

University of California, San Francisco
CURRICULUM VITAE

Name: Andrej Sali, PhD

Position: Professor, Step A/S
Bioengineering & Therapeutic Sciences
School of Pharmacy

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EDUCATION

1983 - 1987	University of Ljubljana, Slovenia	BSC	Chemistry
1987 - 1991	University of London, UK	PhD	Molecular Biophysics

PRINCIPAL POSITIONS HELD

1987 - 1991	Birkbeck College, and Imperial Cancer Research Fund, London, UK. (Mentor: Prof. Thomas L. Blundell, FRS).	PhD student	Crystallography
1991 - 1994	Harvard University, Cambridge, USA. (Mentor: Prof. Martin Karplus).	Postdoctoral Fellow	Chemistry
1995 - 2000	The Rockefeller University	Assistant Professor	
2000 - 2003	The Rockefeller University	Associate Professor	
2003 - present	University of California, San Francisco	Professor	BTS

OTHER POSITIONS HELD CONCURRENTLY

2009 - 2012	California Institute for Quantitative Biosciences (QB3) at UCSF	Director	
2003 - 2015	UCSF	Vice Chair	Department of Bioengineering and Therapeutic Sciences

2003 - present	California Institute for Quantitative Biosciences (QB3)	Faculty Member
2003 - present	UCSF	Faculty Member Pharmaceutical Sciences and Pharmacogenomics Graduate Program
2003 - present	UCSF	Faculty Member Biophysics Graduate Program
2003 - present	UCSF	Faculty Member Bioinformatics and Medical Informatics Graduate Program
2003 - present	UCSF	Faculty Member Chemistry and Chemical Biology Graduate Program
2015 - present	School of Pharmacy, UCSF	Associate Dean for Research

HONORS AND AWARDS

1984	Undergraduate scholarship	J. Stefan Institute, Ljubljana, Slovenia.
1985	British Council Visiting Student	Birkbeck College, London, UK.
1987	British Council Visiting Student	Birkbeck College, London, UK.
1987	Overseas Research Students Award (1987-1990)	Committee of Principals and Vice Chancellors, England.
1987	Scholarship for graduate studies (1987-1988)	Research Council of Slovenia.
1989	Academic Scholarship (1989-1990)	Merck Sharp & Dohm
1991	Postdoctoral Fellow (1991-1994)	Jane Coffin Childs Memorial Fund for Medical Research
1996	Alexandrine and Alexander L. Sinsheimer Scholar (1996-1999)	Alexandrine and Alexander L. Sinsheimer Foundation
1998	Alfred P. Sloan Research Fellow (1998-2000)	Alfred P. Sloan Foundation
2000	Irma T. Hirschl Career Award Scientist (2000-2003)	Irma T. Hirschl Foundation
2007	Zois Award, Science Ambassador	Republic of Slovenia
2014	Fellow	International Society for Computational Biology (ISCB)
2015	Apple Teaching Award	School of Pharmacy, UCSF

2017	Academy Jubilee Professorship	Indian Academy of Sciences
2018	Bijvoet Medal	Utrecht University, Netherlands
2018	Member	National Academy of Sciences, USA

KEYWORDS/AREAS OF INTEREST

Structural biology, computational biology, bioinformatics, proteins, macromolecular complexes, assemblies, macromolecular processes, sequence, structure, function, evolution, modeling of protein structure, prediction of protein function.

We employ the laws of physics and the rules of evolution to develop and apply methods for:

- predicting the structures of proteins;
- determining the structures of macromolecular assemblies;
- annotating the functions of proteins and their assemblies using their structures.

PROFESSIONAL ACTIVITIES

MEMBERSHIPS

1991 - present Protein Society
 1991 - present American Association for the Advancement of Science
 2007 - present Biophysical Society
 2014 - present International Society for Computational Biology

SERVICE TO PROFESSIONAL ORGANIZATIONS

2005 - 2008	Protein Society	Executive Committee
2005 - present	Protein Data Bank	Scientific Advisory Committee
2009 - 2013	PROSPECTS (Proteomics Specification in Time and Space) consortium	Scientific Advisory Committee
2010 - 2010	Keystone Symposia	Scientific Advisory Board (ad hoc)
2011 - 2015	Keystone Symposia	Scientific Advisory Board
2010 - present	Protein Data Bank	Electron Microscopy Validation Task Force (Co-Chair)
2010 - present	Protein Data Bank	Small Angle Scattering Task Force

2014 - present	Protein Data Bank	Hybrid Models Task Force (Co- Chair)
2010 - present	Electron Microscopy Data Bank	Scientific Advisory Committee
2009 - present	PSI Knowledgebase	Working Group on Theoretical Structural Model Validation
2011 - present	Rosetta Commons	Scientific Advisory Board
2017 - 2019	Biophysical Society	Committee member of BPS

SERVICE TO PROFESSIONAL PUBLICATIONS

2003 - present	Editor, Structure.
2004 - present	Editorial Board, PLoS Computational Biology.
2002 - present	Editorial Board, Journal of Computer Aided Molecular Design.
2002 - present	Editorial Board, Molecular and Cellular Proteomics.
2004 - present	Editorial Board, Protein Engineering, Design, and Selection.
2001 - present	Section Head for the Structural Genomics section on BioMed Central
1990 - present	Reviewer for Nature, Science Cell, Proc. Natl. Acad. Sci. USA, Nature Structural and Molecular Biology Nature Genetics, Nature Biotechnology, Structure, Journal of Molecular Biology, Proteins, Protein Engineering, Design, and Selection, Protein Science, Bioinformatics, Nucleic Acids Research, Journal of Biological Chemistry, BMC Structural Biology, Genome Biology, FEBS Letters, Journal of Computer Aided Molecular Design, Biophysical Journal, Biochemical Journal, PLoS Biology, and PLoS Computational Biology.

INVITED PRESENTATIONS - INTERNATIONAL

1999	CERCA CADD Symposium, Montreal, Canada. April 13, 1999.
1999	Data Mining in Crystallography, Erice, Italy. May 15, 1999.
1999	Structural Biology Net, Tallberg, Sweden. June, 1999.
1999	Frontiers in Structural Biology, Indian Institute of Science, Bangalore, India. August 27, 1999.
1999	BRI, Montreal, Canada. November 24, 1999.
1999	University of Toronto, Toronto, Canada. December 9, 1999.

- 2000 Japan Biophysical Society Meeting, Tokyo, Japan. January 17, 2000.
- 2000 Bioinformatics 2000, Elsinore, Denmark. April 28, 2000.
- 2001 University of Zuerich, Zuerich, Switzerland. December 5, 2001.
- 2001 Bioinformatics & Proteomics: From Sequence to Function, Lausanne, Switzerland. December 6, 2001.
- 2001 Structural Genomics and Bioinformatics, Instituto Juan March, Madrid, Spain. March 12-14, 2001.
- 2001 Annual meeting of the Canadian Society for Biochemistry and Molecular and Cellular Biology (CSBMCB), Toronto, Canada. May 31-June 3, 2001.
- 2001 Math/Chem/Comp 2001, Dubrovnik, Croatia. June 25-30, 2001.
- 2001 4th International Conference on Biological Physics, ICBP2001, Kyoto, Japan. July 30-August 3, 2001.
- 2001 4th International Conference on Molecular Structural Biology, ICMSB2001, Vienna, Austria. September 5-9, 2001.
- 2001 Genomics & Proteomics meeting, Barcelona, Spain. October 19, 2001.
- 2002 University of Barcelona, Barcelona, Spain. May 21, 2002.
- 2002 Genomics & Proteomics meeting, Barcelona, Spain. May 22, 2002.
- 2002 Samuel Lunenfeld Research Institute, Toronto, Canada. May 29, 2002.
- 2002 The 19th Congress and General Assembly of the International Union of Crystallography IUCR, Geneva, Switzerland. August 6-15, 2002.
- 2002 Genomics and Bioinformatics Center Inaugural Symposium, Pontificia Universidad Catolica, Santiago, Chile. November 18-20, 2002.
- 2003 Fourteenth Annual World Molecular Engineering Network (WMEN) Conference, San Jose del Cabo, Baja California Sur, Mexico. May 4-8, 2003.
- 2003 5th Meeting of the Slovenian Biochemical Society, Ljubljana, Slovenia. September 24-28, 2003.
- 2004 University of Cologne, Cologne, Germany. January 19, 2004.

- 2004 Ringberg meeting, Schloss Ringberg, Germany. January 21-23, 2004.
- 2004 Fourteenth Annual World Molecular Engineering Network (WMEN) Conference (2004), San Jose del Cabo, Baja California Sur, Mexico. May 2-6, 2004.
- 2004 EMBO conference on Structures in Biology, EMBL, Heidelberg, Germany. November 10-13, 2004.
- 2005 The 7th World Congress of the World Association of Theoretically Oriented Chemists (WATOC), Capetown, South Africa. January 16-21, 2005.
- 2005 Keynote Speaker in XX IUCr Congress in Firenze, Italy. August 23-31, 2005.
- 2005 Speaker at the International Workshop M2CELL, The Royal Abbey of Fontevraud, Paris, France. December 4-6, 2005.
- 2006 Organizer and Speaker at the World Molecular Engineering Network Conference. Cabo San Lucas, Mexico. April 30-May 2nd, 2006.
- 2006 Plenary Speaker at the 11th Symposium on Recent Advances in Biophysics, National Taiwan University, Taipei, Taiwan. May 23-26, 2006
- 2006 2006 Keystone Symposium on Multi-Protein Complexes Involved in Cell Regulation, St. John's College, Cambridge, UK. August 18-23, 2006.
- 2007 Organizer and Speaker at the World Molecular Engineering Network Conference. Cabo San Lucas, Mexico. April 29-May 2nd, 2007.
- 2007 Protein Complexes and Protein Networks Symposium in Martinsried, Germany, May 21-22, 2007.
- 2007 Symposium on Structural Biology and its Application to Drug Development at the University of Tokyo, Tokyo, Japan, 28 January 2007.
- 2008 Invited Speaker at the Basel Computational Biology Conference [BC]2 , Basel, Switzerland, March 13-14, 2008.
- 2008 Organizer and Speaker of the World Molecular Engineering Network Conferenc. Cabo San Lucas, Mexico. May 4-8, 2008.
- 2008 University of Toronto, Canada, 26 July, 2008.
- 2008 Speaker at the 40th Course: From Molecules to Medicines Integrating Crystallography in Drug Discovery, Erice, Italy. May 29 - June 8, 2008.

- 2008 Speaker at the Gordon Research Conference on Macromolecular Organization & Cell Function: Systems Cell Biology, Oxford, England, July 27 to August 2, 2008.
- 2008 Speaker at the 6th National NCCR Symposium on New Trends in Structural Biology, Zurich, Switzerland, September 8-9 2008.
- 2008 Speaker at the Max Planck Institute, Student Workshop, Goettingen, Germany. September 10-13 2008.
- 2008 Speaker at the Max Planck Institute of Biochemistry, INSTRUCT Open Meeting, in Martinsried, Germany, October 16-17 2008.
- 2009 Speaker at the NoE 3DEM final Meeting, Brdo, Slovenia, February 9-13, 2009.
- 2009 McDowell Lecture at the University of British Columbia, Vancouver, BC, Canada, March 10, 2009.
- 2009 Seminar at the University of Ljubljana, Ljubljana, Slovenia, December 17, 2009.
- 2010 Organizer and Speaker at the 20th World Molecular Engineering Network Conference, Cabo San Lucas, Mexico, May 2-5, 2010.
- 2010 Speaker at the Institute of Structural Molecular Biology, Birkbeck Institute, London, England, June 17-18, 2010
- 2010 Speaker at the MPIMP Dahlem Colloquia in Molecular Genetics, Max Planck Institute, Berlin, Germany, August 22-24, 2010.
- 2010 Speaker at Exeter College, Oxford University, England, October 4, 2010.
- 2010 Speaker at the PROteomics SPECification in Time and Space - PROSPECTS Meeting, Taormina, Sicily, Italy, November 2-4, 2010.
- 2010 Speaker at the 6th International Conference on Structural Biology and Functional Genomics, National University of Singapore, Singapore, December 6-8, 2010.
- 2011 Organizer and Speaker at the 21st World Molecular Engineering Network Conference, Cabo San Lucas, Mexico, May 1-4, 2011.
- 2011 Speaker at the International Conference on Structural Genomics, University of Toronto, Toronto, Ontario, Canada, May 10-14, 2011.
- 2011 Speaker at IGBMC, Strasbourg, France, July 17-18, 2011.

