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	NCRR 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 ond 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, Savanah, 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 BBCA)
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

CONTRIBUTIONS TO DIVERSITY

CONTRIBUTIONS TO DIVERSITY
I have been involved in Public Service activities and indirectly even in Clinical activities for diverse patient populations. Perhaps the most significant such contribution is via my role as a co-founder and advisor of Global Blood Therapeutics Inc (NASDAQ GBT), aiming from the outset to develop a small molecule drug for the sickle cell disease, which in the US affects primarily African Americans; there is currently no effective drug for this debilitating and terminal disease. The company produced a drug candidate that is currently in accelerated Phase III clinical trials; GBT announced that FDA will pre-approve the drug as soon as GBT makes an appropriate request within the next few months. Based on all clinical evidence, the drug is efficacious and without significant side affects, and thus poised to significantly benefit hundreds of thousands of patients in the US and Europe, as well as eventually ~20 million patients in Africa. Another similar contribution was my scholarly work on open source drug discovery, with my colleagues Maurer and Rai, published in multiple papers listed in my publication list; this work was motivated by facilitating drug discovery for diseases that are not clearly commerically attractive to commercial drug discovery efforts, such as third world diseases.

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

	Academic Yr	Course No. & Title	Teaching Contribution	School	Class Size
	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
	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

Academic Yr	Course No. & Title	Teaching Contribution	School	Class Size
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

Dates	Name	Program or School	Mentor Type	Role	Current Position
2000 - 2003	Bino John	Rockefeller University		PhD Advisor	Assistant Professor, University of Pittsburg
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.
2005 - 2008	Mark Peterson	BMI		PhD Advisor	The Boston Consulting Group
2006 - 2011	David Barkan	BMI		PhD Advisor	Staff Scientist, Protaganist Therapeutics
2006 - 2011	Keren Lasker	Tel-Aviv University		PhD Advisor	Postdoctoral Fellow, Stanford UniversityWolfson
2007 - 2009	Adam Marko	BMI		MSc Advisor	Asuragen, Inc., Austin, TX Bioinformatics Developer

Dates	Name	Program or School	Mentor Type	Role	Current Position
2007 - 2012	Jeremy Phillips	BMI		PhD Advisor	Bioinformatics 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
2014 - present	Ilan Chemmama	Biophysics		PhD Advisor	Graduate Student
2015 - present	Seth Axen	Biophysics		PhD Advisor	Graduate Student
2018 - present	Laurel Estes	BMI	Research/Scholarly Mentor	Academic Advisor	Graduate Student
2018 - present	Wren Saylor	BMI	Research/Scholarly Mentor	Academic Advisor	Graduate Student
2018 - present	Stephanie Wankowicz	BMI	Research/Scholarly Mentor	Academic Advisor	Graduate Student
2018 - present	Cole Helsell	iPQB	Research/Scholarly Mentor	Academic Advisor	Graduate Student
2018 - present	Bryan Faust	Biophysical	Research/Scholarly Mentor	Academic Advisor	Graduate Student
2018 - present	Nick Hoppe	Biophysical		Academic Advisor	Graduate Student

Dates	Name	Program or School	Mentor Type	Role	Current Position
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-					
-					

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 Insitute, 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 - 2018	Seung-Joong Kim	Postdoc researcher		Research supervision	KAIST, Daejeon, Korea
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 - 2015	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 - 2013	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	Associate Specialist
2014 - 2016	Peter Cimermancic	Postdoc researcher		Research Supervision	Specialist
2014 - present	Shruthi Viswanath	Postdoc researcher		Research Supervision	Postdoc researcher
2014 - 2017	Kate Stafford	Postdoc researcher		Research Supervision	Senior Scientist - Atomwise
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/Scholarly Mentor	Research Supervisor	Postdoc researcher
2018 - present	Thomas-Otavio Peulen	Postdoc researcher	Research/Scholarly Mentor	Research Supervisor	Postdoc researcher
2019 - present	Tanmoy Sanyal	Postdoc researcher	Research/Scholarly Mentor	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. Suprapto, 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. Suprapto, 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 Gõ 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.

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2. P01 GM105537   Co-Investigator   Winey (PI)

	NIH		09/01/2014	08/31/2019
	The Yeast Centrosome-Structure, Assembly & Function		$ 135,000 direct/yr 1	$ 750,000 total

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.

