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EDUCATION

Reed College

B.A. Chemistry

University of California, San Francisco

Ph.D. Pharmaceutical Chemistry

Stanford University

Postdoctoral Fellow

PROFESSIONAL EXPERIENCE

University of Washington

Professor of Bioengineering (9/07- present)

Director of the Biomolecular Structure and Design Program (6/07-present)

Professor of Medicinal Chemistry (7/03- 9/07)

Adjunct Professor of Biochemistry (7/00-present)

Adjunct Professor of Biomedical and Health Informatics (7/02-present)

Adjunct Professor of Bioengineering (2/05-9/07)

Member of Biomolecular Structure and Design Program (9/96-present)

Member of Molecular Biophysics Program (6/93-present)

Member of Neurobiology and Behavior Program (5/02-present)

Member of the Biomedical and Health Informatics Program (6/00-present)

Member of the Computational Molecular Biology Program (6/05-present)

Associate Professor of Medicinal Chemistry (7/98-6/03)

Assistant Professor of Medicinal Chemistry (1/93-6/98)

Cambridge University and Medical Research Council, UK

Visiting Professor, Chemistry Department and Center for Protein Engineering (9/02-1/03)

Member of the Room, Gonville & Caius College

Host: Sir Alan Fersht

Stanford University, Department of Structural Biology

Staff Research Associate (4/92-1/93)

Postdoctoral Fellow (6/90-3/92)

Supervisor: Dr. Michael Levitt

University of California, S.F., Department of Pharmaceutical Chemistry

Physical Chemistry Teaching Assistant (9/86-5/87)

Physical Chemistry Tutor (9/88-12/88)

Graduate Student (9/85-6/90)

Advisors: Drs. Irwin Kuntz and Peter Kollman

Triton Biosciences, Inc.

Consultant (9/88-9/89)

General force field issues and generation of NMR structures.

Rutgers University, Department of Biochemistry and Microbiology

Research Assistant (12/83-9/85)

Development of 2-D electrophoresis methods to screen for the existence of dioxins in the blood of veterans exposed to Agent Orange.

Reed College, Chemistry Department

Senior Thesis Research (5/82-5/83).

Deamidation of proteins and the possible effects of modification on protein folding.

HONORS AND FELLOWSHIPS

US Department of Energy (DOE) Innovative and Novel Computational Impact on Theory and Experiment (INCITE) award for research in "Molecular Dynamematics." Award of 2 million CPU hours, 2005. (one of three awards in the country)

DOE National Research Energy Scientific Computing Center Award of 1,900,000 CPU hours, 2006, 5M hours 2007, 10M hours 2008, 2.5M hours 2009.

Two papers from my group were in the 'Top 5' Downloads from the *Journal of Molecular Biology* in 2005.

National Academy of Sciences: Participated in the First Annual Japanese-American National Academy of Sciences' Frontiers of Science Symposium, August, 1998; Invited to participate in the National Academy of Sciences' Frontiers of Science Symposium, November, 1996 (I was unable to attend); Sackler NAS Colloquium, Frontiers in Bioinformatics: Unsolved Problems and Challenges, 2004, invited participant and session chair.

Young Investigator Award, Office of Naval Research (5/95-4/98), renewed as grant (1/99-12/01, 1/02-9/05, 10/05-9/08).

Invited to Office of Naval Research 50th Anniversary Symposium as a representative of work they are supporting, National Academy of Sciences, 1996.

Office of Naval Research, Two DURIP Equipment Awards (8/96-7/97 and 4/98-3/99).

FIRST Award, National Institutes of Health (8/95-7/00), renewed as R01 (8/00-7/04, 8/04-7/08).

Intel, Computer Equipment, 8/97-7/99, (\$5,900,000, our share ~\$450,000)

Consultant/Co-PI on NIH Program Project Grant on Prion Diseases, Stanley Prusiner, P.D., Fred Cohen, P.I. (1/93-12/98).

American Health Assistance Foundation, Alzheimer's Disease Research Program, two awards (4/93-3/95, 4/95-3/97).

National Science Foundation, RPG Award (7/94-6/95).

Petroleum Research Fund, American Chemical Society, Grant (2/94-8/96).

Sandoz Foundation for Gerontological Research, Grant (5/94-5/95).

Jane Coffin Childs Foundation Postdoctoral Fellowship, (7/90-7/93).

Two separate fellowships from the Katherine McCormick Fund, Stanford University (10/90-10/91, 10/92-10/93).