- 2011 Speaker at Max Planck Institute, Munich, Germany, July 20-21, 2011.
- 2011 Plenary Speaker at the ComBio 2011, Cairns Convention Centre, Cairns, Australia, September 26-29, 2011.
- 2012 Plenary Speaker at the Molecular Modeling Meeting, Queenstown, New Zealand, August 30-September 1, 2012.
- 2013 Speaker at the Swiss Federal Institute of Technology, Lausanne, Switzerland, January 14, 2013.
- 2013 Speaker at the Biozentrum Lecture, Basel, Switzerland, January 15, 2013.
- 2013 Organizer and Speaker at the 23rd World Molecular Engineering Network Conference, Cabo San Lucas, Mexico, May 5-8, 2013.
- 2013 Speaker at the Bioinformatics Meeting, Recife, Brazil, November 3-7, 2013.
- 2014 Speaker at the Lorne Conference, Victoria, Australia, February 9-13, 2014.
- 2014 Speaker at Shanghai Tech University, Shanghai, China, March 14-18, 2014
- 2014 Organizer and Speaker at the 24th World Molecular Engineering Network Conference, Cabo San Lucas, Mexico, May 4-7, 2014
- 2014 Keynote Speaker at the Emerging Trends in Computational Biology Conference, Singapore, June 20-21, 2014
- 2014 Speaker at the PDB Hybrid Methods Task Force Meeting, EMBL-EBI, Hinxton, UK, October 6-7, 2014
- 2015 Seminar at A*Star BII, Singapore, March 12-14, 2015
- 2015 Organizer and Speaker at the 25th World Molecular Engineering Network Conference, Cabo San Lucas, Mexico, May 3-6, 2015
- 2015 Speaker at the GRC on Computational Aspects of Biomolecular NMR, Il Ciocco, Italy, June 7-12, 2015
- 2015 Speaker at the 29th Annual Symposium of the Protein Society, Barcelona, Spain, July 22-25, 2015
- 2015 Seminar at Pasteur Institute, Paris, June 24, 2015
- 2015 Speaker at iHuman Institute, Shanghai Tech University, Shanghai, China, July 27-31, 2015

- 2015 Keynote Speaker at the FEBS3+ Meeting "Molecules of Life", Portoroz, Slovenia, September 16-19, 2015.
- 2015 Speaker at the Hybrid Methods Meeting, Osaka, Japan, October 2-4, 2015
- 2015 Speaker at the Advances in Integrative Biology of Cellular Processes, Shanghai, China, November 10-12, 2015.
- 2016 Speaker at the Graduate School of Quantitative Biosciences Munich (QBM), Munich, Germany, January 11, 2016.
- 2016 Speaker at the EMBL Distinguished Lecture Series, Heidelberg, Germany, January 12, 2016.
- 2016 Organizer and Speaker at the 26th World Molecular Engineering Network Conference, Cabo San Lucas, Mexico, May 7-10, 2016.
- 2016 Speaker at the ETH Zurich Department of Biology Symposium, Zurich, Switzerland, June 13-15, 2016.
- 2016 Speaker at the Max F. Perutz Laboratories, The IMP, Vienna, Austria, June 28-29, 2016.
- 2017 Speaker at the Bioimaging Data Repositories Workshop, EMBL-EBI, Hinxton, UK, Jan 23-24, 2017.
- 2017 Speaker at the Frontiers of NMR in Life Sciences, Keystone, CO, March 12-17, 2017.
- 2017 Organizer and Speaker at the 27th World Molecular Engineering Network Conference, Cabo San Lucas, Mexico, May 6-9, 2017.
- 2017 Seminar at the Sophia College for Women, Mumbai, Jul 24, 2017.
- 2017 Seminar at the Tata Institute for Fundamental Research, Mumbai, Jul 24, 2017.
- 2017 Seminar at the Dept. of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad, Jul 26, 2017.
- 2017 Seminar at the Ahmednagar College, Ahmednagar, Jul 28, 2017.
- 2017 Seminar at the Indian Institute of Science Education and Research, Pune, Jul 31, 2017.
- 2017 Seminar at the Institute of Bioinformatics and Biotechnology, Pune University, Pune, Aug 1, 2017.
- 2017 Seminar at the National Center for Biological Sciences, Bangalore, Aug 2, 2017.

- 2017 Seminar at the Indian Institute of Sciences, Bangalore, Aug 3, 2017.
- 2017 Seminar at the Mysore College, Mysore, Aug 4, 2017.
- 2017 Seminar at the Molecular Biophysics Unit, Indian Institute of Sciences, Bangalore, Aug 7, 2017.
- 2017 Speaker at the Conformational ensembles from experimental data and computer simulations, Biophysical Society, Berlin, Germany, Aug 25-29, 2017.
- 2017 Speaker at the QBI 2017 Cell Mapping Symposium, UCSF, San Francisco, CA, Sep 13-14, 2017.
- 2017 Speaker at the iHuman Institute at ShanghaiTech Symposium, Shanghai, China, Nov 7-8, 2017.
- 2017 Speaker at the EMBL/EMBO Symposium: From Single- to Multiomics: Applications and Challenges Data Integration, Heidelberg, Germany, November 12-14, 2017.
- 2017 Speaker at the Revolutions in Structural Biology: Celebrating the 100th anniversary of Sir John Kendrew, EMBL, Heidelberg, Germany, Nov 16-17, 2017.
- 2018 Speaker at the 3rd DNA Replication and Repair Structures & Cancer Conference, Cancun, Mexico, Feb 11-15, 2018.
- 2018 Keynote Speaker at the 2018 Annual Symposium of the Bijvoet Center of Biomolecular Research, Utrecht, Netherlands, Apr 23-24, 2018.
- 2018 Organizer and Speaker at the 28th World Molecular Engineering Network Conference, Cabo San Lucas, Mexico, May 5-8, 2018.

INVITED PRESENTATIONS - NATIONAL

- 1999 Second International Georgia Tech Conference in Bioinformatics, Atlanta, Georgia, USA. November 12, 1999.
- 1999 2.Structural Genomics Targets Workshop, NIH, Washington DC, USA. February 11, 1999.
- 1999 Advances & Opportunities at the Biology/Math/Computational/Physical Sciences Interface, Rutgers University, New Brunswick, NJ, USA. March 6, 1999.
- 1999 Mount Sinai School of Medicine, New York, NY, USA. March 19, 1999.
- 1999 New York Structural Biology Group, New York Academy of Sciences, New York, NY, USA. March 24, 1999.

- 1999 Columbia University, New York, NY, USA, 1999.
- 1999 Chemistry Dept., New York University, New York, NY, USA, 1999.
- 1999 Protein Sequence Structure Function Meeting, UCSF, San Francisco, CA, USA. April 23, 1999.
- 1999 The Scripps Institute, La Jolla, CA, USA. August 13, 1999.
- 1999 Mathematical Problems in the Molecular Sciences, Courant Institute, New York, NY, USA. October 10, 1999.
- 1999 City College of New York, New York, USA. October 20, 1999.
- 1999 Agouron Pharmaceuticals, San Diego, California, USA. October 28, 1999.
- 1999 Structural Genomics Conference, ANL, Chicago, Illinois, USA. November 16, 1999.
- 1999 Structural Genomics and the Pharmaceutical Industry, Princeton, New Jersey, USA. November 18, 1999.
- 2000 Quantitative Challenges in the Post Genomic Sequence Era, La Jolla Interfaces in Science, San Diego, California, USA. January 12, 2000.
- 2000 UCSD, Dept of Physics, San Diego, California, USA. January 19, 2000
- 2000 UCSF, San Francisco, California, USA. January 20, 2000.
- 2000 Center for Physics and Biology, Rockefeller University, New York, New York, USA. January 24, 2000.
- 2000 Biological Chemistry Seminar Series, University of Penn, Philadelphia, Pennsylvania, USA. February 17, 2000.
- 2000 ABRF 2000 "From Singular to Global Analyses of Biological Systems", Bellevue, Washington, USA. February 22, 2000.
- 2000 AAAS conference, Washington DC, USA. March 20, 2000.
- 2000 Keystone Symposium on Macromolecular Assemblies at Work: Application of Physics, Chemistry, and Mathematics to Biology, Durango, Colorado, USA. March 25, 2000.
- 2000 Bio2000, Boston, Massachusetts, USA. March 28, 2000
- 2000 Computational Challenges of the Post Genomic Age, SUN, San Francisco, California, USA. May 12, 2000.
- 2000 Biopolymers Gordon Conference, Newport, Rhode Island, USA. June 18-22, 2000.

- 2000 2000 FASEB Summer Research Conference on Protein Folding in the Cell, Saxton River, Vermont, USA. July 22-27, 2000.
- 2000 Monsanto/Pharmacia lectureship series, Univ. of Saint Louis, Missouri, USA. September 28, 2000.
- 2000 Workshop on Structural Genomics. NIGMS, Washington DC, USA. October 23, 2000.
- 2000 Genomics and Bioinformatics, UMD, New Brunswick, New Jersey, USA. November 2, 2000.
- 2000 University of Minnesota, Minneapolis, Minnesota, USA. November 27, 2000.
- 2001 Oncogenomics: Dissecting Cancer Through Genome Research, Nature Genetics, Tuscon, Arizona, USA. January 25-27, 2001.
- 2001 UAB, Birmingham, Alabama, USA. February 26, 2001.
- 2001 Bard College, New York, USA. April 18, 2001.
- 2001 Physics/Chemistry. CSUN, Northridge, California, USA. May 2, 2001.
- 2001 ACS Meeting, Chicago, Illinois, USA. August 26-30, 2001.
- 2001 University of Maryland, Maryland, USA. October 2, 2001.
- 2001 Columbia University, New York, New York, USA. October 15, 2001.
- 2001 Mast Cell Workshop, Bethesda, Maryland, USA. November 26-30, 2001.
- 2002 Genomics Seminar Series, Skirball Institute, New York, New York, USA. February 6, 2002.
- 2002 Mining the Human Genome for New Drug Discovery - New Ways of Handling Orphan Targets. NYAS, New York, New York, USA. February 26, 2002.
- 2002 Biological Processes for New and Innovative Engineering Systems and Applications, ARO workshop, Research Triangle Park, North Carolina, USA. February 26-27, 2002.
- 2002 New York City Blood Centre, New York, New York, USA. March 7, 2002.
- 2002 Proteomics - The New Frontiers: Discovery, Separation, Prediction & Modeling, University of Delaware, Newark, Delaware, USA. March 14-15, 2002.

- 2002 Harvard University, Cambridge, Massachusetts, USA, March 28, 2002.
- 2002 Molecular Cell Biology and Biochemistry Seminar Series, Virginia Tech, Blacksburg, Virginia, USA. April 5, 2002.
- 2002 UCSF, San Francisco, California, USA, April 15, 2002.
- 2002 A Workshop on large biological structures, Asilomar, California, USA. April 20-22, 2002.
- 2002 SCBMB Program, Baylor College of Medicine, Houston, Texas, USA. May 15, 2002.
- 2002 50th ASMS conference American Society of Mass Spectrometry, Orlando, Florida, USA. June 2-6, 2002.
- 2002 The 5th Summer Session of the New York Structural Biology Discussion Group , Cold Spring Harbor Laboratory, New York, USA. June 26, 2002
- 2002 Berkeley-Stanford summer school for protein crystallography, SSRL, Stanford, California, USA. July 8-12, 2002.
- 2002 Gordon Conference on Diffraction Methods in Structural Biology, Connecticut College, New London, Connecticut, USA. July 14-19, 2002.
- 2002 NYCBS New York Computational Biology Society seminar, NAS, New York, New York, USA. September 18, 2002.
- 2002 Center for Biological Modeling, Michigan State University, East Lansing, Michigan, USA. September 27, 2002.
- 2002 Bioinformatics seminar, Texas A&M University, Tamu, TX, USA. November 7, 2002.
- 2002 Structure and Function of the Proteome, Argonne National Laboratory, Argonne, Illinois, USA. November 23-24, 2002.
- 2003 Keystone Symposium in Proteomics: Technologies and Applications, Keystone Resort in Keystone, Colorado, USA. March 25-30, 2003.
- 2003 NCCR sponsored Workshop on Structural Proteomics of Complexes, Bethesda, Maryland, USA. April 7-8, 2003.
- 2003 American Society for Biochemistry and Molecular Biology meeting, San Diego, California, USA. April 11-15, 2003.
- 2003 St. Jude Children's Research Hospital, Memphis, TN, USA. April 22, 2003.
- 2003 Genentech, Inc., South San Francisco, CA, USA. April 29, 2003.

