemistry and minor in Mathematics Fourah Bay College, Freetown, Sierra Leone	1989 - 1993

PROFESSIONAL EXPERIENCE

Bioinformatics Specialist Howard Hughes Medical Institute Investigator: Prof. J. Andrew McCammon University of California at San Diego La Jolla, California	2005 – present
Postgraduate Research Howard Hughes Medical Institute Department of Chemistry and Biochemistry, University of California at San Diego La Jolla, California	2003 – 2005
Postdoctoral Research National Center for Data mining Laboratory for Advanced Computing, University of Illinois Chicago, Illinois	2001 – 2003
Academic Exchange Visitor Data Mining Group/Imperial College Parallel Research Center Imperial College of Science Technology and Medicine, University of London, England Visitor of Prof. Yike Guo research group	Summer 2002
Graduate Research and Teaching Assistant Department of Chemistry, Georgia State University Atlanta, Georgia	1996 - 2001
Commercial Sales Engineer Mobil Oil Company, Freetown, Sierra Leone	1993 - 1995

AWARDS

Chair Award Chemistry Department, Georgia State University	Spring 2001
David W. Boykin Graduate Fellowship Chemistry Department, Georgia State University	Fall 1999
Teaching Award Chemistry Department, Georgia State University	Winter 1998
Workshop grant Pittsburgh Supercomputing Center	August 1998

PROFESSIONAL MEMBERSHIP

American Chemical Society
Biophysical Society
American Association for the Advancement of Science
Protein Society

PROFESSIONAL ACTIVITIES

Mentoring

- Howard Hughes Medical Institute summer research undergraduates at University of California, San Diego: Jennifer Greene, 2004, University of Maryland, Baltimore; Shayri Greenwood, 2005, SUNY Stony Brook
- Visiting research graduate students at University of California, San Diego: Erik Johan Qvist, 2006, Lund University Sweden; Jesper Sorensen, visitor 2006, M.S. student, University of Aarhus, Denmark
- Several rotation students at University of California, San Diego
- M.S. students at the National Center for Data Mining, University of Illinois, Chicago between 2001-2003: Pavan Kasturi; Priya Raghunath

Teaching

- Chemistry 115/215: Modeling Biological Macromolecules. Lectures on molecular dynamics simulation and analysis. University of California at San Diego (2005)
- Lecture on Accelerating conformational transition in biomolecules at a research workshop and summer school "Theory and Computation in Molecular Biological Physics" Center for Theoretical and Biological Physics at University of California at San Diego (2004)
- Chemistry 8510: Biophysical Chemistry, teaching assistant, Georgia State University (2000)
- Chemistry 6450: Molecular Modeling Methods, teaching assistant, Georgia State University (1999)
- Chemistry 6110: Physical Chemistry, teaching assistant, Georgia State University (1998-2001)

Journal manuscript review

- Journal of the American Chemical Society
- Protein Engineering Design and Selection
- Bioorganic and Medicinal Chemistry Letters

COMPUTER SKILLS

- Unix system administrator with 5+ years of experience
- Experienced in Unix shell scripting and C++ object oriented programming
- Write C/C++ and Fortran codes as part of my research project
- Familiar with Pascal, Java, Fortran, TCP/IP, networking and the Linux operating system

PUBLICATIONS (*Total Citations: 270+ times*)

Sørensen, J., **Hamelberg, D.**, Schiøtt, B., McCammon, J.A. (2007). Comparative MD analysis of the stability of transthyretin providing insight into the fibrillation mechanism. *Biopolymers*, **86**, 73-82 (Issue Cover Story)

Oliveira C. A. F., **Hamelberg D.**, McCammon J. A., (2006). On the Application of Accelerated Molecular Dynamics to Liquid Water Simulations. *Journal of Physical Chemistry B*, **110**, 22695-22701

Hamelberg D., Shen T., McCammon J. A., (2006). Insight into the role of hydration on protein dynamics. *Journal Chemical Physics*, **125**, 094905