National Institutes of Health Postdoctoral Fellowship (1990, declined).

Graduate Opportunity Fellowship, University of California, S.F. (9/85-9/86).

Coca Cola Academic Scholarship, Reed College, (9/79-6/81).

Oregon Scholar, Reed College, (9/79-5/83).

PROFESSIONAL ACTIVITIES AND SERVICE

- Senior Editor of *Protein Engineering Design and Selection (PEDS)* with Alan Fersht (January 2004-present)
- Editorial Boards (current): *Biochemistry* (2003-present), *Structure* (1995-present), *Biomedical Computation Review (BCR)* (2005-present).
- Member of NIH Macromolecular Structure and Function B Study Section, July 2005 - 2008.
Contributing faculty member to 'Faculty of 1000 Biology', February 2005 – June 2007.
- Co-Editor with Alan Fersht of *Current Opinion in Structural Biology* issue on Folding and Binding, 2007 and 2009.
- Elected Biophysical Society Council Member, 2007-2010.
- Chair of 2009 Cellular Osmoregulation Gordon Conference. Vice Chair 2007.
- Chair of 2004 Biopolymers Gordon Conference. Vice Chair 2002.
- Co-organizer of the 2002 Protein Society Meeting.
- Editor of a 2003 volume on Protein Simulations for *Advances in Protein Chemistry*
- Editorial Boards (past): Principal Editor for *TheScientificWorld* (2000-2001), Structural Biology section of Biomed Central, electronic publications (2001-2003), *Protein Science* (1996-1999, 2000-2003).
- Participant/lecturer for Royal Society Discussion Meeting on New Science from High Performance Computing, I represented Biomolecular Modeling (10/2001)
- Elected to the Nominating Committee for the Protein Society (2000-2003)
- Steering and Admissions Committees (1994-2002) and founding member of interdisciplinary program for Biomolecular Structure and Design at U. of WA
- Acting Director for Biomolecular Structure and Design Program, 1999-2000.
- Member of the Biophysics Group at U. of WA since 1993, Selection Committee for Trainees for NIH Biophysics Training Grant, 1995, 1998, 1999, 2003.
- Member of the Steering Committee, Molecular Biophysics Training Grant, U of WA (2002-2006)
- Member of the Biomedical and Health Informatics Program at U. of WA since 2000, Selection Committee for Trainees and Admissions.
- Manuscript reviews: *Biochemistry*, *Biopolymers*, *Biophysical Journal*, *Journal of Molecular Biology*, *Proceedings of the National Academy of Sciences*, *Structure*, *Protein Engineering Design and Selection*, *Protein Science*, *Chemical Physics*, *J. Comp. Physics*, *Nature Structural Biology*, *Nature*, *Journal of Biological Chemistry*, *Proteins: Structure, Function and Genetics*, *International Journal of Quantum Chemistry*, *J. Comp. Chem.*, plus others on an occasional basis.
- Professional Societies: American Chemical Society, Protein Society, New York Academy of Sciences, Neuroscience Society, Biophysical Society.
- Special Programs Grant Reviews: National Institutes of Health; National Academy of Sciences/ National Research Council; Department of Energy; Research Corporation--A Foundation for the Advancement of Science; Medical Research Council, U.K., The Wellcome Trust, UK, Hereditary Disease Foundation, Biotechnology and Biological Sciences Research Council (BBSRC UK); plus other private and local foundations.
- Grant/Program Reviews NIH: Special Study Section Member for Project Site Visit, April 1997; Special Study Section Member for Human Genome RFA, July 1997; Special Study Section Member for Program Project Grant, March 2003; Ad hoc for BBCA, February 2003.
- Grant/Program Reviews DOE: Workshop addressing future of biological computations, July 2003 (could not attend), panel member to review INCITE proposals for 2007 (Nov. 2006).