- 2003 Structure and Function of Proteome, SBC, Argonne National Laboratory, Argonne, Illinois, USA. Spring, 2003.
- 2003 "Frontiers of Bioinformatics" symposium, Center of Excellence in Bioinformatics, University at Buffalo, Buffalo, New York, USA. June 6-8, 2003.
- 2003 IBM Thomas J. Watson Research Center, New York, New York, USA. June 11, 2003.
- 2003 2003 Gordon Research Conference on 3D Electron Microscopy of Macromolecules, Colby Sawyer College, New London, New Hampshire, USA. June 22-26, 2003.
- 2003 PSI workshop on data management, NIH Campus, Bethesda, MD, USA. July 10-11, 2003.
- 2003 GTL and Beyond: Data and Computational Needs Workshop, San Francisco, CA, USA. September 10-11, 2003.
- 2003 2003 Pharmaceutical Sciences and Pharmacogenomics Retreat, Marshall, CA, USA. September 11-13, 2003.
- 2003 Structure and Chemistry Seminar at Scripps, San Diego, CA, USA. September 18, 2003.
- 2003 Seminar at Northeastern University, Boston, MA, USA. October 6, 2003
- 2003 Workshop on Visualization of Biological Complexes, Four Points Sheraton Hotel, Emeryville, San Francisco Bay Bridge, CA, USA. October 11-12, 2003
- 2003 Seminar at PARC, Palo Alto, CA, USA. October 15, 2003.
- 2003 NIGMS Homology Modeling Workshop, Bethesda, MD, USA. October 21-22, 2003.
- 2003 Seminar at Purdue University, West Lafayette, IN, USA. October 24-25, 2003.
- 2003 PSI Target Selection Workshop, Bethesda, MD, USA. November 13-14, 2003.
- 2003 Biophysics/CCB Retreat, Asilomar Conference Center, Pacific Grove, CA, USA. December 7-9, 2003.
- 2004 Licensing Executives Society meeting, San Francisco, CA, USA. February 12, 2004
- 2004 The Structural, Functional and Evolutionary Gordon Conference, Four Points Sheraton Harbortown, Ventura, CA, USA. February 15-20, 2004.
- 2004 Seminar at Berkeley, Berkeley, CA, USA. March 8, 2004.

- 2004 Seminar at UCSC, Santa Cruz, CA, USA. March 11, 2004.
- 2004 Workshop on Structure Determination of Macromolecular Machines and Assemblies by Hybrid Methods, Granlibakken/Lake Tahoe Conference Center, CA, USA. March 17-20, 2004.
- 2004 Workshop on Structural Determination of Environmentally Responsive Gene (ERG) Products for Diagnostics & Drug Discovery (NIEHS/DERT), Snowbird Resort, Snowbird, Utah, USA April 12-13, 2004.
- 2004 2004 Keystone Symposium on Structural Genomics, Snowbird Resort, Snowbird, Utah, USA April 13-19, 2004.
- 2004 BayGenomics PGA, San Francisco, CA, USA. April 27, 2004.
- 2004 Gladstone Scientific Retreat, Asilomar in Monterey County, CA, USA. May 18-20. 2004.
- 2004 Seminar at Caltech, Pasadena, CA, USA. October 12, 2004.
- 2004 ICSG 2004 Meeting, Washington, DC, USA. November 17-24, 2004.
- 2004 Workshop of the Center of Protein Folding Machinery, Stanford University, CA, USA. December 4-5, 2004.
- 2004 Biological and Medical Informatics/Biophysics/Chemistry and Chemical Biology graduate groups retreat, Asilomar Conference Center, Pacific Grove, CA, USA. December 5-7, 2004.
- 2005 ABRF meeting, Biomolecular Technologies:Discovery to Hypothesis, Savannah, Georgia, USA. February 5-8, 2005.
- 2005 Frontiers in Computational Biophysics Symposium, NIH campus in Bethesda, MD, USA. April 29-30, 2005.
- 2005 NIH Symposium on Structural Analysis of Large Assemblies: Sizing up the Challenges, NIH campus in Bethesda, MD, USA. June 2-3, 2005.
- 2005 SRI's Computational Biology series, SRI International, Menlo Park, CA, USA. June 29, 2005.
- 2005 19th Annual Symposium of the Protein Society, Boston, MA, USA. July 30 – August 3, 2005.
- 2005 GRC 2005 Computer-aided design meeting, Tilton School, NH, USA. July 31 – August 5, 2005.
- 2005 Seminar at the Biochemical and Biophysical Methods Course Fall 2005, The Rockefeller University, New York, NY, USA. October 11, 2005.

- 2005 Seminar at the Novartis Institutes for BioMedical Research, Cambridge, MA, USA. November 9, 2005.
- 2005 Workshop on Biological Macromolecular Structure Models, The State University of New Jersey, Piscataway, NJ, USA. November 19-20, 2005.
- 2006 Organizer and Speaker of the Theme "Macromolecular Structure and Dynamics" with 4 Symposia. ASBMB 2006 meeting, San Francisco, CA, USA. April 1-5, 2006.
- 2006 Seminar at UC Davis, CA. June 1, 2006.
- 2006 Symposium at Wyeth Research, Cambridge, MA, USA. October 16, 2006.
- 2006 Seminar at the University of Massachusetts, Dept. of Biochemistry and Molecular Pharmacology, Worcester, MA, USA. October 18, 2006.
- 2006 Seminar at the Fifth Annual Systems Biology Course at the Institute for Systems Biology, Seattle, WA, USA. 9 November 2006.
- 2006 Seminar at UC Merced Center for Computational Biology, Merced, CA, USA. 30 November 2006.
- 2006 TDR/WHO Drug Target Selection Meeting in Seattle, OR, USA. 1 December, 2006.
- 2006 Biological and Medical Informatics/Biophysics/Chemistry and Chemical Biology Graduate Groups Retreat, Monterey, CA, USA. 3-5 December, 2006.
- 2007 Collaborative Drug Discovery meeting, UCSF, San Francisco, USA. 1 March 2007
- 2007 The Protein Folding Center Annual Retreat, Stanford, CA, USA. 27-29 May 2007.
- 2007 Seminar at the Center for Theoretical Biological Physics. UCSD, San Diego USA. 1 June, 2007.
- 2007 Institute for Systems Biology, Seattle, WA, 12 July 2007.
- 2007 Seminar at Genentech, San Francisco, CA, 25 September 2007.
- 2007 Seminar at the SCRIPPS Institute, La Jolla, CA, USA. September 27-28
- 2007 Speaker and Organizer of the Modeling of Protein Interactions Meeting, MPI-2007, Lawrence, KA, USA, September 30 – October 2, 2007.

- 2007 Seminar at the Albert Einstein College of Medicine, New-York, NY. 16 October 2007.
- 2007 Seminar at University of California Berkeley, New-York, NY. 25 October 2007.
- 2007 Seminar at the Carolina Center for Genomic Sciences colloquium, UNC, Chapel Hill, NC, USA. 9 November 2007.
- 2007 Seminar at the Duke University Computational Biology Series, Durham, NC, USA. 12 November 2007.
- 2008 Keystone Symposium on Structural Genomics and Its Applications to Chemistry, Biology and Medicine, Steamboat Springs, Colorado, CO, USA, 6-11 January 2008.
- 2008 Seminar for the Biochemical and Biophysical Methods Course at the Rockefeller University, New York, NY. 30 January 2008
- 2008 Seminar at the University of Utah, February 25 2008.
- 2008 Seminar at The Buck Institute for Age Research, Novato, CA, USA, July 1 2008.
- 2008 Speaker and Organizer of the Protein Modeling Workshop, University of California, San Francisco, CA, USA, July 11-12 2008.
- 2008 Speaker at the 2008 Senior Vice Chancellor's Laureate Lecture Series at the University of Pittsburgh, July 18 2008.
- 2008 Protein Structure Initiative (PSI3), Washington DC, USA, October 29-30, 2008.
- 2008 Seminar at UT Southwestern Medical Center, 5-6 Nov 2008.
- 2008 Biology and Mathematics in the Bay Area (BaMBA), University of California, Davis, CA, USA, November 15, 2008.
- 2008 Biological and Medical Informatics/Biophysics/Chemistry and Chemical Biology Graduate Groups Retreat, Monterey, CA, USA. 7-9 December, 2008.
- 2008 NCMI Single Particle Reconstruction Workshop, Baylor College of Medicine, Houston, TX, USA, December 10-13, 2008.
- 2009 Seminar at the University of Pennsylvania School of Medicine, Philadelphia, PA, USA, January 29, 2009.
- 2009 Mesilla Chemistry Workshop Multi-Scale Modeling of Biological Molecules, Mesilla, TX, USA, February 1-4, 2009.
- 2009 Technology Centers for Networks and Pathways Annual All Hands Meeting, Washington DC, USA, March 12-13, 2009

- 2009 2009 Symposium on Molecular Systems Biology of the Cell, Seattle, WA, USA, April 19, 2009.
- 2009 Seminar at the University of Minnesota, Minneapolis, MN, USA, April 22, 2009.
- 2009 Seminar at the University of Washington, Seattle, WA, USA, May 14, 2009.
- 2009 Seminar at Indiana University, Indianapolis, IN, USA, May 18, 2009.
- 2009 Seminar at University of Texas Southwestern, Dallas, TX, USA, May 20-21, 2009.
- 2009 23rd Annual Symposium of the Protein Society, Boston, MA, USA, July 25-29, 2009.
- 2009 Speaker at the Pharmaceutical Sciences and Pharmacogenomics Retreat, Tomales Bay, CA, USA, September 9-10, 2009.
- 2009 Beckman Institute 20th Anniversary Symposium, University of Illinois at Urbana-Champaign, Urbana, IL, USA, September 20-23, 2009.
- 2009 Seminar at University of Southern California, Los Angeles, CA, USA, November 19, 2009.
- 2009 Speaker at the Annual Computational and Theoretical Biology Symposium, Houston, TX, USA, December 4-6, 2009.
- 2010 Speaker and Co-Organizer of the Keystone Symposia on Structural Biology/Structural Genomics, Steamboat Springs, CO, USA, January 8-13, 2010.
- 2010 Speaker at the Modeling of Cryo-EM Map Workshop, Baylor College of Medicine, Houston, TX, USA, January 14-17, 2010.
- 2010 Chair and Speaker at the Biophysical Society 54th Annual Meeting, San Francisco, CA, USA, February 20-24, 2010.
- 2010 Speaker at the Hybrid Methods Symposium, Lake Tahoe, CA, USA, March 10-14, 2010.
- 2010 Speaker at the Structural Biology Symposium, Case Western Reserve University, Cleveland, OH, USA, May 19, 2010.
- 2010 Keynote Speaker at the 3Dsig Satellite Meeting, Boston, MA, USA, July 9-10, 2010.
- 2010 Speaker at the 18th International Conference on Intelligent Systems for Molecular Biology (ISMB 2010), Boston, MA, USA, July 11-13, 2010.

- 2010 Seminar at Vanderbilt University, Nashville, TN, USA, October 12, 2010.
- 2010 Seminar at Ohio State University, Columbus, OH, USA, October 26, 2010.
- 2010 Speaker at the MPI Meeting, University of Kansas, Lawrence, KS, USA, October 28-30, 2010.
- 2010 Seminar at the University of California, San Diego, CA, USA, December 12, 2010.
- 2011 Speaker at the Design of Drugs and Chemicals that Influence Biology Workshop, University of California, Los Angeles, CA, USA, April 4-8, 2011.
- 2011 Keynote Speaker at the Sanford-Burnham Structural Systems Biology Symposium, La Jolla, CA, USA, June 7, 2011.
- 2011 Speaker at the Institute for Systems Biology Symposium and Workshop, University of Washington, Seattle, WA, USA, July 24-27, 2011.
- 2011 Speaker at the Accelerating Predictive Drug Development Through Quantitative Pharmacology Symposium University of California, San Francisco, California, USA, September 22-23, 2011.
- 2011 Speaker at the Worldwide Protein Data Bank (wwPDB) Symposium, Cold Spring Harbor, NY, USA, October 28-30, 2011.
- 2011 Seminar at St. Jude Children's Research Hospital, Memphis, TN, USA, November 15, 2011.
- 2011 Seminar at Duke University, Durham, NC, USA, November 18, 2011.
- 2012 Speaker and Co-organizer of the Keystone Symposia on High Throughput and Hybrid Approaches to Structural Biology, Keystone, CO, USA, January 22-27, 2012.
- 2012 Speaker at Eli Lilly Symposium, Indianapolis, IN, USA, February 13-14, 2012.
- 2012 Seminar at the University of Michigan, Ann Arbor, MI, USA, February 15, 2012.
- 2012 Seminar at the Scripps Research Institute, San Diego, CA, USA, March 1-2, 2012.
- 2012 Co-organizer of the 6th International Conference on Structural Analysis of Supramolecular Assemblies by Hybrid Methods, Lake Tahoe, CA, USA, March 14-18, 2012.