Shen T., **Hamelberg D.**, McCammon J. A., (2006). Elasticity of peptide omega bonds. *Physical Review E*, **73**, 041908

Vera C., Lao J., **Hamelberg D.**, Sung L. A., (2005). Mapping the tropomyosin isoform 5 binding site on human erythrocyte tropomodulin: Further insights into E-Tmod/TM5 interaction. *Archives of Biochemistry and Biophysics*, **444**, 130-138 (Issue Cover Story)

Hamelberg D., McCammon J. A., (2005). Fast Peptidyl cis-trans Isomerization within the Flexible Gly-Rich Flaps of HIV-1 Protease. *Journal of the American Chemical Society*, **127**, 13778 -13779

Shen TY, Zong CH, **Hamelberg D**, McCammon J. A., Wolynes, P. G, (2005). The folding energy landscape and phosphorylation: modeling the conformational switch of the NFAT regulatory domain. *FASEB Journal*, **19**, 1389-1395

Hamelberg D., Shen T., McCammon J. A., (2005). Relating kinetic rates and local energetic roughness by accelerated molecular-dynamics simulations. *Journal of Chemical Physics*, **122**, 241103

Hamelberg D., Shen T., McCammon J. A., (2005). Phosphorylation effects on cis/trans isomerization and the backbone conformation of serine-proline motifs: Accelerated molecular dynamics analysis. *Journal of the American Chemical Society*, **127**, 1969-1974

Chaires J. B., Ren .J, **Hamelberg D.**, Kumar A., Pandya V., Boykin D. W., Wilson W. D., (2004). Structural selectivity of aromatic diamidines. *Journal of Medicinal Chemistry*, **47**, 5729-5742

Hamelberg D., McCammon J. A., (2004). Standard free energy of releasing a localized water molecule from the binding pockets of proteins: double-decoupling method. *Journal of the American Chemical Society*, **126**, 7683-7689

Hamelberg D., Mongan J., McCammon J. A., (2004). Accelerated molecular dynamics: A promising and efficient simulation method for biomolecules. *Journal of Chemical Physics*, **120** (24), 11919-11929

Grossman R., Kasturi, P., **Hamelberg, D.**, Liu, B. (2004). An empirical study of the universal chemical key algorithm for assigning unique keys to chemical compounds. *Journal of Bioinformatics and Computational Biology*, **2**, 155-171

Tanious F. A., **Hamelberg D.**, Bailly C., Czarny, A., Boykin D. W., Wilson, W. D., (2004). DNA sequence dependent monomer-dimer binding modulation of asymmetric benzimidazole derivatives. *Journal of the American Chemical Society*, **126**, 143-153

Nguyen B, **Hamelberg D.**, Bailly C., Colson P., Stanek J., Brun R., Neidle S., Wilson W. D. (2004). Characterization of Novel DNA minor-groove complex. *Biophysical Journal*. **82**, 1028-1041

Grossman R. L., Gu Y. H., **Hamelberg D.**, Hanley D., Hong X. W., Levera J., Lillethun D., Mazzucco M., Mambretti J., Weinberger J., (2003). Experimental studies using photonic data services at IGrid 2002. *Future Generation Computer Systems*, **19**, 945-955

Nguyen B, Lee M. P. H., **Hamelberg D.**, Joubert A., Bailly C., Brun R., Neidle S., Wilson W. D. (2002). Strong Binding in the DNA Minor Groove by an Aromatic Diamidine With a Shape That Does Not Match the Curvature of the Groove. *Journal of the American Chemical Society*. **124**, 13680-13681

Hamelberg D., Williams, L. D., Wilson, W. D., (2002). The Effect of Neutralized Phosphate Backbone on the Minor Groove Structure of B-DNA: Molecular Dynamics Simulation Studies. *Nucleic Acid Research*, **30**, 3615-3623

Hamelberg D., Williams, L. D., Wilson, W. D., (2001). Influence of the Dynamic Positions of Cations on the Structure of the DNA Minor: Sequence Dependent Effects. *Journal of the American Chemical Society*, **123**, 7745-7755