INVITED TALKS

2009

Boston, biophys soc
Chicago, amyloid mtg
Acs mtg salt lake city
WSU
Cuernavaca
China
Bioe mtg
Faseb mt
Doe mtg
Schulten mtg
Undergrad mtg, shields
Georgia Tech mtg

2008

Gordon Research Conference on Protein Folding, Ventura, CA, January 6-11, 2008.
Prion Research Network of Canada, February 4-6, Toronto, March 8, Vancouver (declined, conflict)
University of Oregon, Eugene, March 11, 2008.
Fibrous Proteins: Transforming structural knowledge into new materials, Melbourne, Australia, March 31-April 4, 2008.
American Chemical Society Meeting, New Orleans, April 6-10, 2008 (declined, conflict).
Gordon Research Conference, Computational Aspects of Biomolecular NMR, Italy, May 18-23, 2008.
Gordon Research Conference, Biopolymers, Rhode Island, June 8-13, 2008.
EMBO Conference on Protein Modeling, Paris, July 1-8, 2008.
Human Frontiers of Science Annual Meeting, Berlin, July 6-9, 2008 (declined, conflict).
American Chemical Society Meeting, Philadelphia, August 17-21, 2008 (declined, conflict).
8th KIAS International conference on Protein Structure and Function scheduled on 10/9/2008-10/11/2008 in Seoul, Korea.
Biomedical High Performance Computing Leadership Summit 2008, Boston MA, Oct. 6-7 (declined).
Jane Coffin Childs Annual Meeting, Connecticut, October 17-19, 2008.
BIT's 6th Annual Congress of International Drug Discovery Science and Technology, Session 27: Bioinformatics, Bio-IT, LIMS to Data Visualization in Drug Discovery, Beijing China, October 18-22, 2008 (declined, conflict).

Other Work Travel: Annual editorial board meeting for *Biochemistry*, October 2008; Annual council meeting for Biophysical Society, February, 2008; NIH MSFB study section, February and June, 2008.

2007

Indiana University, Seminar Chemistry Department and School of Medicine, March, 2007.
Albert Einstein College of Medicine, Yeshiva University, Seminar Biophysics Department, March, 2007.
Gordon Research Conference on Osmoregulation, France, June, 2007, declined, conflict with NIH study section meeting.
American Chemical Society Meeting, Boston, declined, conflict, August, 2007.
2007 Frontiers of Macromolecular Simulations, Atlanta, GA, Nov, 2007.
University of California, San Francisco, Biochemistry Seminar Series, October 2007.
Stanford University, Seminar, September, 2007.

Other Work Travel: Annual editorial board meeting for *Biochemistry*, October 2007; Annual council meeting for Biophysical Society, February, 2007; Three meetings a year for NIH study section.

2006

Gordon Research Conference on Protein Folding, Ventura, CA, January 8-13, 2006.
Keystone Meeting on Structural Biology, Keystone, CO, January 29- February 3, 2006.
DARPA's Control of Protein Conformation Workshop, Arlington, VA, February 16-17, 2006 (declined, conflict with NIH study section meeting).
Computational/Experimental Approaches to Protein Defects in Human Disease, Rutgers University, April 20-21, 2006.
International Symposium on Biomolecules: Proteins, DNA/RNA, and Their Interactions, Taipei, Taiwan, June 19-20, 2006.
EMBO Practical Course on Biomolecular Simulation, Pasteur Institute, Paris, June 28 – July 5, 2006.
University of Texas Medical Branch, Neurology Department, Protein Misfolding Seminar Series, Spring, 2006.
Protein Folding in the Cell, FASEB Conference, Vermont, July 29 – August 3, 2006.
American Chemical Society Meeting, Alfred Bader Award Symposium, Award recipient Alan Fersht, San Francisco, CA, September 10-14, 2006.
CECAM workshop on Protein folding and misfolding: Bringing theory close to experiment, Lyon, Paris, September 26-29, 2006.

2005

7th Congress of the World Association of Theoretically Oriented Chemists, Cape Town, South Africa, 16-21 January, 2005.
Biophysical Society Annual Meeting, Chair and Speaker, Symposium on Protein Folding: Theory, Experiment and Design, Long Beach, CA, February 12-16, 2005.
Science Forum Colloquium, University of Washington, March 4, 2005.
Biophysical Aspects of Protein and Peptide Aggregation: Experiment and Theory, American Chemical Society Meeting Symposium, San Diego, March 13-17, 2005.
Cornell Biophysics Colloquia Series, Cornell University, NY, March 30, 2005.
Mayo Clinic, Biochemistry Seminar Series, Minnesota, April 5, 2005.
Flexibility in Biomolecules Workshop, Tempe Arizona, May 2005 (declined, conflict)
Instituto de Biocomputacion y Fisica de Sistemas Complejos, Universidad de Zaragoza, BIFI Colloquia, April 25-28, 2005.
Symposium on Protein Folding, Dynamics and Function, Peking University, Beijing, China, 4-7 July 2005.
Gordon Conference on Cellular Osmoregulation: Sensors, Transducers and Regulators, Salve Regina College in Newport RI, August 7-12.
Telluride Summer Research Workshop on "Vibrational dynamics of biological molecules", August 13-20, 2005 in Telluride, CO (declined, conflict).
XX Congress of the International Union of Crystallography, Florence, Italy, August 23-31, 2005. (not attending, conflict)
CECAM workshop on 'Multiscale Modeling of Macromolecule/Membrane Interactions' in Lyon, France, August 29-31, 2005 (conflict, unable to attend).
Spetsai Summer School, Protein Misfolding, Protein Modification and Age-Related Diseases, Spetses Island, Greece, 5-15 September 2005.
International Molecular Graphics and Modelling Society (MGMS) Meeting, Biomolecular Simulations - from Prediction to Practice, Dublin, Ireland 11th-14th September 2005. (not attending, conflict)