- 2012 Keynote Speaker at the ISMB, Long Beach, CA, USA, July 14-17, 2012.
- 2012 Speaker at the NRAMM Workshop, Scripps Research Institute, San Diego, CA, USA, November 16, 2012.
- 2013 Seminar at NIH, Bethesda, MD, USA, January 17, 2013.
- 2013 Speaker at the Herron Lecture, Florida State University, Tallahassee, FL, USA, February 15, 2013.
- 2013 Speaker at the Hauptman-Woodward Medical Research Institute, Buffalo, NY, USA, March 28, 2013.
- 2014 Seminar at Harvard University, Cambridge, MA, USA, February 3, 2014
- 2014 Seminar at Columbia University, New York, NY, USA, February 5, 2014
- 2014 Seminar at the Scripps Research Institute, San Diego, CA, USA, February 24-25, 2014
- 2014 Seminar at UC Berkeley, Berkeley, CA, USA, March 10, 2014
- 2014 Keynote Speaker at the 2014 Biopolymers Gordon Research Conference, Newport, RI, USA, June 1-6, 2014
- 2014 Keynote Speaker at the 2014 Annual RosettaCon, Leavenworth, WA, USA, July 30 - August 1, 2014
- 2014 Speaker at the Peter Wright Symposium, University of California, San Francisco, CA, USA, September 15, 2014
- 2014 Speaker at the NCI Workshop at the Houston Methodist Research Institute at Texas Medical Center, Houston, TX, USA, September 18-19, 2014
- 2014 Organizer of the Martin Karplus Celebration Symposium, San Francisco, CA, USA, October 1, 2014
- 2014 Speaker at the International Society for the Study of Xenobiotics meeting, San Francisco, CA, USA, October 19-23, 2014
- 2014 Seminar at Rutgers University, New Brunswick, NJ, USA, October 29, 2014
- 2015 Seminar and Biophysics Course at the Scripps Research Institute, San Diego, CA, USA, February 26-27, 2015
- 2015 Speaker at the U.S. Human Proteome Organization (US-HUPO) Annual Meeting, Tempe, AZ, USA, March 15-18, 2015
- 2015 Speaker at the American Chemical Society National Meeting, Denver, CO, USA, March 22-26, 2015

- 2015 Seminar at the University of Florida, Gainesville, FL, USA, April 14, 2015
- 2015 Seminar at the Oregon Health and Science University, Portland, OR, USA, May 19, 2015
- 2015 Seminar at Department of Chemistry and Biochemistry, UCSD, San Diego, November 2-3, 2015.
- 2016 Speaker at the 2016 ASBMB Annual Meeting, San Diego, USA, April 6, 2016.
- 2016 Speaker at the 5th International Symposium on Higher Order Structure of Protein Therapeutics, Long Beach, USA, April 12, 2016.
- 2016 Organizer and Speaker at the Computational Biophysics Workshop, San Francisco Dec 12-16, 2016.
- 2017 Speaker at the QBI 2017 Cell Mapping Symposium, UCSF, San Francisco, CA, Sep 13-14, 2017.
- 2017 Seminar at the Rockefeller University, New York City, NY, Oct 24, 2017
- 2018 Speaker at the 2018 Keystone Symposia on Cryo-EM from Cells to Molecules: Multi-Scale Visualization of Biological Systems, Granlibakken, CA, Feb 4-9, 2018.
- 2019 Organizer of the 63rd Annual Meeting of the Biophysical Society, Baltimore, MD, Mar 2-6, 2019.

GOVERNMENT AND OTHER PROFESSIONAL SERVICE

- | | | |
|----------------|----------------------------------|--|
| 2004 - 2009 | National Institutes of Health | MSF-B Study
Section (successor
of BBICA) |
| 1995 - present | NIH, National Science Foundation | ad hoc Grant
Reviews |
| - | DOE, European Community | |
| - | Burroughs Welcome Fund | |
| - | Binational Science Foundation | |

UNIVERSITY AND PUBLIC SERVICE

SERVICE ACTIVITIES SUMMARY

I serve on a large number of committees at UCSF, as detailed on the cv; these include graduate program leadership, technical infrastructure, and faculty search committees. In addition, I am engaged in public service, for example as an editor of several scientific journals,

a reviewer for a number of funding agencies, and an advisor for a number of scientific initiatives, as outlined above.

UCSF CAMPUSWIDE

2003 - present	Ad hoc Faculty reviews (~30)
2003 - 2003	Future of Computing at UCSF Committee
2003 - 2007	MD/PhD Scientist in QB3 Search Committee
2003 - 2005	Byers Hall (QB3) Building Committee
2003 - 2005	Pharmaceutical Sciences and Pharmacogenomics Graduate Program Admissions Committee
2003 - present	Bioinformatics and Medical Informatics Graduate Program Executive Committee
2003 - 2004	Bioinformatics and Medical Informatics Graduate Program Admissions Committee
2003 - 2004	Biophysics Graduate Program Admissions Committee
2005 - present	iPQB Curriculum committee
2005 - present	iPQB Executive Committee
2005 - 2009	iPQB Admissions Committee
2004 - 2004	Chancellor's Council committee
2004 - 2004	Academic Information Technology Coordinator search committee
2004 - present	QB3 Executive Committee
2005 - 2008	Basic Sciences Research Resources Oversight Committee
2005 - 2011	Rock Hall Governance Committee
2005 - 2006	QB3 Governance/Community Committee, Chair
2005 - 2009	Mission Bay leadership committee
2006 - present	Faculty steering committee for the shared computer cluster at QB3, Chair
2003 - 2004	Bioinformatics and Computational Biology Faculty Search Committee, Co-Chair
2005 - 2010	Systems Biology Faculty Search Committee
2005 - 2008	Systems Biology HHMI/NIBIB Training Grant Leadership Committee
2007 - present	BMI Training Grant Leadership Committee
2007 - 2007	Quantitative Imaging Faculty Search Committee

2008 - 2008 Human Genetics Faculty Search Committee, Co-Chair
2011 - 2011 Pharmacometrics Faculty Search Committee
2011 - present Bioinformatics Task Force
2011 - present IT Governance Committee on Research Technology
2012 - present Enabling Technologies Advisory Committee
2012 - 2012 Gladstone Institute Faculty Search Committee
2012 - present ICHS Infrastructure Committee
2012 - present Funding Shared Equipment Awards Committee
2012 - present Bioimaging Faculty Search Committee
2013 - present Data Center Services Advisory Board
2013 - present 2.0-Ideation for the Future of UCSF Committee
2013 - present Shared Research Facilities Roadmap Steering Committee
2014 - present Institute for Neurodegenerative Diseases Faculty Search Committee, Co-Chair
2015 - present Chair, QB3 Shared Cluster Steering Committee
2016 - present Basic Research - IT interactions committee
2016 - present Executive Committee of Institute for Computational Health Sciences (ICHS)

SCHOOL OF PHARMACY

2003 - 2008 SOP Information Technology Committee
2005 - 2005 SOP Strategic Planning Committee
2007 - 2007 SOP Advisory committee for sharing software royalties
2007 - 2007 SOP Advisory committee for developing the SOP price / performance metric
2007 - 2007 SOP Space allocation committee
2009 - present SOP Outreach to industry program
2010 - 2011 SOP Faculty Awards Committee
2012 - 2014 SOP Educational Policy Committee
2014 - present SOP Frontiers in Science and Practice of Therapeutics Committee
2015 - present Associate Dean of Research
2015 - present SOP leadership group

DEPARTMENTAL SERVICE

2003 - present BTS Internal Advisory Committee

2013 - present PSPG Graduate Program Admissions Committee

TEACHING AND MENTORING**TEACHING SUMMARY**

When I arrived to UCSF in January 2003, I joined Prof. Patsy Babbit in leading the graduate and professional students' courses in Bioinformatics (BMI-206 and BPS-114). In 2008-09, I took the primary responsibility for these two courses. I also gave many of the lectures and supervised student activity associated with the courses (eg, student seminars, exercise sets). Since 2010, I contribute several lectures to BMI-206, but the course is led by others (BPS-114 does not exist anymore). I also participate as a guest lecturer in a number of other courses, such as Macromolecules and Chem 204. Since 2014, I began to be increasingly involved in BPS-134, a course for pharmacy students, led by Nancy Sambol. Finally, I am involved in the shaping of the curriculum for the graduate programs in the iPQB umbrella program, as a member of the iPQB curriculum committee and a contributor to the training grant re-submissions.

FORMAL TEACHING

	Academic Yr	Course No. & Title	Teaching Contribution	School	Class Size
	2004 - 2004	Bioinformatics BMI-206	Co-Organizer, Lecturer		15
	2005 - 2005	Bioinformatics BMI-206	Co-Organizer, Lecturer		15
	2005 - 2005	Bioinformatics BPS-114	Co-Organizer, Lecturer		130
	2006 - 2006	Bioinformatics BMI-206	Co-Organizer, Lecturer		15
	2006 - 2006	Bioinformatics BPS-114	Co-Organizer, Lecturer		130
	2007 - 2007	Bioinformatics BMI-206	Co-Organizer, Lecturer		15
	2007 - 2007	Bioinformatics BPS-114	Co-Organizer, Lecturer		130
	2007 - 2007	Bioinformatics BMI-206	Co-Organizer, Lecturer		15
	2007 - 2007	Bioinformatics BPS-114	Co-Organizer, Lecturer		130
	2008 - 2008	Bioinformatics BMI-206	Organizer, Lecturer		15

	Academic Yr	Course No. & Title	Teaching Contribution	School	Class Size
	2008 - 2008	Bioinformatics BPS-114	Organizer, Lecturer		130
	2009 - 2009	Bioinformatics BMI-206	Organizer, Lecturer		15
	2009 - 2009	Bioinformatics BPS-114	Lecturer		130
	2010 - 2010	Bioinformatics BMI-206	Organizer, Lecturer		15
	2012 - 2012	Bioinformatics BMI-206	Lecturer		15
	2013 - 2013	Bioinformatics BMI-206	Lecturer		15
	2013 - 2013	BPS 134	Lecturer		6
	2013 - 2013	NSF Proposal Course	Lecturer		
	2014 - 2014	NSF Proposal Course	Lecturer		
	2014 - 2014	Bioinformatics BMI-206	Lecturer		15
	2014 - 2014	BPS 134	Lecturer		6
	2003 - present	Macromolecular Interactions BP-204	Occasional Guest Lecturer		20
	2011 - present	Chem 204	Guest Lecturer		3
	2015 - present	Systems Pharmacology, Pharmacogenomics 245B	Guest Lecturer		15
	2015 - 2015	BPS 134	Lecturer		6
	2016 - 2016	BPS 134	Lecturer		10
	2017 - 2017	BPS 134	Lecturer		10
	2018 - 2018	BPS 134	Lecturer		10

MENTORING SUMMARY

I have been involved in both formal and informal teaching at UCSF, as illustrated by my contributions to the graduate courses, professional courses, and mentoring of students and postdocs in my laboratory, detailed in the corresponding sections of this cv.

