



**Curriculum Vitae  
Jennifer M. Bui, Ph.D.**



**Hughes Hall**

University of Cambridge  
Department of Chemistry  
Lensfield Road  
Cambridge CB2 1EW UK

Phone: +44 (0)1223 336311  
Fax: +44 (0)1223-336362  
Email: jbb39@cam.ac.uk  
National: United States of America

**Education**

- 2006-present      **NSF** Postdoctoral Fellow in Structural Biology and Chemical Information  
University of Cambridge, Cambridge, UK.  
Project: Target Protein Flexibility in Molecular Recognition and Binding  
Advisor: Prof. **Christopher M. Dobson**
- 2005-2006      Postdoctoral Fellow in Computational Chemistry  
University of California, San Diego, USA.  
Project: Protein Conformational Conversions upon Binding Recognition  
Advisor: Prof. **J. Andrew McCammon**
- 2000-2005      Ph.D. in Theoretical Chemistry  
University of California, San Diego, USA.  
Dissertation: Structural Transitions, Functions, and Dynamics of Acetylcholinesterase and its  
Inhibitors.  
  
Advisor: Prof. **J. Andrew McCammon**
- 1997-1999      Ph.D. Program in Theoretical Chemistry with Emphasized in Mathematical Biology  
University of California, Davis, USA.  
Project: The Initiation Mechanisms of Repetitive Calcium Waves in Mouse Oocyte upon  
Fertilization.  
Advisor: The late Prof. Joel E. Keizer
- 1995-1997      B.S. in Chemistry  
University of California, Davis, USA.  
Project: *Ab initio* Study of Charge Effects on Electronic Configuration of Noble Gases  
Advisor: Prof. William H. Fink

**Honors and Fellowship**

- 2007-2009      Research Fellow, Hughes Hall, Cambridge, UK.
- 2006-2009      **National Institutes of Health Ruth L. Kirschstein/NRSA Postdoctoral Fellowship**, University of  
Cambridge, UK
- 2006-2009      **National Science Foundation Postdoctoral Research Fellowship in Biological Informatics**,  
**University of Cambridge, UK.**

2003-2006 Trainee, NSF Center for Theoretical Biological Physics, UC-San Diego  
2001-2006 Affiliated Trainee, NIH Molecular Biophysics Training Grant, UC-San Diego  
1998-1999 Affiliated Trainee, NSF Institute of Theoretical Dynamics Training Grant, UC-Davis  
1997 **University of California Regents:** The Bradford Borge Graduate Fellowship, UC-Davis  
1997 Departmental Citation for the most meritorious undergraduate achievement, UC-Davis  
1996 Clorox Chemical Scholarship, UC-Davis  
1996 The Dean's List of College of Letters and Science, UC-Davis

## **Publications**

- **Jennifer M. Bui** and J. Andrew McCammon. Protein Complex Formation Mechanism: Fast Conformational Transitions of Neurotoxin Fasciculin-2 in Complex with Acetylcholinesterase. in press. *Proc. Natl. Acad. Sci USA*, **103** 15451-16456, (2006).
- **Jennifer M. Bui** , Zoran Radic, Palmer Taylor, J.A. McCammon; Conformational Transitions in Protein-Protein Binding: The Neurotoxin Fasciculin-2 Binding to Acetylcholinesterase *Biophysical Journal*, **90**, 3280-3287 (2006)
- Sanjib Senapati, **Jennifer M. Bui**, and J.A. McCammon; Induced Fit in Mouse Acetylcholinesterase upon Binding syn-TZ2PA6: A Molecular Dynamics Study. *J. Med. Chem. Soc.*, **48**, 8155-8162 (2005).
- David D.L. Minh, **Jennifer M. Bui**, Chia-en Chang, Tushar Jain, Jessica M.J. Swanson, and J. Andrew McCammon. Molecules Losing Space: An External Entropy Calculation of Protein-Protein Association, Fas2 binding to AChE. *Biophysical Journal*, **89**, L25-27 (2005).
- **Jennifer M. Bui** and J.A. McCammon; Acetylcholinesterase: Pivotal Roles of its Long Omega Loop (CYS69-CYS96) in Regulating Substrate Binding. *J. Chem-Biol. Interact.*, Vol:157, 357 (2005)
- **Jennifer M. Bui**; Kaihsu Tai; J.A. McCammon; Acetylcholinesterase: Enhanced Fluctuations and Alternative Routes to the Active Site in the Complex with Fasciculin-2. *J. Amer. Chem. Soc.*, **126**, 7198-7205 (2004).
- **Jennifer M. Bui** and J.A. McCammon; The Displacement of Ligand through the Bottleneck Region of the Acetylcholinesterase Gorge. In *Proceedings of the International Symposium on Cholinesterases and Related Proteins*, Chile, N.C. Inestrosa and E.O. Campos, Eds., pp 207-211 (2004)
- **Jennifer M. Bui**; R..H. Henchman; J.A. McCammon; The Dynamics of the Ligand Barrier Crossing inside the Acetylcholinesterase Gorge, *Biophysical Journal*. **85**, 2267-2272 (2003).

## Invited Talks

- February 14-18, 2004 “Conformational Variations of Fasciculin Associated with Protein-Protein Binding Interaction”. Presented at the 48<sup>th</sup> **Biophysical Society** Annual Meeting, Baltimore, Maryland
- March 25-April 1, 2004 “Conformational Variations of Fasciculin Associated with Protein-Protein Binding Interaction” Presented at the 228<sup>th</sup> **American Chemical Society** National Meeting, Anaheim, California.
- June 3-5, 2005 “Computational Modeling of Biomolecules: The Roles of Dynamics in Acetylcholinesterase Activity and Inhibition”. Presented at the 6<sup>th</sup> VACETS Technical International Conference, Milpitas, California.
- September 10-14 2006 “Protein binding mechanism: Fast induced-fit conformational transitions of neurotoxin Fasciculin-2 in complex with acetylcholinesterase” Presented at 232<sup>nd</sup> **American Chemical Society** National Meeting, San Francisco, CA

## Professional Activities

- **Chairwoman**, Biophysical Society Meeting Platform, Baltimore (02/2004)
- Referee, Proteins: Structure, Function and Bioinformatics (06/2004)
- Referee, Biophysical Journal (07/2003)
- Member, American Chemical Society (2004)
- Member, Biophysical Society (2002)
- Member, Protein Society (2002)
- Member, NFS Institute of Theoretical Dynamics, UC-Davis (1997-1999)
- Elected Member, Phi Kappa Phi Honors Society (1996-present)
- Editorial Board Member of the Vietnamese Public Library of Knowledge Journal (2006-present)

## Teaching

2000-2005 *Teaching Assistant, Department of Chemistry and School of Pharmacy University of California, San Diego*

Taught undergraduate physical chemistry: quantum mechanics and kinetics courses, a graduate course in computational modeling, and a physical chemistry course to pharmacy students.

1997-1999 *Teaching Assistant, Department of Chemistry, University of California, Davis*

Taught general chemistry courses and a graduate course in neurophysiology and computational biology.