International Bunsen Discussion Meeting, 'Mechanically Induced Chemistry: Theory and Experiment', Tutzing near Munich, October 3 - 6, 2005 (not attending, conflict).
Center for Computational Biology Seminar series at Washington University, St Louis, 7 October 2005.
Prion 2005---Between fundamentals and society's needs. German TSE Research Platform, Dusseldorf, Germany, October 19-21, 2005.

2004

Gordon Research Conference, Protein Folding Dynamics, Discussion Leader, Ventura, CA January 2004.
Gordon Research Conference, Computational Aspects of Biomolecular NMR, January 2004 (conflict, declined)
Southwestern Medical Center at Dallas, Molecular Biophysics Graduate Program Seminar Series, February 2004.
Annual Suddath Symposium, Computational Biology, Georgia Institute of Technology, March, 2004.
Isaac Newton Workshop 2004, Statistical Mechanics of Molecular and Cellular Biological Systems, Cambridge, UK, Spring 2004 (declined, conflict).
Materials Research Society, Proteins as Materials, San Francisco, April 2004 (conflict, declined)
Keystone Symposium, Frontiers in Structural Biology, Snowbird, Utah, April 2004 (conflict, declined)
University of Maryland, College Park, Biochemistry Department, Student-selected speaker, May 2004.
The Role of Theory in Biological Physics and Materials NSF Workshop, Tempe Arizona, May 2004 (declined, conflict)
91st Statistical Mechanics Conference, Rutgers University, May 2004 (declined, conflict)
Dubrovnik 2004 Conference, From Solid State to Biophysics III, Dubrovnik, Croatia, June 2004. (declined, conflict)
Elastin 2004, Third European Symposium, Manchester, UK, June 2004 (declined, conflict)
FASEB Meeting on Folding in the Cell, Vermont, July 2004.
Gordon Research Conference on Water and Aqueous Systems, New Hampshire, August 2004 (declined due to conflict)
Hereditary Disease Foundation Meeting, Panel Member regarding structural properties of poly-glutamine, Boston, MA, August, 2004.
Yale University, MB&B Seminar Series, September 2004.
VIP Scientific Forum of the International Internet, Processing, Systems for e-education/e-business, and Interdisciplinaries -2004 PESCARA Conference, Italy, July 2004 (declined, conflict)
Congress on Tilted Peptides, Namur, Belgium, October 2004.
Sackler Colloquia of the National Academy of Sciences, Frontiers in Bioinformatics: Unsolved Problems and Challenges, Irvine CA, October 2004. Session Chair.
Protein Folding and Misfolding in Alzheimer's Disease, Satellite symposium of the Society for Neuroscience, organized by Elsevier and Neurobiology of Aging, October, 2004 (declined due to conflict)
Karolinska Institute, Huddinge, Sweden, Seminar and external examiner for a dissertation, November, 2004.

2003

American Chemical Society Meeting, March 2003 (conflict, declined).
University of Pennsylvania, April 2003.
University of Arizona, April 2003.
Birthday Symposium for Alan Fersht, Cambridge University, April 2003.

Johns Hopkins University, Spring 2003 (conflict, postponed)
State University of New York, Spring 2003 (conflict, postponed)
19th International Congress of Biochemistry and Molecular Biology, Toronto, Canada, July 2003
(changed to Montreal, October 2003 because of SARS).
DOE Symposium on Protein Folding and Structure Prediction, July 2003 (did not attend)
CECAM Meeting, France, September 2003.
Seoul Korea, September 2003 (declined)
Duke University, November 2003.
New York University, November 2003.
40th Anniversary Symposium of the Chinese University of Hong Kong, Hong Kong, China,
December 2003.