PREDOCTORAL STUDENTS SUPERVISED OR MENTORED

Dates	Name	Program or School	Mentor Type	Role	Current Position
1995 - 2000	Roberto Sanchez	Rockefeller University		PhD Advisor	Associate Professor, Mount Sinai School of Medicine, NY
1999 - 2001	Eric Feyfant	Rockefeller University		PhD Advisor	Senior Scientist, Wyeth Inc. Cambridge, MA.
1999 - 2003	Nebojsa Mirkovic	Rockefeller University		PhD Advisor	Postdoctoral fellow with Diana Murray at Weill Medical College of Cornell University, NY
2000 - 2003	Bino John	Rockefeller University		PhD Advisor	Assistant Professor, University of Pittsburgh
2002 - 2008	Ranyee Chiang	BMI		PhD Advisor	Postdoc at New York University
2003 - 2007	Fred Davis	Biophysics		PhD Advisor	Postdoc at Janelia Farm, HHMI
2003 - 2008	Michael Kim	BMI		PhD Advisor	The Mechanical Zoo
2003 - 2008	Libusha Kelly	BMI		PhD Advisor	Postdoc at MIT, with Penny Chisholm
2004 - 2008	David Eramian	Biophysics		PhD Advisor	Patent Counsel, eBay Inc.

Dates	Name	Program or School	Mentor Type	Role	Current Position
2005 - 2008	Mark Peterson	BMI		PhD Advisor	The Boston Consulting Group
2006 - 2011	David Barkan	BMI		PhD Advisor	Staff Scientist, Protagonist Therapeutics
2006 - 2011	Keren Lasker	Tel-Aviv University		PhD Advisor	Postdoctoral Fellow, Stanford UniversityWol fson
2007 - 2009	Adam Marko	BMI		MSc Advisor	Asuragen, Inc., Austin, TX Bioinformatic s Developer
2007 - 2012	Jeremy Phillips	BMI		PhD Advisor	Bioinformatic s Analyst, Genome Institute/LBL
2009 - 2014	Peter Cimermancic	BMI		PhD Advisor	UCSF Specialist
2011 - 2015	Natalia Khuri	Biophysics		PhD Advisor	Educational Program Director, UCSF-Stanford CERSI Lecturer,
2010 - 2016	Charles Greenberg	BMI		PhD Advisor	Lumiata, Inc of San Mateo, CA
2012 - present	Adrian Stecula	PSPG		PhD Advisor	Graduate Student
2012 - 2016	Sara Calhoun	Biophysics		PhD Advisor	Lawrence Berkeley National Lab

Dates	Name	Program or School	Mentor Type	Role	Current Position
2014 - present	Ilan Chemmama	Biophysics		PhD Advisor	Graduate Student
2015 - present	Seth Axen	Biophysics		PhD Advisor	Graduate Student

POSTDOCTORAL FELLOWS AND RESIDENTS MENTORED

Dates	Name	Fellow	Mentor Role	Faculty Role	Current Position
1995 - 1997	Ilya Vakser	Postdoc researcher		Research supervision	Professor, University of Kansas, Lawrence, KS
1996 - 1999	Azat Badretdinov	Postdoc researcher		Research supervision	Senior scientific programmer at Accelrys Inc., San Diego
1997 - 2002	Andras Fiser	Postdoc researcher		Research supervision	Associate Professor, Albert Einstein College of Medicine, Bronx, NY
1998 - 2001	Francisco Melo	Postdoc researcher		Research supervision	Associate Professor, Pontificia Universidad Catolica de Chile
1999 - 2003	Ash Stuart	Postdoc researcher		Research supervision	Assistant Professor, Ramapo College, Mahwah, NJ

Dates	Name	Fellow	Mentor Role	Faculty Role	Current Position
1999 - 2006	Marc Marti-Renom	Adjunct Assistant Professor		Research supervision	Assistant Professor, Prince Felipe Research Center, Valencia, Spain
2000 - 2002	Valya Ilyin	Scientific Programmer		Research supervision	Associate Professor, Northeastern University, Boston
2000 - 2006	Andrea Rossi	Postdoc researcher		Research supervision	Senior Scientist, Rinat Laboratories, Pfizer Inc.
2000 - 2007	M.S. Madhusudhan	Postdoc researcher		Research supervision	Assistant Professor, Bioinformatics Institute, Singapore
2000 - 2008	Narayanan Eswar	Scientific Programmer		Research supervision	Group Leader, Du Pont Inc.
2000 - 2014	Ursula Pieper	Scientific Programmer		Research supervision	Web Applications Specialist, National Agricultural Library
2001 - 2007	Frank Alber	Postdoc researcher		Research supervision	Assistant Professor, University of Southern California

Dates	Name	Fellow	Mentor Role	Faculty Role	Current Position
2002 - 2003	Bozidar Yerkovich	Scientific Programmer		Research supervision	Head of Structural Bioinformatics at Rosetta Inpharmatics Inc., Seattle
2002 - 2006	Damien Devos	Postdoc researcher		Research supervision	Senior postdoc with Rob Russell, EMBL, Heidelberg
2002 - 2007	Dmitry Korkin	Postdoc researcher		Research supervision	Assistant Professor, University of Missouri at Columbia
2003 - 2004	Niu Huang	Postdoc researcher		Research supervision	Assistant Professor, Beijing, China
2003 - 2006	Maya Topf	Postdoc researcher		Research supervision	Lecturer, Department of Crystallography, Birkbeck College, London
2003 - 2006	Rachel Karchin	Postdoc researcher		Research supervision	Assistant Professor, Johns Hopkins University
2003 - 2008	Min-yi Shen	Postdoc researcher		Research supervision	Postdoc researcher
2003 - present	Ben Webb	Scientific Programmer		Research supervision	Scientific Programmer
2005 - 2008	Friedrich Foerster	Postdoc researcher		Research supervision	Postdoc researcher

Dates	Name	Fellow	Mentor Role	Faculty Role	Current Position
2006 - 2013	Javier Velazquez	Postdoc researcher		Research supervision	Cypher Genomics Bioinformatics Analyst
2006 - 2014	Hao Fan	Postdoc researcher		Research supervision	A*STAR, Singapore Principal Investigator
2007 - 2014	Daniel Russel	Postdoc researcher		Research supervision	AltSchool Senior Research Engineer
2008 - 2012	Avner Schlessinger	Postdoc researcher		Research supervision	Mount Sinai School of Medicine Assistant Professor
2008 - 2015	Dina Schneidman	Postdoc researcher		Research supervision	Specialist
2008 - present	Seung-Joong Kim	Postdoc researcher		Research supervision	Specialist
2009 - 2011	Sebnem Essiz	Postdoc researcher		Research supervision	Assistant Professor, Kadir Has University, Istanbul
2009 - 2014	Guangqiang Dong	Postdoc researcher		Research supervision	Data Scientist, Facebook
2009 - 2014	Patrick Weinkam	Postdoc researcher		Research supervision	Lead Engineer, Data Science, Baselayer
2009 - present	Elina Tjioe	Scientific Programmer		Research supervision	Scientific Programmer

Dates	Name	Fellow	Mentor Role	Faculty Role	Current Position
2010 - 2011	Backy Chen	Postdoc researcher		Research Supervision	Institute of Biomedical Science, Academia Sinica, Taiwan, Postdoc Researcher
2010 - 2013	Massimiliano Bonomi	Postdoc researcher		Research Supervision	Postdoc researcher
2010 - present	Riccardo Pellarin	Postdoc researcher		Research Supervision	Postdoctoral Fellow, Institut Pasteur
2011 - 2012	Lan Hua	Postdoc researcher		Research Supervision	Postdoc researcher
2012 - 2013	Miriam Sgobba	Postdoc researcher		Research Supervision	Postdoc researcher
2012 - present	Barak Raveh	Postdoc researcher		Research Supervision	Postdoc researcher
2014 - 2016	Peter Cimermanic	Postdoc researcher		Research Supervision	Specialist
2014 - present	Shruthi Viswanath	Postdoc researcher		Research Supervision	Postdoc researcher
2014 - present	Kate Stafford	Postdoc researcher		Research Supervision	Postdoc researcher
2014 - present	Daniel Saltzberg	Postdoc researcher		Research Supervision	Postdoc researcher
2015 - present	Ignacia Echeverria	Postdoc researcher		Research Supervision	Postdoc researcher
2016 - present	Sai Ganesan	Postdoc researcher		Research Supervisor	Postdoc researcher
2016 - present	Nikita Chopra	Postdoc researcher		Research Supervisor	Postdoc researcher
2017 - present	Kala Pilla	Postdoc researcher		Research Supervisor	Postdoc researcher

Dates	Name	Fellow	Mentor Role	Faculty Role	Current Position
2017 - present	Jeremy Tempkin	Postdoc researcher		Research Supervisor	Postdoc researcher
2017 - present	Rakesh Ramachandran	Postdoc researcher	Research/Scholarly Mentor	Research Supervisor	Postdoc researcher
2018 - present	Leah Ray	Postdoc researcher		Research Supervisor	Postdoc researcher

FACULTY MENTORING

Dates	Name	Position while Mentored	Mentor Type	Mentoring Role	Current Position
2013 - present	Sourav Bandyopadhyay	Assistant Professor		Mentor	Assistant Professor, BTS
2012 - present	Graham Johnson	Fellow		Mentor	QB3 Fellow, BTS
2010 - present	Ryan Hernandez	Assistant Professor		Mentor	Assistant Professor, BTS
2011 - present	Rada Savic	Assistant Professor		Mentor	Assistant Professor, BTS
2004 - 2013	Tanja Kortemme	Assistant Professor		Mentor	Professor, BTS
2007 - 2008	Mats Gustafsson	Assistant Professor		Mentor	Assistant Professor, Physiology

RESEARCH AND CREATIVE ACTIVITIES

RESEARCH AND CREATIVE ACTIVITIES SUMMARY

I have a broad background in computational structural biology, with the emphasis on structural modeling and simulations: I have developed and applied methods for comparative protein structure modeling, functional annotation of proteins, and integrative structure determination of macromolecular assemblies, as well as contributed to the understanding of the protein folding process. For example, in the field of protein structure prediction, I introduced homology or comparative modeling by satisfaction of spatial restraints, which utilizes both physical and statistical information, thereby improving its accuracy and applicability. The corresponding program, MODELLER, has been licensed to over 50,000 academic users, as well as many pharmaceutical groups, and is perhaps the most widely used program for comparative modeling. The resulting database of models for approximately 6 million known protein sequences, ModBase, is linked bi-directionally to a number of key biological databases,

including UniProt. My major current research objective is to develop and apply a computational system for enumerating structures of protein assemblies that are consistent with all available information from experimental methods, physical theories, and statistical inference. Such an integrative system will maximize efficiency, accuracy, resolution, and completeness of the structural coverage of macromolecular assemblies. The current version of the corresponding program, Integrative Modeling Platform (IMP), is being used to determine the structures of a number of macromolecular assemblies, in collaboration with experimentalists. Most prominently, the approach already enabled the determination of the configuration of the 456 proteins in the yeast Nuclear Pore Complex and 19 proteins in the 19S subunit of the 26S proteasome.

1. Integrative structural biology. Samples of many biological macromolecules prove recalcitrant to mainstream structural biology methods. In such cases, structures can often be determined by consideration of complementary information from multiple methods. Thus, we are developing mathematical formalism and open source computer software for enumerating structures of macromolecular assemblies that are consistent with all available information from experimental methods, physical theories, and statistical preferences extracted from biological databases (IMP; <http://integrativemodeling.org>). To achieve this objective, we formulated the problem as an optimization task, requiring a hierarchical representation of the modeled system, a scoring function that incorporates input information, and a sampling scheme that finds good scoring solutions. The integrative approach facilitates maximizing the accuracy, precision, completeness, and efficiency of the structural coverage of biomolecular systems. In addition, we are contributing to the nucleation of the scientific community concerned with computation, validation, visualization, archival, and dissemination of integrative structures, in part through several advisory groups associated with the Protein Data Bank, Keystone Symposia SAB, and editing of Structure.

F. Alber, S. Dokudovskaya, L. Veenhoff, W. Zhang, J. Kipper, D. Devos, A. Suprpto, O. Karni, R. Williams, B.T. Chait, M.P. Rout, A. Sali. "Determining the architectures of macromolecular assemblies." *Nature* **450**, 683-694, 2007. PMID: 18046405

F. Alber, F. Förster, D. Korkin, M. Topf, A. Sali. "Integrating Diverse Data for Structure Determination of Macromolecular Assemblies." *Ann Rev Biochem* **77**, 443-477, 2008. PMID: 18318657

F. Forster, B. Webb, K.A. Krukenberg, H. Tsuruta, D.A. Agard, A. Sali. "Integration of small-angle X-ray scattering data into structural modeling of proteins and their assemblies." *J Mol Biol* **382**, 1089-1106, 2008. PMCID: PMC2745287

Russel D, Lasker K, Webb B, Velazquez-Muriel J, Tjioe E, Schneidman-Duhovny D, Peterson B, Sali A. Putting the pieces together: integrative structure determination of macromolecular assemblies. *PLoS Biol* **10**, e1001244, 2012. PMCID: PMC3260315

2. Determining structures of macromolecular assemblies. It is essential for developers of computational methods to collaborate with experimentalists in applying their methods to practical problems. Such applications provide a validation of the methods as well as feedback for further development. Since 2001, we applied our integrative structure determination approach to over 20 macromolecular assemblies, exemplified by the four papers listed below. The resulting structures often facilitated insights into their evolution, function, and modulation.