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9. HARC P50   Webb (PI)

HARC   09/01/2017   08/31/2019

Integrative Modeling of HIV-Human Protein Complexes $ 63,046 direct/yr
1

Integrative Modeling of HIV-Human Protein Complexes

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10. DBI 1756250   Co-Investigator   Berman (PI)

Rutgers University, National Science Foundation   09/01/2018   08/31/2021

Collaborative Research: ABI Development: Building a Pipeline for Validation, Curation and Archiving of Integrative/Hybrid Models

The goal is to develop new methods for validating integrative structures.

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11. USC Fellowship Subcontract   PI   Sali (PI)

NIH/NIGMS   09/01/2017   08/31/2019

Integrative Modeling of the Human Pancreatic Beta Cell

This award primarily supports a Postdoc. Goal is to develop and apply computer modeling for a combined experimental and computational effort on mapping the pancreatic beta cell.

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12. R01GM117370   Co-Investigator   Taatjes (PI)

University of CO, Boulder/NIH/NIGMS   04/01/2017   03/31/2020

Mediator Kinases and Transcription Regulation

The goal is to compute integrative structures of the Mediator complexes within the scope of the project.

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13. P50GM082250   Co-investigator   Krogan (PI)

NIH/NIGMS   09/01/2017   08/31/2022

HARC Center: HIV Accessory and Regulatory Complexes (Core 5)

The overall goal of the Integrative Modeling Core is to facilitate the analysis and interpretation of multiple datatypes to identify and characterize the cellular proteins and networks that influence HIV virus replication.

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

   Nucliear 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   PI

   NSF   10/01/1996   09/30/1998

   Acquisition of a Multiprocessor Computer for Computational Physics and Structural Biology

6. Gift   PI

   Molecular Simulations, Inc.   07/01/1998   07/01/1998

7.	Alfred P. Sloan Fellowship	PI		
	Alfred P. Sloan Foundation		10/01/1998	9/30/2000

8.	R01 HL63284	Collaborator		
	NIH/NHLBI		09/01/1999	08/31/2003
	Disruption and Expression of Mast Cell Protease Genes			

9.	Mathers Foundation Award	PI		
	Mathers Foundation		01/01/2000	12/31/2002
	Comparative Annotation of Eukaryotic Genomes: From Gene Detection to Protein Structure Modeling			

10.	Career Scientist Award	PI		
	Irma T. Hirschl Monique Weill-Caulier Trust		01/01/2000	12/31/2004
	Comparative Protein Structure Modeling for Genomics			

11.	The Merck Genome Research Institute Award	PI		
	The Merck Genome Research Institute		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

NYSGRC: 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   Collaborator

Sandler Family Supporting Foundation   07/01/2003   06/30/2010

Bioinformatics of Host-Pathogen Interactions

19. California Institute for Quantitative Biomedical Research   PI

     08/01/2003   07/31/2005

Towards a Comprehensive Map of Protein-Ligand Interactions

20. SUR Equipment Award   PI

IBM, Inc.		08/03/2003	08/03/2003
Large-Scale Protein Structure Modeling and Ligand Docking			

21. Equipment Award	PI		
Intel, Inc.		09/15/2003	09/15/2003
Large-Scale Protein Structure Modeling and Ligand Docking			

22. EIA-0324645	Co-PI		
NSF		11/01/2003	10/31/2006
Subnanometer Structure-Based Fold Determination of Biological Complexes			

23. Opportunity Award	PI		
Sandler Program in Basics Sciences		02/15/2004	02/14/2006
Hierarchical Framework for Structural Biology			

24. P01 AI035797	Core PI		
NIH/AI		07/01/2004	06/30/2009
Targeting Cysteine Proteases - Antiparasitic Chemotherapy			

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 Perfomance 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 direct/yr 1	$ 750,000 total

39. R21	coPI		Charly Craik (PI)
NIH		4/1/2014	3/31/2016
Extracellular Proteolysis as a Molecular Stratification Tool for Cancer		$ 20000 direct/yr 1	$ 40000 total
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 direct/yr 1	$ 225000 total

The goal is to find small molecules that activate the human 20S proteasome.

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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 direct/yr 1	$ 650,000 total

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42. S10OD021596	PI		Sali (PI)
NIH		07/01/2016	06/30/2017
High Performance Computer for Computational Biosciences	$ 443,460 direct/yr 1		$ 443,460 total

Equipment grant for high performance computer for computational bioscience.

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43. 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.

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 cystatis: 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 dolocanje kineticnih konstant pri interakciji encima s kompetitivnim inhibitorjem (A new method for rapid

determination of kinetic constants for competitive inhibition of enzymes)." Vestnik Slovenskaga 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.