2002

NSF Meeting on Folding, Function and Funnels, Co-sponsored by the US and Japanese National
Science Foundations, Hawaii, January 2002.
Gordon Conference, Protein Dynamics and Folding, Ventura, CA, January 2002.
Program in Mathematics and Molecular Biology, Symposium on Modeling across the Scales-
Atoms to Organisms, Santa Fe, NM, January 2002 (conflict, I had to decline).
Satellite Meeting of the Biophysical Society to honor Peter Kollman, San Francisco, February
2002.
42nd Sanibel Symposium, Saint Augustine, FL, February-March 2002.
Lise Meitner Symposium, University of Lund, Sweden, Sponsored by the Nobel Committee for
Chemistry, Organized in response to media discussions in Sweden regarding the lack of
women laureates, March 2002.
Annual American Chemical Society Meeting, Award Symposium for Tack Kuntz, Computers in
Chemistry Award, Orlando, Florida, April 2002.
Western Washington University, Chemistry Department Seminar Series, Bellingham, WA, April
2002.
University of California, Santa Cruz, April 2002.
CECAM Workshop on Protein Dynamics, Lyon, France, May 2002 (declined, conflict with
teaching).
Hereditary Disease Foundation workshop on Structural Studies of Huntingtin, Dedicated to the
memory of Max Perutz, May, 2002.
Javits Meeting on Prion Diseases, San Francisco, CA, May 2002.
Department of Environment, Food and Rural Affairs, Transmissible Spongiform Encephalopathy
Research Unit, UK, Workshop to discuss BSE and other TSE diagnostics, London,
England, May 2002 (declined, conflict).
Biopolymers Gordon Conference, Rhode Island, June 2002.
FASEB Meeting on Folding in the Cell, Vermont, July 2002.
Center for Biologically Inspired Materials and Materials Systems, Duke University, 2002
(conflict).
Structural Informatics Symposium, Georgia State University, Fall, 2002 (declined, conflict)

2001

ACS Meeting, Symposium on Energy Landscapes of Proteins, Glasses and Clusters, San Diego,
April 2001.
Javits Meeting on Prion Diseases, San Francisco, CA, May 2001.
International Center for Theoretical Physics, Protein Folding, Structure and Design, Trieste, Italy,
June 2001 (conflict, I had to decline).
Proteins Gordon Conference, New Hampshire, June 2001.
Telluride Summer Workshop on Conformational Dynamics in Proteins, August 2001 (conflict, I
had to decline)

Protein Society Meeting, Philadelphia, PA, July 2001.
University of California, Berkeley, Structural Biology Seminar Series, September 2001.
Royal Society Discussion Meeting: New Science from High Performance Computing, London, England, October 2001.
Novartis Foundation Discussion Meeting on Biological Computing, London, England, October 2001.

2000

The Lorne Conference on Protein Structure and Function, Lorne, Australia, Organized by Richard Simpson, February 2000.
Sydney Protein Structure Group, Sydney, Australia, Organized by Brett Church, February 2000.
5th Johns Hopkins Protein Folding Meeting, Coolfont, WV, March 2000.
European Biochemical Society Symposium, From Protein Folding to New Enzymes, Leeds, England, Organized by Sheena Radford and Alan Berry, April 2000.
Ettore Majorana Center International Summer School of Biophysics: Structural Biology, Sicily, Italy, Organized by Vincent Torre and Antonino Cattaneo, May 2000. Meeting cancelled by NATO.
Biopolymers Gordon Conference, Co-organized by Peter Kollman, Rhode Island, June 2000.
Interdisciplinary Workshop on Protein Flexibility and Folding, sponsored by Michigan State University, August 2000.
Martinsrieder Symposium 2000, Munich, Germany, Organized by Wolfgang Baumeister, Ulrich Hartl, the Max Planck Institute, October 2000.
Hereditary Disease Foundation workshop on Structural Studies of Huntingtin, December, 2000.