C.M. Spahn, R. Beckmann, N. Eswar, P.A. Penczek, A. Sali, G. Blobel, J. Frank. "Structure of the 80S ribosome from *Saccharomyces cerevisiae* tRNA-ribosome and subunit-subunit interactions." *Cell* **107**, 373-386, 2001. PMID: 11701127

F. Alber, S. Dokudovskaya, L. Veenhoff, W. Zhang, J. Kipper, D. Devos, A. Suprpto, O. Karni, R. Williams, B.T. Chait, A. Sali, M.P. Rout. "The Molecular Architecture of the Nuclear Pore Complex." *Nature* **450**, 695-701, 2007. PMID: 18046406

Lasker K, Forster F, Bohn S, Walzthoeni T, Villa E, Unverdorben P, Beck F, Aebersold R, Sali A, Baumeister W. Molecular architecture of the 26S proteasome holocomplex determined by an integrative approach. *Proc Natl Acad Sci USA* **109**, 1380-1387, 2012. PMCID: PMC3277140

J. Erzberger, F. Stengel, R. Pellarin, S. Zhang, T. Schaefer, C. Aylett, P. Cimermancic, D. Boehringer, **A. Sali**, R. Aebersold, N. Ban. "Molecular architecture of the 40S•eIF1•eIF3 translation initiation complex." *Cell* **158**, 1125-1135, 2014. PMCID: PMC4151992

3. Development of comparative protein structure modeling. The accuracy of homology or comparative modeling is limited by the information that can be used in model calculations. Thus, we introduced comparative modeling by satisfaction of spatial restraints, which utilizes both physical and statistical information, thereby improving its accuracy and applicability. The corresponding program, MODELLER, has been distributed to over 50,000 academic users as well as many pharmaceutical groups, and is perhaps the most widely used program for comparative modeling. Because the genomic scale of biological data sets and accessibility require automation, we improved and implemented the entire process of comparative modeling, including fold assignment, sequence-structure alignment, model building, and model assessment, allowing us to calculate useful models for domains in ~65% of all known protein sequences. The resulting database, ModBase, is linked bi-directionally to UniProt at EBI and several other major biological databases. Our comparative modeling results led us to suggest some key aspects of the target selection strategies for the structural genomics initiative.

A. Sali, T.L. Blundell. Comparative protein modelling by satisfaction of spatial restraints. *J Mol Biol* **234**, 779-815, 1993. PMID: 8254673

A. Fiser, R.K.G. Do, A. Sali. "Modeling of loops in protein structures." *Protein Sci* **9**, 1753-1773, 2000. PMID: 11045621

B. John, A. Sali. "Comparative protein structure modeling by iterative alignment, model building and model assessment." *Nucleic Acids Res* **31**, 3982-3992, 2003. PMID: 12853614

M.-Y. Shen, A. Sali. "Statistical Potential for Assessment and Prediction of Protein Structure" *Protein Science* **15**, 2507-2524, 2006. PMID: 17075131

4. Development of methods for annotation of protein function. We have contributed a number of concepts, methods, programs, web servers, and databases in the bioinformatics toolbox for structure-based functional annotation of proteins (<http://salilab.org>). Examples include a machine-learning method for predicting functional consequences of single point mutations in proteins, optimized protocols for virtual screening against comparative models, various methods for predicting functional sites and localizing cryptic sites on protein structures, as well as databases of protein-protein interfaces and protein-small molecule interactions. To maximize our impact, we are also applying these tools in collaboration with biologists. An example is our extensive characterization of ABC and SLC membrane transporters, including mapping their evolution by classification, identification of their ligands by virtual screening and experimental validation, and prediction of functional impact of their point mutants; these studies contributed to structural genomics of ABC and SLC transporters.

R. Karchin, M. Diekhans, L. Kelly, D.J. Thomas, U. Pieper, N. Eswar, D. Haussler, A. Sali. "LS-SNP: large-scale annotation of coding non-synonymous SNPs based on multiple information sources." *Bioinformatics* **21**, 2814-2820, 2005. PMID: 15827081

F.P. Davis, A. Sali. "PIBASE: a comprehensive database of structurally defined protein interfaces." *Bioinformatics* **21**, 1901-1907, 2005. PMID: 15657096

A. Schlessinger, E. Geier, H. Fan, J. Irwin, B. Shoichet, K. Giacomini, A. Sali. "Structure-based Discovery of Prescription Drugs that Interact with the Norepinephrine Transporter, NET." *Proc Natl Acad Sci USA* **108**, 15810-15815, 2011. PMID: 21885739

U. Pieper, B. Webb, G.Q. Dong, D. Schneidman-Duhovny, H. Fan, S.J. Kim, N. Khuri, Y. Spill, P. Weinkam, M. Hammel, J. Tainer, M. Nilges, A. Sali. "ModBase, a database of annotated comparative protein structure models, and associated resources." *Nucleic Acids Res* **42**, 336-346, 2014. PMCID: PMC3965011

5. Insights into protein folding and allostery. We used a simple 3D lattice model of a protein chain to contribute to the current view of protein folding, which suggests that proteins can often fold via an ensemble of pathways, not a single one. Simulations suggested that the necessary and sufficient condition for a sequence to fold rapidly was a pronounced energy minimum for the native state. This finding was explained by an elementary, three-stage random search mechanism of folding. The rate-limiting step was a random search by local chain rearrangement in the semi-compact part of the phase space; a resolution of the Levinthal paradox without recourse to a folding pathway was made possible by a sufficiently small ratio between the numbers of states in the semi-compact and transition regions. The pronounced energy minimum of a folding sequence allowed the search to take place at a temperature that was high enough for the chain to rearrange efficiently, but also low enough for the native state to remain thermodynamically stable. More recently, we used realistic multi-minima Gō models to simulate allostery at atomic resolution, and predict impact of point mutations on the allostery mechanism.

A. Sali, E. Shakhnovich, M. Karplus. "How does a protein fold?" *Nature* **369**, 248-251, 1994. PMID: 7710478

A. Sali, E. Shakhnovich, M. Karplus. "Kinetics of protein folding. A lattice model study of the requirements for folding to the native state." *J Mol Biol* **235**, 1614-1636, 1994. PMID: 8107095

P. Weinkam, J. Pons, A. Sali. "Structure-based Model of Allostery Predicts Coupling Between Distant Sites." *Proc Natl Acad Sci USA* **109**, 4875-4880, 2012. PMCID: PMC3324024

P. Weinkam, Y.C. Chen, J. Pons, A. Sali. "Impact of mutations on the allosteric conformational equilibrium." *J Mol Biol* **425**, 647-661, 2013. PMCID: PMC3557769

RESEARCH AWARDS - CURRENT

1. P41 GM109824	Co-Investigator	Rout (PI)
NIH	08/01/2014	04/30/2019
National Center for Dynamic Interactome Research	\$ 189,269 direct/yr	\$ 995,000 total
	1	

The central goal of the proposed National Center for Dynamic Interactome Research (NCDIR) is to address the urgent need for technologies that can rapidly, reliably and routinely reveal and interpret the dynamic cellular interactome.

2. P01 GM105537	Co-Investigator	Winey (PI)
NIH	09/01/2014	08/31/2019
The Yeast Centrosome-Structure, Assembly & Function	\$ 135,000 direct/yr	\$ 750,000 total
	1	

The goal of this project is to understand the structure and function of centrosomes.

3.	P01AG002132	Co-Investigator	Prusiner (PI)
	NIH	6/16/2015	03/31/2020
	Degenerative and Dementing Diseases of Aging	\$ 140,000 direct/yr 1	\$ 700,000 total
	The central goal is mapping protein self-assemblies that lead to a number of neurodegenerative and systemic disorders.		
4.	R01GM112108	Co-Investigator	Michael P. Rout (PI)
	NIH	08/01/2014	02/28/2019
	Structure-Function Mapping of the Nuclear Pore Complex	\$ 48,000 direct/yr 1	\$ 192,000 total
	The goal is to construct a model of the transport through the Nuclear Pore Complex, based on varied theoretical considerations and experimental datasets.		
5.	P01 GM111126	Co-Investigator	Stroud (PI)
	NIH	08/01/2015	07/31/2020
	Mapping the conformational cycle of transmembrane transporters	\$ 200,000 direct/yr 1	\$ 1,000,000 total
	The goal is to apply integrative structure determination to select ABC transporters.		
6.	R01 GM083960	PI	Sali (PI)
	NIH/NIGMS	04/01/2017	03/31/2021
	IMP: Software for Hybrid Determination of Macromolecular Assembly Structures	\$ 220,000 direct/yr 1	\$ 880,000 total
	The goal is to develop and implement methods for integrative modeling of macromolecular assembly structures in the open source IMP package and to support its distribution.		
7.	U54DK107981	Co-Investigator	Alber (PI)
	NIH/NIDDK		
	Mapping the 3D Genome Landscape	\$ 79,701 direct/yr 1	\$ 398,505 total
	The aim is to upgrade IMP to allow for mapping the three-dimensional organization of the genome.		
8.	P01 GM118303	Co-Investigator	Gerlt (PI)
	University of Illinois/NIH/NIGMS	04/01/2016	06/30/2021
	Discovery of Microbial Metabolic Pathways Guided by Ligand Binding	\$ 78,768 direct/yr 1	

Program project focuses on the development and application of novel computational and experimental strategies for the discovery of novel metabolic pathways in microbial species for which complete genome sequences are available.

9.	R01GM117370	CoPi	Taatjes (PI)
	NIH	01/01/2017	03/31/2018
	Mediator kinases and transcription regulation	\$ 33,000 direct/yr	
		1	
	This collaborative project seeks to gain a deep mechanistic understanding of the Mediator kinases (CDK8 and CDK19) and the CDK8 module study CDK8 and CDK19 function in the context of serum response signaling, which is fundamentally important for cell physiology, development, and cancer biology.		
10.	HARC		Webb (PI)
	HARC	09/01/2015	08/31/2018
	Integrative Modeling of HIV-Human Protein Complexes	\$ 63,046 direct/yr	
		1	
	Integrative Modeling of HIV-Human Protein Complexes		

RESEARCH AWARDS - PAST

1.	R01 GM54762	PI		
	NIH/NIGMS		07/01/1996	06/30/2010
	Protein Modeling by Satisfaction of Spatial Restraints		\$ 200,000 direct/yr 1	\$ 2,500,000 total
2.	U54 GM103511	Co-PI		
	NIH/NIGMS		06/10/2005	07/31/2014
	Nuclear Information Pathway Center		\$ 273,439 direct/yr 1	\$ 2,100,000 total
3.	P01 GM71790	Collaborator		
	NIH/NIGMS		07/01/2004	06/30/2014
	Deciphering Enzyme Specificity		\$ 96,350 direct/yr 1	\$ 800,000 total
4.	Sinsheimer Scholar Award	PI		
	Alexandrine and Alexander L. Sinsheimer Fund		09/01/1996	08/31/1998

Knowledge-Based Protein Structure Modeling for Genome Projects

5.	BIR-9601845 NSF Acquisition of a Multiprocessor Computer for Computational Physics and Structural Biology	PI	10/01/1996	09/30/1998
6.	Gift Molecular Simulations, Inc.	PI	07/01/1998	07/01/1998
7.	Alfred P. Sloan Fellowship Alfred P. Sloan Foundation	PI	10/01/1998	9/30/2000
8.	R01 HL63284 NIH/NHLBI Disruption and Expression of Mast Cell Protease Genes	Collaborator	09/01/1999	08/31/2003
9.	Mathers Foundation Award Mathers Foundation Comparative Annotation of Eukaryotic Genomes: From Gene Detection to Protein Structure Modeling	PI	01/01/2000	12/31/2002
10.	Career Scientist Award Irma T. Hirschl Monique Weill-Caulier Trust Comparative Protein Structure Modeling for Genomics	PI	01/01/2000	12/31/2004
11.	The Merck Genome Research Institute Award The Merck Genome Research Institute	PI	02/01/2000	01/31/2002