7. V. Turk, R. Jerala, B. Lenarcic, A. Sali. "Structural and functional aspects of human cathepsins B." In: Intracellular Proteolysis: Mechanisms and Regulations. Ed: N. Katunuma, E. Kominami, pp. 27 -37, Japan Scientific Societies Press, Berlin, West Germany; New York, New York, USA., 1989.

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. Mantafounis, 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 A 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.

16. M.S. Johnson, A. Sali, T.L. Blundell. "Phylogenetic relationships from three-dimensional protein structures." Methods Enzymol 183, 670-690, 1990.

17. M.S. Johnson, J.P. Overington, A. Sali. "Knowledge-based protein modelling: Human plasma kallikrein and human neutrophil defensin." In: Chemistry: Techniques Structure and Function. Ed: J.J. Vilafranca, pp. 567-574, Academic Press, Inc., London, 1990.

18. M.S. Johnson, J. Overington, A. Sali, Z. Zhu, D. Donnelly, P. Thomas, A. McLeod, R. Goold, C. Topham, T.L. Blundell. "From comparative structure analysis to protein engineering: Knowledge-based protein modelling and design." Fresenius Journal of Analytic Chemistry 337, 1-3, 1990.

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20. T.L. Blundell, J.B. Cooper, A. Sali, Z.Y. Zhu. "Comparisons of the sequences, 3-D structures and mechanisms of pepsin-like and retroviral aspartic proteinases." Adv Exp Med Biol 306, 443-453, 1991.

21. T.L. Blundell, J.B. Cooper, D. Donnelly, H. Driessen, Y. Edwards, F. Eisenmenger, C. Frazao, M. Johnson, K. Niefind, M. Newman, J. Overington, A. Sali, C. Slingsby, V. Nalini, Z.Y. Zhu. "Patterns of sequence variation in families of homologous proteins." In: Methods in Protein Sequence Analysis. Ed: H. Jornval, J.O. Hoog, A.M. Gustavsson, pp. 373-385, Birkhauser Verlag, Basel, Switzerland, 1991.

22. A. Sali, J.P. Overington, M.S. Johnson, T.L. Blundell. "From modelling homologous proteins to prediction of structure." In: Protein design and the development of new therapeutics and vaccines. Ed: J.M. Goodfellow, D.S. Moss, pp. 231-245, Ellis Horwood Ltd., LYNGBY, DENMARK, 1991.

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.

24. B. Veerapandian, J.B. Cooper, A. Sali, T.L. Blundell, R.L. Rosati, B.W. Dominy, D.B. Damon, D.J. Hoover. "Direct observation by X-ray analysis of the tetrahedral "intermediate" of aspartic proteinases." Protein Sci 1, 322-328, 1992.

25. Z.Y. Zhu, A. Sali, T.L. Blundell. "A variable gap penalty function and feature weights for protein 3-D structure comparisons." Protein Eng 5, 43-51, 1992.

26. J. Overington, D. Donnelly, M.S. Johnson, A. Sali, T.L. Blundell. "Environment-specific amino acid substitution tables: tertiary templates and prediction of protein folds." Protein Sci 1, 216-226, 1992.

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30. A. Sali, R. Matsumoto, H.P. McNeil, M. Karplus, R.L. Stevens. "Three-dimensional models of four mouse mast cell chymases. Identification of proteoglycan-binding regions and protease-specific antigenic epitopes." J Biol Chem 268, 9023-9034, 1993.

31. A. Sali, T. Blundell. "Comparative protein modeling by statisfaction of spatial restraints." In: Protein Structure by Distance Analysis. Ed: H. Bohr, S. Brunak, pp. 64-86, TECH UNIV DENMARK, CTR BIOL SEQUENCE ANAL, LYNGBY, DENMARK, 1994.

32. A. Sali, J.P. Overington. "Derivation of rules for comparative protein modeling from a database of protein structure alignments." Protein Sci 3, 1582-1596, 1994.

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35. A. Dinner, A. Sali, M. Karplus, E. Shakhnovich. "Phase diagram of a model protein derived by exhaustive enumeration of the conformations." J Chem Phys 101, 1444-1451, 1994.

36. M. Karplus, A. Sali. "Theoretical studies of protein folding and unfolding." Curr Opin Struct Biol 5, 58-73, 1995.

37. M. Karplus, A. Caflisch, A. Sali, E. Shakhnovich. "Protein dynamics: From the native to the unfolded state and back again." In: Modelling of Biomolecular Structures and Mechanisms. Ed: A.Pullmanet al, pp. 69-84, Kluwer Academic Publishers, London, 1995.