1999

University of Wisconsin, Madison, Molecular Biophysics Seminar Series, Organized by the Training Grant Students, January 1999.
24th Taniguchi International Symposium, Old and New Views of Protein Folding, Tokyo, Japan, Organized by Kunihiro Kuwajima, March 1999.
Research Development Corporation of Japan, Simulations of Biological Functions--- Computational Biology, Tokyo, Japan, Organized by Nobuhiro Go and Shigeo Ihara, March 1999.
NIH Meeting on Opportunities in Molecular Biomedicine in the Era of Pentaflop Computing, Organized by Klaus Schulten, March 1999. Unable to attend.
University of Illinois, Urbana-Champaign, Theoretical Biophysics Seminar Series, Organized by Klaus Schulten, March 1999.
Tri-institutional Structural Biology Seminar Series, Rockefeller University, Sloan-Kettering Institute and the Weill Medical College of Cornell University, Organized by Andrej Sali, September 1999

1998

European Molecular Biology Organization Workshop: Protein Folding and Misfolding Inside and Outside the Cell, Oxford, U.K., Organized by Chris Dobson, March 1998.
University of Cambridge, Chemistry Department, Two seminars, Organized by Alan Fersht, March 1998.
University of California, San Francisco, Department of Pharmaceutical Chemistry, Organized by Vladimir Basus and Lucy Waskell, June 1998.
University of Iowa, Biochemistry Departmental Seminar Series, Organized by Ken Murphy, October, 1998.
Javits Meeting on Prion Diseases, San Francisco, Organized by Stanley Prusiner, November, 1998.

1997

Johns Hopkins Meeting on Protein Folding, Coolfont, WV, Organized by Bob Matthews, March 1997.

University of California, San Francisco, Organized by Peter Kollman, Biophysics Seminar Series, May 1997.

Javits Meeting on Prion Diseases, San Francisco, Organized by Stanley Prusiner, May 1997.

Annual Meeting of the Protein Society, Boston, Organized by David Eisenberg, July 1997.

Spetsai Summer School on Molecular and Cellular Biology: Biomolecular Recognition, Spetsai, Greece, Organized by Alan Fersht, September, 1997.

1996-1993

Javits Meeting on Prion Diseases, San Francisco, Organized by Stanley Prusiner, April, 1996.

Western Washington University, Chemistry Department Seminar Series, Organized by Mark Bussell, May 1996.

University of Minnesota, Biochemistry Department Seminar Series, Organized by Clare Woodward, June 1996.

NEC Princeton Lectures on Biophysics, Organized by Bill Bialek, June, 1996.

American Chemical Society Meeting: 2 separate talks in the Computers in Chemistry Division. Organized by Alex Tropsha, August 1996, Florida.

University of California, Berkeley, Structural Biology Seminar Series, Chemistry Department and the Department of Cellular and Molecular Biology, Organized by Susan Marqusee, October 1996.

Ohio State University, Physics Department Seminar Series, November 1996.

American Chemical Society Meeting: Invited to give two talks: Physical Chemistry Division and in the Division of Computers in Chemistry, Anaheim, CA, Organized by Laura Lerner and Peter Kollman, April, 1995,

Symposium of the European Network on Protein Folding and Stability, San Feliou, Spain, Organized by Rainer Jaenicke, April, 1995.

Javits Meeting on Prion Diseases, San Francisco, Organized by Stanley Prusiner, May 1995.

Aspen Center for Physics, Workshop on Statistical Mechanics and Protein Structure, Organized by Ron Elber, August 1994.

Fairchild Symposium November, 1994, San Francisco, CA. Symposium on Prion Diseases.

International Society of Biochemists and Biophysicists, Asilomar, Organized by Peter Kollman, December 1993.

OTHER WORK EXPERIENCE/ACTIVITIES

Alumni representative for Reed College Admissions Office (9/85-1993).

Volunteer teacher, Science Education Partnership (1/89-6/90). This was a partnership between scientists at U.C.S.F. and local high school teachers.

Other seasonal employment includes: escorting orphans from Latin America to Scandinavia for the Swedish Center for International Child Welfare; and 3 years as a professional downhill ski instructor. Also, I was in a Warren Miller ski movie, 1980.

PUBLICATIONS

(As of 7/09: 163 publications with 6,623 citations, ~700 citations/yr last 4 yrs, h-index = 47)

V. Daggett, Protein Degradation: The Role of Mixed-Function Oxidases, *Pharmaceutical Research* **4**: 278-284, 1987.

P. Kollman, S. Rao, F. Brown, **V. Daggett**, G. Seibel and U.C. Singh. Free Energy Perturbation Methods Can Give Exciting Insights Into the Effect of Site-Specific Mutants on Both Binding and Catalysis: Applications to Subtilisin, Trypsin and Triose Phosphate Isomerase and the Description of a Free Energy Component Analysis. In *Protein Structure, Folding and Design* **2**, D. Oxender, ed., A. Liss & Co., 215-225, 1987.