Database of Comparative Protein Structure Model for
Genomics

12. R33 CA84699	Co-PI		
NIH/NCI		02/01/2000	01/31/2003
Target Selection for the Structural Genomics of Cancer			
13. Gift	PI		
Prospect Genomics, Inc.		07/01/2000	07/01/2000
14. U54 GM074945	Co-PI		
SGX/NIH		09/30/2000	08/31/2010
NYSGRG: A Large-Scale Center for the Protein Structure Initiative		\$ 261,032 direct/yr 1	\$ 2,700,000 total
15. R33 C89810	Collaborator		
NIH/NCI		06/01/2001	03/31/2004
Comprehensive Map of Cellular Protein Interactions			
16. EDUD-7824-020257-US	PI		
Sun Academic Equipment Grant		07/03/2001	07/03/2001
Development of an Integrated Software Environment for High-Throughput Structural Biology and Automated Comparative Protein Structure Modeling			
17. RGP67/2003	Co-PI		
Human Frontier Science Program Organization		07/01/2003	06/30/2006
3-D Reconstruction and Identification of Postsynaptic Molecular Complexes Images by Electron Cryotomography			

18. Sandler Center for Basic Research in Parasitic Diseases Sandler Family Supporting Foundation Bioinformatics of Host-Pathogen Interactions	Collaborator	07/01/2003	06/30/2010
19. California Institute for Quantitative Biomedical Research Towards a Comprehensive Map of Protein-Ligand Interactions	PI	08/01/2003	07/31/2005
20. SUR Equipment Award IBM, Inc. Large-Scale Protein Structure Modeling and Ligand Docking	PI	08/03/2003	08/03/2003
21. Equipment Award Intel, Inc. Large-Scale Protein Structure Modeling and Ligand Docking	PI	09/15/2003	09/15/2003
22. EIA-0324645 NSF Subnanometer Structure-Based Fold Determination of Biological Complexes	Co-PI	11/01/2003	10/31/2006
23. Opportunity Award Sandler Program in Basics Sciences Hierarchical Framework for Structural Biology	PI	02/15/2004	02/14/2006
24. P01 AI035797 NIH/AI Targeting Cysteine Proteases - Antiparasitic Chemotherapy	Core PI	07/01/2004	06/30/2009

25. IIS-0705196	PI		
NSF		08/01/2007	07/31/2009
Integrated Modeling of Biological Nanomachines			
26. EF 0626651	Collaborator		
NSF		01/01/2008	10/31/2010
The PhyloFacts Phylogenomic Encyclopedia of Microbial Protein Families		\$ 17,261 direct/yr 1	\$ 35,387 total
27. Pfizer / QB3 Award	PI		
Pfizer, Inc.		09/01/2008	08/31/2009
Epitope Mapping by Combining Protein-Protein Docking and Varied Low-Resolution Structural Data			
28. S10 RR027100-01	PI		
NIH/NIGMS		04/01/2010	03/31/2011
High Performance Computing Cluster for Bioimaging and Computational Biology		\$ 499,512 direct/yr 1	
29. Pfizer, Inc.	PI		
California Institute for Quantitative Biosciences (QB3)		07/01/2010	06/30/2011
A Computational Model of Allostery with Application to Antibody Design		\$ 70,000 direct/yr 1	\$ 70,000 total
30. PN2 EY016525	Co-PI		
NIH		09/30/2005	09/29/2011
Center for Protein Folding Machinery		\$ 50,000 direct/yr 1	\$ 600,000 total
31. SP41 RR001081-32S1	Collaborator		
NIH		09/15/2009	09/14/2011

Resource for Biocomputing, Visualization, and Informatics		\$ 7,140 direct/yr 1	\$ 14,500 total
32.	PI		
Pfizer, Inc.		10/01/2013	09/30/2014
A Computational Model of Allostery with Application to Antibody Design		\$ 55,000 direct/yr 1	\$ 55,000 total
33.	PI		
Bayer Inc.		12/15/2012	12/15/2014
Modeling of ternary MHCII-peptide-TCR complexes		\$ 73,877 direct/yr 1	\$ 147,755 total
34. U01 GM61390	Collaborator		
NIH/NIGMS		04/01/2003	06/30/2015
Pharmacogenetics of Membrane Transporters		\$ 45,000 direct/yr 1	\$ 600,000 total
35. U54 GM0094625	Co-PI		
NIH/NIGMS		07/01/2005	06/30/2015
CSMP: Centers for Membrane Protein Structure Determination		\$ 65,000 direct/yr 1	\$ 650,000 total
36. U54 GM093342	Co-PI		
NIH/NIGMS		04/01/2010	04/30/2015
Collaborative Center for an Enzyme Function Initiative		\$ 170,000 direct/yr 1	\$ 850,000 total
37. U01 GM098256	Co-PI		
NIH/NIGMS		07/01/2011	07/31/2015
Nucleocytoplasmic Transport: A Target for Cellular Control		\$ 50,000 direct/yr 1	\$ 200,000 total

38. U54 GM094662	Co-PI		
NIH/NIGMS		07/01/2010	06/30/2015
New York Structural Genomics Research Consortium		\$ 150,000	\$ 750,000
		direct/yr 1	total
39. R21	coPI		Charly Craik (PI)
NIH		4/1/2014	3/31/2016
Extracellular Proteolysis as a Molecular Stratification Tool for Cancer		\$ 20000	\$ 40000 total
		direct/yr 1	
The goal is to apply machine learning to cancer proteolysis data sets.			
40.	PI		Andrej Sali (PI)
QB3		1/1/2014	12/31/2015
Small molecular activators of the 20S proteasome		\$ 125000	\$ 225000 total
		direct/yr 1	
The goal is to find small molecules that activate the human 20S proteasome.			
41. P01 AI09575	Co-PI		Sali (PI)
NIH/NIGMS		07/13/2011	06/30/2016
Protein Homeostasis Mechanism Underlying Enterovirus Replication and Evolution		\$ 130,000	\$ 650,000
		direct/yr 1	total
42. S10OD021596	PI		Sali (PI)
NIH		07/01/2016	06/30/2017
High Performance Computer for Computational Biosciences		\$ 443,460	\$ 443,460
		direct/yr 1	total
Equipment grant for high performance computer for computational bioscience.			

PEER REVIEWED PUBLICATIONS

1. M. Renko, A. Sali, V. Turk, M. Pokomy, I. Kregar. "A neutral metalloproteinase from *Streptomyces rimosus*." *Vestnik Slovenskega Kemijskega Drustva* 32/2, 161-173, 1985.
2. B. Lenarcic, A. Ritonja, A. Sali, M. Kotnik, V. Turk, W. Machleidt. "Properties and structure of human spleen stefin B - a low molecular weight protein inhibitor of cysteine proteinases." In: *Cysteine Proteinases and Their Inhibitors*; First International Symposium, Portoroz, Yugoslavia, September 15-18, 1985. Xvi+846p. Ed: V. Turk, pp. 473-488, Walter De Gruyter and Co., Berlin, West Germany; New York, New York, USA., 1986.

3. V. Turk, J. Brzin, B. Lenarcic, A. Sali, W. Machleidt. "Human stefins and cystatins: their properties and structural relationships." In: Cysteine Proteinases and Their Inhibitors; First International Symposium, Portoroz, Yugoslavia, September 15-18, 1985. Xvi+846p. Ed: V. Turk, pp. 429-442, Walter De Gruyter and Co., Berlin, West Germany; New York, New York, USA., 1986.
4. M. Kotnik, A. Sali, J. Kos, B. Turk, V. Turk. "Nova metoda za hitro določanje kinetičnih konstant pri interakciji encima s kompetitivnim inhibitorjem (A new method for rapid determination of kinetic constants for competitive inhibition of enzymes)." Vestnik Slovenskega Kemijskega Drustva 34, 369-377, 1987.
5. A. Sali, V. Turk. "Prediction of the secondary structures of stefins and cystatins, the low-molecular mass protein inhibitors of cysteine proteinases." Biol Chem Hoppe Seyler 368, 493-499, 1987.
6. T. Lah, I. Kregar, A. Sali, B. Lenarcic, M. Kotnik, V. Kostka, V. Turk. "Circular dichroism studies of different aspartyl proteinases and their interactions with pepstatin." Periodicum Biologorum 90, 31-38, 1988.
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8. A. Sali, B. Veerapandian, J.B. Cooper, S.I. Foundling, D.J. Hoover, T.L. Blundell. "High-resolution X-ray diffraction study of the complex between endothiapepsin and an oligopeptide inhibitor: the analysis of the inhibitor binding and description of the rigid body shift in the enzyme." Embo Journal 8, 2179-2188, 1989.
9. T.L. Blundell, G. Elliott, S.P. Gardner, T. Hubbard, S. Islam, M. Johnson, D. Mantaounis, P. Murrayrust, J. Overington, J.E. Pitts, A. Sali, B.L. Sibanda, J. Singh, M.J.E. Sternberg, M.J. Sutcliffe, J.M. Thornton, P. Travers. "Protein engineering and design." Philosophical Transactions of the Royal Society of London Series B-Biological Sciences 324, 447-460, 1989.
10. T.L. Blundell, D. Carney, T. Hubbard, M.S. Johnson, A. McLeod, J.P. Overington, A. Sali, M.S. Sutcliffe, P. Thomas. "Knowledge-based protein modelling and design." In: Advances in Protein Design: International Workshop 1988 GBF Monographs. Ed: H. Bloecker, J. Collins, R.D. Schmid, D. Schomburg, 12, pp. 39-43, VCH, London, UK, 1989.
11. A. Sali, T.L. Blundell. "Definition of general topological equivalence in protein structures. A procedure involving comparison of properties and relationships through simulated annealing and dynamic programming." J Mol Biol 212, 403-428, 1990.
12. A. Sali, J.P. Overington, M.S. Johnson, T.L. Blundell. "From Comparisons of protein sequences and structures to protein modelling and design." Trends Biochem Sci 15, 235-240, 1990.
13. B. Veerapandian, J.B. Cooper, A. Sali, T.L. Blundell. "X-ray analyses of aspartic proteinases. III Three-dimensional structure of endothiapepsin complexed with a transition-state isostere inhibitor of renin at 1.6 Å resolution." J Mol Biol 216, 1017-1029, 1990.
14. J. Overington, M.S. Johnson, A. Sali, T.L. Blundell. "Tertiary structural constraints on protein evolutionary diversity: templates, key residues and structure prediction." Procedures in Biological Science 241, 132-145, 1990.

15. J.P. Overington, M.S. Johnson, C. Topham, A. McLeod, A. Sali, Z.Y. Zhu, L. Sibanda, T.L. Blundell. "Applications of environment specific amino acid substitution tables to identification of key residues in protein tertiary structure." *Curr Sci* 59, 867-874, 1990.
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23. A. Sali, B. Veerapandian, J.B. Cooper, D.S. Moss, T. Hofmann, T.L. Blundell. "Domain flexibility in aspartic proteinases." *Proteins* 12, 158-170, 1992.
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SIGNIFICANT PUBLICATIONS

1. Comparative protein modelling by satisfaction of spatial restraints

A Sali, TL Blundell

Journal of Molecular Biology 234, 779-815, 1993

Dr. Sali conceived and performed the research, as well as wrote the paper.

2. How does a protein fold?

A Sali, E. Shakhnovich, M Karplus

Nature 369, 248-251, 1994

Dr. Sali conceived of the research, performed it, and co-wrote the paper.

3. Determining the architectures of macromolecular assemblies

F Alber, S Dokudovskaya, LM Veenhoff, W Zhang, J Kipper, D Devos, ...

Nature 450 (7170), 683-694, 2007

Dr. Sali conceived of the research, performed part of it, and co-wrote the paper.

4. Integrative Structure and Functional Anatomy of a Nuclear Pore Complex

4. S.J. Kim, J. Fernandez-Martinez, I. Nudelman, Y. Shi, W. Zhang, B. Raveh, T. Herricks, B.D. Slaughter, J. Hogan, P. Upla, I.E. Chemmama, R. Pellarin, I. Echeverria, M. Shivaraju, A.S. Chaudhury, J. Wang, R. Williams, J.R. Unruh, C.H. Greenberg, E.Y. Jacobs, Z. Yu, M.J. de la Cruz, R. Mironska, D.L. Stokes, J.D. Aitchison, M.F. Jarrold, J.L. Gerton, S.J. Ludtke, C.W. Akey, B.T. Chait, A. Sali, M.P. Rout

Nature 555, 475-482, 2018

Dr. Sali co-led the research and co-wrote the paper.