38. A. Sali. "MODELLER: Implementing 3D protein modeling." In: mc^2, 2, pp. 5, Molecular Simulations Inc., Totowa, NJ, 1995.

39. X.D. Wu, B. Knudsen, S.M. Feller, J. Zheng, A. Sali, D. Cowburn, H. Hanafusa, J. Kuriyan. "Structural basis for the specific interaction of lysine-containing proline-rich peptides with the amino-terminal SH3 domain of c-Crk." Structure 3, 215-226, 1995.

40. R. Matsumoto, A. Sali, N. Ghildyal, M. Karplus, R.L. Stevens. "Packaging of proteases and proteoglycans in the granules of mast cells and other hematopoietic cells. A cluster of histidines on mouse mast cell protease 7 regulates its binding to heparin serglycin proteoglycans." J Biol Chem 270, 19524-19531, 1995.

41. A. Sali. "Comparative protein modeling by satisfaction of spatial restraints." Mol Med Today 1, 270-277, 1995.

42. A. Sali, E. Shakhnovich, M. Karplus. "Protein Folding Studied by Monte Carlo Simulations." In: Protein Folds: A Distance Based Approach. Ed: H. Bohr, S. Brunak, pp. 202-216, CRC Press Inc., LYNGBY, DENMARK, 1995.

43. A. Sali, E. Shakhnovich, M. Karplus. "Thermodynamics and kinetics of protein folding from lattice Monte Carlo simulations." In: DIMACS Series in Discrete Mathematics and Theoretical Computer Science. Ed: D. Shalloway, G. Xue, P. Pardalos, 23, pp. 199-213, American Mathematical Society, LYNGBY, DENMARK, 1995.

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402. D.E. Gordon, G.M. Jang, M. Bouhaddou, J. Xu, K. Obernier, M.J. O Meara, J.Z. Guo, D.L. Swaney, T.A. Tummino, R. Hüttenhain, R.M. Kaake, A.L. Richards, B. Tutuncuoglu, H. Foussard, J. Batra, K. Haas, M. Modak, M. Kim, P. Haas, B.J. Polacco, H. Braberg, J.M. Fabius, M. Eckhardt, M. Soucheray, M.J. Bennett, M. Cakir, M.J McGregor, Q. Li, Z.Z.C. Naing, Y. Zhou, S. Peng, I.T. Kirby, J.E. Melnyk, J.S. Chorba, K. Lou, S.A. Dai, W. Shen, Y. Shi, Z. Zhang, I. Barrio-Hernandez, D. Memon, C. Hernandez-Armenta, C.J.P. Mathy, T. Perica, K.B. Pilla, S.J. Ganesan, D.J. Saltzberg, R. Ramachandran, X. Liu, S.B. Rosenthal, L. Calviello, S. Venkataramanan, Y. Lin, S.A. Wankowicz, M. Bohn, R. Trenker, J.M. Young, D. Cavero, J. Hiatt, T. Roth, U. Rathore, A. Subramanian, J. Noack, M. Hubert, F. Roesch, T. Vallet, B. Meyer, K.M. White, L. Miorin, D. Agard, M. Emerman, D. Ruggero, A. García-Sastre, N. Jura, M. Zastrow, J. Taunton, O. Schwartz, M. Vignuzzi, C. d Enfert, S. Mukherjee, M. Jacobson, H.S. Malik, D.G. Fujimori, T. Ideker, C.S. Craik, S. Floor, J.S. Fraser, J. Gross, A. Sali, T. Kortemme, P. Beltrao, K. Shokat, B.K. Shoichet, N.J. Krogan. A SARS-CoV-2 protein interaction map reveals targets for drug repurposing. Nature 583, 459-468, 2020. PMCID7431030

403. Y. Kwon, R. Kaake, I. Echeverria, M. Suarez, M.K. Shamsabadi, C. Stoneham, P.W. Ramirez, J. Kress, R. Singh, A. Sali, N. Krogan, J. Guatelli, X. Jia. Structural Basis of CD4 Downregulation by HIV-1 Nef. Nat Struct Mol Biol, 2020. PMCID7483821

404. F.D. Mast, A.T. Navare, A.M. van der Sloot, J. Coulombe-Huntington, M.P. Rout, N.S. Baliga, A. Kaushansky, B.T. Chait, A. Aderem, C.M. Rice, A. Sali, M. Tyers, J.D. Aitchison. Crippling life support for SARS-CoV-2 and other viruses through synthetic lethality. J Cell Biol 219, 2020. PMCID7659715