- V. Daggett**, P.A. Kollman, and I.D. Kuntz, Molecular Dynamics Simulations of Small Peptides, *Conference Proceedings for the Fourth International Conference on Supercomputing II*: 348-356, 1989.
- V. Daggett**, P.A. Kollman and I.D. Kuntz, Free Energy Perturbation Calculations of Charge Interactions with the Helix Dipole, *Chemica Scripta* **29A**: 205-215, 1989.
- V. Daggett**, F. Brown, and P. Kollman, Free Energy Component Analysis: A Study of the Glu 165 → Asp 165 Mutation in Triose Phosphate Isomerase, *J. Am. Chem. Soc.* **111**: 8247-8256, 1989.
- L.A. Williams, K. Kirshenbaum, **V. Daggett**, C. Sorace, and P.C. Kahn, Two-Dimensional Electrophoresis of Liver Microsomal Proteins from Rats Treated with 2,3,7,8-tetrachloro-dibenzo dioxin, 3-methyl cholanthrene and phenobarbital, *Chemosphere* **18**: 947-954, 1989.
- V. Daggett** and P.A. Kollman, Molecular Dynamics Simulations of Active Site Mutants of Triosephosphate Isomerase, *Protein Engineering* **3**: 677-690, 1990.
- V. Daggett**, P.A. Kollman, and I.D. Kuntz, Molecular Dynamics Simulations of Small Peptides: Dependence on Dielectric Model and pH, *Biopolymers* **31**: 285-304, 1991.
- V. Daggett**, P.A. Kollman, and I.D. Kuntz, A Molecular Dynamics Simulation of Polyalanine: An Analysis of Equilibrium Motions and Helix-Coil Transitions, *Biopolymers* **31**: 1115-1134, 1991.
- P. Kollman, **V. Daggett**, and L. Dang, The Application of Computational Methods to the Study of Enzyme Catalysis by Triose Phosphate Isomerase and Stabilities of variants of Bacteriophage T4 Lysozyme, in *The Ciba Foundation Symposium Series*, Wiley Press, Chichester, **161**: 91-107, 1991.
- S. Schröder, **V. Daggett**, and P.A. Kollman, A Comparison of the AM1 and PM3 Semiempirical Models for Calculation of the Catalytic Properties of the Serine Proteases, *J. Am. Chem. Soc.* **113**: 8922-8925, 1991.
- Daggett V.**, Schröder, S. and P.A. Kollman, The Catalytic Pathway in Trypsin: Classical and Quantum Mechanical Calculations, *J. Am. Chem. Soc.* **113**: 8926-8935, 1991.
- Daggett V.** and M. Levitt, A Molecular Dynamics Simulation of the C-Terminal Fragment of the L7/L12 Ribosomal Protein in Solution, *Chemical Physics*, **158**: 501-512, 1991.
- V. Daggett** and M. Levitt, Molecular Dynamics Simulations of Helix Denaturation, *J. Mol. Biol.*, **223**: 1121-1138, 1992.
- V. Daggett** and M. Levitt, A Model of the Molten Globule State from Molecular Dynamics Simulations, *Proc. Natl. Acad. Sci. USA*, **89**: 5142-5146, 1992.
- V. Daggett** and P.A. Kollman, The Use of Theoretical Methods in Protein Engineering, in *Protein Engineering: A Practical Approach*, A. Rees, M.J. Sternberg, and R. Wetzel, Eds., Oxford University Press, Chapter **6**: 143-163, 1992.
- V. Daggett**, A Model for the Molten Globule State of CTF Generated Using Molecular Dynamics, in *Techniques in Protein Chemistry IV*, R.H. Angeletti, Ed., Academic Press, 525-532, 1993.
- V. Daggett** and M. Levitt, Realistic Simulation of Native Protein Dynamics in Solution and Beyond, *Ann. Rev. of Biophys. and Biomol. Struct.* **22**: 353-380, 1993.
- V. Daggett** and M. Levitt, Protein Unfolding Pathways Explored through Molecular Dynamics Simulations, *J. Mol. Biol.* **232**: 600-619, 1993.
- V. Daggett** and M. Levitt., Protein folding/unfolding dynamics. *Current Opinion in Structural Biology.* **4(2)**: 291-295, 1994.
- A. Li and **V. Daggett**. Characterization of the Transition State of Protein Unfolding Using Molecular Dynamics: Chymotrypsin Inhibitor 2, *Proc. Natl. Acad. Sci. USA*, **91**: 10430-10434, 1994.