5. Prediction of enzymatic pathways by integrative pathway mapping

S. Calhoun, M. Korczynska, D.J. Wichelecki, B. San Francisco, S. Zhao, D.A. Rodionov, M.W. Vetting, N.F. Al-Obaidi, H. Lin, M.J. O'Meara, D.A. Scott, J.H. Morris, D. Russel, S.C. Almo, A.L. Osterman, J.A. Gerlt, M.P. Jacobson, B.K. Shoichet, A. Sali

eLife 7, e31097, 2018

Dr. Sali conceived of the research and co-wrote the paper.

ACADEMIC LEADERSHIP

Dr. Sali is involved in the leadership of Protein Data Bank, the key community database in structural biology. His roles have included membership on the Scientific Advisory Board, organizing a number of PDB workshops, and contributing as well as leading the writing of White Papers that made recommendations about the organization of the PDB and validation of various types of structures deposited in the database. In particular, Dr. Sali has co-led the establishment of PDB-Dev, the nascent PDB archive for integrative structures.

OTHER CREATIVE ACTIVITIES

OTHER MENTORING:

2004-now Coaching of iQPB student journal club presentations (approx. 3 students each year).

2006-now The Academic Advisor for approximately one third of students in BMI.

2008-now Coaching iPQB graduate students on submitting NSF research proposals.

Dates	Name	Program	Role
2004	Nima Fayazmanesh	Biophysics	Supervised Graduate Rotation
2003	Greg Friedland	Biophysics	Supervised Graduate Rotation
2005	Michael Mysinger	PSPG	Supervised Graduate Rotation
2004	Dale Webster	BMI	Supervised Graduate Rotation
2003	Alex Adai	BMI	Supervised Graduate Rotation
2003	Brian Tuch	BMI	Supervised Graduate Rotation
2006	Alan Barber	PSPG	Supervised Graduate Rotation
2008	Adam Marko	BMI	Supervised Graduate Rotation
2008	Rocco Varela	BMI	Supervised Graduate Rotation
2004	Tiba Ayunechi	BMI	Thesis Committee member
2004	Barbara Novak	BMI	Orals Committee member
2004	Alan Graves	Biophysics	Orals Committee member
2004-now	Alexandra Schnoes	BMI	Orals, thesis Committee member
2005	Ben Sellers	Biophysics	Orals Committee member
2005	Nathan Salomonis	PSPG	Orals Committee member
2005	Jerome Nilmeir	Biophysics	Orals Committee member
2005-07	Tuan Pham	BMI	Orals, Thesis Committee member
2006-07	Marco Sorani	BMI	Thesis committee member
2006-07	David Lomelin	BMI	Orals Committee member
2006-08	Ben Sellers	BMI	Thesis committee member
2006	Nima Fayazmanesh	Biophysics	Orals Committee member
2006	Arjun Narayanan	Biophysics	Orals Committee member
2006	Veena Thomas	PSPG	Orals Committee member
2006	Dale Webster	BMI	Orals Committee member
2006	Holly Atkinson	BMI	Orals Committee member
2006	Dan Mandel	BMI	Orals Committee member
2006-now	Mike Keiser	BMI	Orals, Thesis Committee Member
2007-now	Elisabeth Humphris	Biophysics	Orals, Thesis Committee member
2007-now	Colin A. Smith	BMI	Orals Committee member
2005-08	Greg Friedland	Biophysics	Orals, Thesis Committee member
2007	Rafaela Ferreira	BMI	Orals Committee member
2007	Michelle Dimon	BMI	Orals Committee member
2007	Michael Hicks	PSPG	Orals Committee member
2008	Matt Eames	Biophysics	Thesis Committee member

2008	Jason Fernandez	PSPG	Orals Committee member
2008	Leonard Apeltsin	BMI	Orals, Thesis Committee member
2009	Alan Barber	PSPG	Orals Committee member
2009	Hannes Braberg	Biophysics	Orals Committee member
2009	Noah Ollikainen	BMI	Orals, Thesis Committee member
2009	Peter Skewes-Cox	BMI	Orals Committee member
2009	Monica Tremont	Biophysics	Orals Committee member
2009	Kiyoshi Egami	Biophysics	Orals Committee member
2009	Martin Turk		Visiting Scholar
2010	Rocco Varela	BMI	Thesis Committee member
2010	Russell Spitzer	BMI	Orals Committee member
2010	Henry Lin	BMI	Orals Committee member
2010	Jeremy Phillips	BMI	Thesis Committee member
2010	Geoff Rollins	Biophysics	Orals Committee member
2010	Laurens Kraal	BMI	Orals Committee member
2010	Ethan Geier	PSPG	Orals Committee member
2010	Davide Bau		Visiting Scholar
2010	Benjamin Schwartz		Visiting Scholar
2010	Yannick Spill		Visiting Scholar
2011	Brittany Fotsch	CCB	Supervised Graduate Rotation
2011	Zac Apte	Biophysics	Orals Committee member
2011	Yi Song	BMI	Supervised Graduate Rotation
2011	Argyris Politis		Visiting Scholar
2011	Amrita Choudhury		Visiting Scholar
2011	Javona White Bear	BMI	Supervised Graduate Rotation
2011	Natalia Khuri	Biophysics	Supervised Graduate Rotation
2011	Pia Unverdorben		Visiting Scholar
2011	Bart Lenselink		Visiting Scholar
2011	Yannick Spill		Visiting Scholar
2012	Sara Calhoun	Biophysics	Supervised Graduate Rotation
2012	Diego Garrido Ruiz	Biophysics	Supervised Graduate Rotation
2012	Kale Kundert	Biophysics	Supervised Graduate Rotation
2012	Adrian Stecula	PSPG	Supervised Graduate Rotation
2012	Miriam Sgobba		Visiting Scholar
2012	Jeff Yunes	Bioengineering	Orals Committee member
2012	James Webber	BMI	Orals Committee member
2013	Kyle Barlow	iPQB	Orals Committee member

2013	Joel Karpiak	CCB	Orals Committee member
2013	Rahel Woldeyes	CCB	Orals Committee member
2013	Andrew Vanbenschoten	Biophysics	Thesis Committee member
2013	Daniel Himmelstein	BMI	Orals Committee member
2014	Dorota Latek		Visiting Scholar
2014	Ilan Chemmama	Biophysics	Supervised Graduate Rotation
2014	Melissa Lemke		Visiting Scholar
2014	Reed Stein	PSPG	Supervised Summer Rotation
2014	Leo Gendele	Biophysics	Orals Committee member
2014	Ibai Irastorza		Visiting Scholar
2015	Yiran Wu		Visiting Scholar
2015	Seth Axen	Bioinformatics	Supervised Graduate Rotation
2015	Leon Bichman		Visiting Scholar
2015	Sam Ivry	PSPG	Quals Committee Member
2015	Rebecca Davidson	BMI	Quals Committee Member
2015	Neville Bethel	Biophysics	Quals Committee Member
2015	Sara Calhoun	Biophysics	Thesis Committee Member
2015	Diego Garrido Ruiz	Biophysics	Thesis Committee Member
2015	Kale Kundert	Biophysics	Thesis Committee Member
2016	Daniel Himmelstein	Bioinformatics	Thesis Committee Member
2016	Ilan Chemmama	Biophysics	Thesis Committee Member
2016	Charles Greenberg	Biophysics	Thesis Committee Member
2016	Brak Mensa	CCB	Quals Committee Member
2016	James Webber	BMI	Quals Committee Member
2016	Elena Caceres	BMI	Quals Committee Member
2016	Kyle Barlow	BMI	Thesis Committee Member
2017	Kale Kundert	Biophysics	Thesis Committee Member
2017	Charlotte Nelson	BMI	Thesis Committee Member
2017	Alexander Wolff	Biophysics	Thesis Committee Member

2017	Benjamin Barad	Biophysics	Thesis Committee Member
2018	James Lucas	Bioengineering	Thesis Committee Member

ORGANIZATION OF MEETINGS:

1999-2001 Program Committee, Georgia Tech Intl. Conference on Bioinformatics, Atlanta GA

2001 Program Committee, Math/Chem/Comp 2001, Dubrovnik, Croatia

2005 Program Committee, Protein Society 19th Symposium in Boston, MA

2005 Program Committee, Protein Structure Modeling Workshop, Rutgers University, NJ

2006 Program Committee, American Society for Biochemistry and Molecular Biology

2007 Program Committee, 4th Conference on Modeling of Protein Interactions (MPI)

2008 Organizer, Workshop on Applications of Protein Structure Models in Biomedical Research, UCSF, CA

2010 Program Committee, 3DSIG symposium at ISMB conference, Boston

2010 Co-Organizer, Keystone Symposia on Frontiers in Structural Biology

2012 Co-Organizer, Keystone Symposia on High-Throughput Structural Biology

2012 Co-Organizer, Conference on Structural Analysis of Supramolecular Assemblies by Hybrid Methods, Lake Tahoe

2013 Organizer, Keystone Symposia on Structural Analysis of Supramolecular Assemblies by Hybrid Methods, Lake Tahoe

2014 Organizer, Martin Karplus Celebration Symposium

2006-now Organizer, World Molecular Engineering Network, annual TSRI & UCSF meeting in San Jose del Cabo, Mexico

2019 Organizer, 63rd Annual Meeting of the Biophysical Society, Baltimore, MD, Mar 2-6, 2019.

FELLOWSHIPS TO LAB MEMBERS:

Howard Hughes Predoctoral Fellowship (R. Sanchez)

Howard Hughes Predoctoral Fellowship (F. Davis)

Burroughs Wellcome Fund Predoctoral Fellowship (R. Chiang)

Alfred P. Sloan Postdoctoral Fellowship (A. Stuart)

Burroughs Wellcome Fund Postdoctoral Fellowship (A. Fiser, M.A. Marti-Renom)

Rockefeller University Presidential Fellowship (M.A. Marti-Renom)

Charles Revson Foundation Postdoctoral Fellowship (A. Fiser, M.S. Madhusudhan)

NIH Postdoctoral Fellowship (R. Karchin)

Burroughs Wellcome Predoctoral Fellowship (M. Kim, R. Chiang)

DOE Predoctoral Fellowship (M. Peterson)

Genentech Award (M. Peterson)

Human Frontier Sciences Program Postdoctoral Fellowship (F. Foerster)

Spanish Minister of Education Postdoctoral Fellowship (J. Velazquez)

Clore Foundation Predoctoral Fellowship (K. Lasker)

Weizmann Institute Advancing Women in Science Postdoctoral Fellowship (D. Schneidman)
UC Cancer Research Coordinating Committee Fellowship (D. Barkan)
NIH NRSA Postdoctoral Fellowship (A. Schlessinger)
Chancellor's Graduate Research Fellowship (P. Cimermancic)
Swiss National Science Foundation Perspective Researcher Fellowship (R. Pellarin)
NSC Taiwan Postdoctoral Fellowship (B. Chen)
NSF Graduate Research Fellowship (C. Greenberg)
Howard Hughes Medical Institutes Predoctoral Fellowship (P. Cimermancic)
Frank M. Goyan Award for Excellence in Physical Chemistry (J. Phillips)
2012 School of Pharmacy Research Award (P. Cimermancic)
QB3 Rogers Award (P. Cimermancic)
NIH Fellowship (K. Stafford)
PhRMA Fellowship in Pharmacology/Toxicology (A. Stecula)
Mel Jones Excellence in Graduate Student Research Award (C. Greenberg)
PhRMA Fellowship in Pharmacology/Toxicology (A. Stecula)
AFPE Pre-Doctoral Award in Pharmaceutical Science (A. Stecula)
NSF Fellowship (I. Chemmama)

SOFTWARE:

1993 MODELLER, a program for comparative protein structure modeling by satisfaction of spatial restraints; licensed to Accelrys Inc. since 1994.
2000 MODPIPE, a program for large-scale comparative protein structure modeling; licensed to Accelrys Inc. and Structural Genomix Pharmaceuticals Inc. (2000-2004).
2000 MODBASE, a comprehensive database of comparative protein structure models; licensed to Structural Genomix Pharmaceuticals Inc. (2000-2004).
2010 IMP, a program for integrative structure determination of macromolecular assemblies, open source.