Hamelberg D., McFail-Isom, L., Williams, L. D., Wilson, W. D., (2000). Flexible Structure of DNA: Ion Dependence of Minor-Groove Structure and Dynamics. *Journal of the American Chemical Society* **122**, 10513-10520

BOOK CHAPTERS

Hamelberg D., McCammon J. A., (2007). Dealing with bound waters in a site: Do they leave or stay? In "Computational and Structural Approaches to Drug Discovery," R.M. Stroud, Ed., Royal Society of Chemistry, (in press)

Hamelberg D., McCammon J. A., (2006). Accelerating conformational transitions in biomolecular systems. *Annual Reports in Computational Chemistry*, **2**, 221-232

INVITED TALKS, CONFERENCE PAPERS, AND POSTERS

Hamelberg D., Mongan, J. T., Shen, T. Y., McCammon J. A. (2005). Exploring the energy landscapes of biomolecules. *ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 230th ACS Spring National Meeting, Washington, D. C, August, 2005*

Hamelberg D., Shen, T. Y., McCammon J. A. (2005). Relating local energetic roughness and kinetic rates: All-atom accelerated molecular dynamics of CIS/TRANS isomerization of serine-proline motifs. *ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 228th ACS Spring National Meeting, San Diego, CA, March, 2005*

Hamelberg D., Shen, TY., McCammon J. A. (2005). Accelerating conformational transitions in biomolecules using all atom molecular dynamics simulation: Cis/trans isomerization of serine-proline motifs. *BIOPHYSICAL JOURNAL* **88** (1): 183A-183A Part 2 Suppl. S, Long Beach, CA JAN 2005

Hamelberg D., McCammon J. A. (2004). Free energy of releasing a localized water molecule from the binding pockets of proteins: Double-decoupling method. *ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 227th ACS Spring National Meeting, Anaheim, CA, March 27-April 1, 2004*

Nguyen B, **Hamelberg D**, Tanious F, Wilson WD. (2004). Energetic basis for drug - DNA minor groove interactions. *ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 227th ACS Spring National Meeting, Anaheim, CA, March 27-April 1, 2004*

Nguyen B, **Hamelberg D**, Wilson D. (2004). The energetics of molecular recognition of the DNA minor groove. *BIOPHYSICAL JOURNAL* **86** (1): 138A-138A Part 2 Suppl. S, JAN 2004

Grossman R., **Hamelberg D.**, Kasturi, P., Liu, B. (2003). Experimental Studies of the Universal Chemical Key (UCK) Algorithm on the NCI Database of Chemical Compounds. *IEEE Computer Society Bioinformatics Conference (CSB'03)*, IEEE Computer Society, Los Alamitos, California, p. 244

Nguyen B, Tanious F, **Hamelberg D.**, Wilson W. D. (2003). Thermodynamics of DNA minor groove interactions: Sequence dependence of the binding enthalpy and entropy. *226th ACS National Meeting, New York, NY, September 7-11, 2003*

Nguyen B, Lee M. P. H., **Hamelberg D.**, Joubert A., Bailly C., Brun R., Neidle S., Wilson W. D. (2002). Structure and Dynamics of an Antitrypanosomal Agent Binding to DNA. *The University System of Georgia Research Symposium: Georgia State University*

Donald Hamelberg, Lori McFail-Isom, Loren D. Williams, W. David Wilson (2001). Effect of Cations on the Structure of DNA. *The 9th Annual Suddath Memorial Symposium: Georgia Institute of Technology*

Donald Hamelberg, Fariel A. Tanious, Donald A. Patrick, Richard R. Tidwell, W. David Wilson (1999) Relative Binding Energies of a 2, 7-diamidinium carbazole and several analogs to d(GCGAATTCGC)₂: A Free Energy Perturbation Study. *The 7th Annual Suddath Memorial Symposium: Georgia Institute of Technology*