- M. Levitt, M. Hirshberg, R. Sharon, and **V. Daggett**, Potential Energy Function and Parameters for Simulations of the Molecular Dynamics of Proteins and Nucleic Acids in Solution, *Computer Physics Commun.* **91**: 215-231, 1995.
- D.O.V. Alonso and **V. Daggett**, Molecular Dynamics Simulations of Protein Unfolding and Limited Refolding: Characterization of Partially Unfolded States of Ubiquitin in Methanol and in Pure Water, *J. Mol. Biol.*, **247**: 501-520, 1995.
- Kirshenbaum, K. and **V. Daggett**, pH Dependent Conformations of the Amyloid β (1-28) Peptide Fragment Explored Using Molecular Dynamics, *Biochemistry*, **34**: 7629-7639, 1995.
- Kirshenbaum, K. and **V. Daggett**, Sequence Effects on the Conformational Properties of the β (1-28) Amyloid Peptide Fragment: Testing a Proposed Mechanism for $\alpha \rightarrow \beta$ Transitions, *Biochemistry*, **34**: 7640-7647, 1995.
- Kazmirski, S., D.O.V. Alonso, F.E. Cohen, S. Prusiner and **V. Daggett**. Theoretical Studies of Sequence Effects on the Conformational Properties of a Fragment of the Prion Protein: Implications for Scrapie Formation. *Chemistry & Biology*, **2**: 305-315, 1995.
- Storch, E. and **V. Daggett**, Molecular Dynamics Simulations of Cytochrome b_5 : Implications for Protein-Protein Recognition, *Biochemistry*, **34**: 9682-9693, 1995.
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Articles about, or including, our research:

The [Dyneomics Project](#), which began running on the supercomputers at NERSC in 2005 with the goal of simulating the unfolding pathways of all known protein folds, it was recently listed as [a major accomplishment in Advanced Scientific Computing Research](#) by the Office of Science, US Department of Energy.

Microsoft released a press release about our work at <http://www.microsoft.com/presspass/press/2008/nov08/11-06AlzHeavensPR.mspx> which was picked up by The New York Times, Forbes, CNBC and others.

A Case Study was done by Microsoft in August of 2008 investigating the data management scheme the group has developed for the Dyneomics Database. Microsoft SQL Server 2005 and OLAP are used to mine over 20 terabytes of simulation data which reside on three servers. (<http://www.microsoft.com/casestudies/casestudy.aspx?casestudyid=4000002488>).

The Washington Research Foundation highlighted the Group's in house molecular dynamics software, *in lucem* molecular mechanics, in their 2007 Annual Report (http://www.wrfseattle.org/2007_Annual_Report.pdf).

Bioinform, one of GenomeWeb's Application-Focus Newsletters: "The integrated informatics news source", featured the Daggett Group's research in an article entitled UW Team Creates High-Performance Workflow To Explore Molecular Dynamics of Proteins by Vivien Marx, July 7, 2008 (http://depts.washington.edu/daglab/downloads/Bioinform_2008.pdf).

Microsoft featured the Group's integration of Windows software in a Case Study in June of 2008 (<http://www.microsoft.com/casestudies/casestudy.aspx?casestudyid=4000002104>). High-performance computing clusters running Windows Compute Cluster Server are used to run the lab's molecular dynamics software with better performance than the optimized Linux version, and Microsoft SQL Server powers the 14-terabyte Dyneomics Database.

The group's application of Microsoft's software was also featured in a Press Release (<http://www.microsoft.com/presspass/press/2008/jun08/06-11HPCResearchPR.msp>).

Bleeding Edge Biotech, a blog hosted by Carnegie Mellon computational biologist Adam Kraut, highlighted the Dynameomics Project in April of 2008 (<http://www.bleedingedgebiotech.com/blog/bioengineering/dynameomics-mass-annotation-of-protein-dynamics/>).

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Department of Energy press release December 22, 2004, "DOE Allocates Massive Supercomputer Resources to Drive Advances in Combustion, Astrophysics and Protein Structure Research", (<http://www.energy.gov/news/1563.htm>)

This press release was followed by approximately 200 secondary articles and announcements in magazines, websites, newspapers, etc. (not listed here)

Nature, "New Role for Pauling's Ribbons" by Christopher Surridge, **430**, 739, 2004.

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IRIS Universe Magazine. "Romancing the Molten Globule" by Grant Ellis, **23**: 58-61, SGI Inc., 1993.

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