405. Y. Qiao, Z. Wang, F. Tan, J. Chen, J. Lin, J. Yang, H. Li, X. Wang, A. Sali, L. Zhang, G. Zhong. Enhancer Reprogramming within Pre-existing Topologically Associated Domains Promotes TGF-β-Induced EMT and Cancer Metastasis. Mol Ther 28, 2083-2095, 2020

406. H. Braberg, I. Echeverria, S. Bohn, P. Cimermancic, A. Shiver, R. Alexander, J. Xu, M. Shales, R. Dronamraju, S. Jiang, G. Dwivedi, D. Bogdanoff, K.K. Chaung, R. Hüttenhain, S. Wang, . Mavor, . D, R. Pellarin, D. Schneidman, J.S. Bader, J.S. Fraser, J. Morris, J.E. Haber, B.D. Strahl, C.A. Gross, J. Dai, J.D. Boeke, A. Sali, N.J. Krogan. Genetic interaction mapping informs integrative structure determination of protein complexes. Science 370, 2020.

407. A. Leitner, A.M.J.J. Bonvin, C.H. Borchers, R.J. Chalkley, J. Chamot-Rooke, C.W. Combe, J. Cox, M. Dong, L. Fischer, M. Götze, F.C. Gozzo, A.J.R. Heck, M.R. Hoopmann, L. Huang, Y. Ishihama, A.R. Jones, N. Kalisman, O. Kohlbacher, K. Mechtler, R.L. Moritz, E. Netz, P. Novak, E. Petrotchenko, A. Sali, R.A. Scheltema, C. Schmidt, D. Schriemer, A. Sinz, F. Sobott, F. Stengel, K. Thalassinos, H. Urlaub, R. Viner, J.A. Vizcaíno, M.R. Wilkins, J. Rappsilber. Toward Increased Reliability, Transparency, and Accessibility in Cross-linking Mass Spectrometry. Structure 28, 1259-1268, 2020.

408. K.L. White, J. Singla, V. Loconte, J.H. Chen, A. Ekman, L. Sun, X. Zhang, J.P. Francis, A. Li, W. Lin, K. Tseng, G. McDermott, F. Alber, A. Sali, C. Larabell, R.C. Stevens. Visualizing subcellular rearrangements in intact β cells using soft x-ray tomography. Sci Adv 6, 2020. PMCID7725475

409. M. Hepburn, D.J. Saltzberg, L. Lee, S. Fang, C. Atkinson, N.C.J. Strynadka, A. Sali, S.P. Lees-Miller, D.C. Schriemer. The active DNA-PK holoenzyme occupies a tensed state in a staggered synaptic complex. Structure, 2020.

410. T.H. Tran, J.V. Nguyen, A. Stecula, J. Akutagawa, A.V. Moorman, B.S. Braun, A. Sali, C.G. Mullighan, N.P. Shah, Y. Dai, M. Devidas, K.G. Roberts, C.C. Smith, M.L. Loh. The EBF1-PDGFRB T681I mutation is highly resistant to imatinib and dasatinib in vitro and detectable in clinical samples prior to treatment. Haematologica, in press, 2021.

411. S.K. Burley, C. Bhikadiya, C. Bi, S. Bittrich, L. Chen, G. Crichlow, C.H. Christie, K. Dalenberg, L. Di Costanzo, J.M. Duarte, S. Dutta, Z. Feng, S. Ganesan, D.S. Goodsell, S. Ghosh, R.K. Green, V. Guranović, D. Guzenko, B.P. Hudson, C.L. Lawson, Y. Liang, R. Lowe, H. Namkoong, E. Peisach, I. Persikova, C. Randle, A. Rose, Y. Rose, A. Sali, J. Segura, M. Sekharan, C. Shao, Y. Tao, M. Voigt, J.D. Westbrook, J.Y. Young, C. Zardecki, M. Zhuravleva. RCSB Protein Data Bank: Powerful new tools for exploring 3D structures of biological macromolecules for basic and applied research and education in fundamental biology, biomedicine, biotechnology, bioengineering, and energy sciences. Nucleic Acids Res 49, D437-D451, 2021. PMCID7779003

412. D.J. Saltzberg, S. Viswanath, I. Echeverria, I.E. Chemmama, B. Webb, A. Sali. Using Integrative Modeling Platform to Compute, Validate, and Archive a Model of a Protein Complex Structure. Prot Sci 30, 250-261, 2021. PMCID7737781

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

1.
   OTHER MENTORING:

   2004-now Coaching of iPQB 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

Visting 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 Gendelev
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
Elena Caceres

Thesis Committee Member

FORMAL COURSES ELSEWHERE:

ADDITIONAL RELEVANT INFORMATION

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.