UNIVERSITY OF CALIFORNIA AT SAN FRANCISCO

Curriculum vitæ

Name: **Andrej Sali**

Position: Professor, Step IX
Department of Bioengineering and Therapeutic Sciences (BTS)
Department of Pharmaceutical Chemistry
California Institute for Quantitative Biosciences (QB3)
School of Pharmacy

Integrative Program in Quantitative Biology (iPQB):
- Bioinformatics and Medical Informatics Graduate Program
- Biophysics Graduate Program
- Graduate Program in Complex Biological Systems

Chemistry and Chemical Biology Graduate Program
Pharmaceutical Sciences and Pharmacogenomics Graduate Program

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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-now	University of California, San Francisco	Professor	BTS

OTHER POSITIONS HELD CONCURRENTLY:

2009-2012	Director, California Institute for Quantitative Biosciences (QB3) at UCSF
2003-now	Vice Chair, Department of Bioengineering and Therapeutic Sciences
2003-now	Faculty member, California Institute for Quantitative Biosciences (QB3)
2003-now	Faculty member, Pharmaceutical Sciences and Pharmacogenomics Graduate Program
2003-now	Faculty member, Biophysics Graduate Program
2003-now	Faculty member, Bioinformatics and Medical Informatics Graduate Program
2003-now	Faculty member, Chemistry and Chemical Biology Graduate Program

HONORS AND AWARDS:

1984-1987	Undergraduate scholarship from J. Stefan Institute, Ljubljana, Slovenia.
1985	British Council Visiting Student at Birkbeck College, London, UK.
1987	British Council Visiting Student at Birkbeck College, London, UK.
1987-1990	Overseas Research Students Award from the Committee of Principals and Vice Chancellors, England.
1987-1988	Scholarship for graduate studies from the Research Council of Slovenia.
1989-1990	Merck Sharp & Dohm academic scholarship.
1991-1994	Jane Coffin Childs Memorial Fund for Medical Research Postdoctoral Fellow.
1996-1999	Alexandrine and Alexander L. Sinsheimer Scholar.
1998-2000	Alfred P. Sloan Research Fellow.
2000-2003	Irma T. Hirschl Career Award Scientist.
2007	Zois Award, Science Ambassador of Republic of Slovenia.

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:

PROFESSIONAL ORGANIZATIONS:

Memberships

1991-now	Protein Society
1991-now	American Association for the Advancement of Science
2007-now	Biophysical Society

Service to Professional Organizations

2005-2008	Protein Society	Executive Committee
2005-now	Protein Data Bank	Scientific Advisory Committee
2009-now	PROSPECTS (Proteomics Specification in Time and Space) consortium	Scientific Advisory Committee
2010	Keystone Symposia	Scientific Advisory Board (*ad hoc*)
2011-2014	Keystone Symposia	Scientific Advisory Board
2010-now	Protein Data Bank	Electron Microscopy Validation Task Force (Co-Chair)
2010-now	Protein Data Bank	Small Angle Scattering Task Force
2010-now	Electron Microscopy Data Bank	Scientific Advisory Committee
2009-now	PSI Knowledgebase	Working Group on Theoretical Structural Model Validation
2011-now	Rosetta Commons	Scientific Advisory Board

SERVICE TO PROFESSIONAL PUBLICATIONS:

2003-now	Editor, Structure.
2004-now	Editorial Board, PLoS Computational Biology.
2002-now	Editorial Board, Journal of Computer Aided Molecular Design.
2002-now	Editorial Board, Molecular and Cellular Proteomics.
2004-now	Editorial Board, Protein Engineering, Design, and Selection.
2001-now	Section Head for the Structural Genomics section on BioMed Central
1990-now	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.

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

INVITED PRESENTATIONS (since 1999):

INTERNATIONAL

1. CERCA CADD Symposium, Montreal, Canada. April 13, 1999.
2. Data Mining in Crystallography, Erice, Italy. May 15, 1999.
3. Structural Biology Net, Tallberg, Sweden. June, 1999.
4. Frontiers in Structural Biology, Indian Institute of Science, Bangalore, India. August 27, 1999.
5. BRI, Montreal, Canada. November 24, 1999.
6. University of Toronto, Toronto, Canada. December 9, 1999.
7. Japan Biophysical Society Meeting, Tokyo, Japan. January 17, 2000.
8. Bioinformatics 2000, Elsinore, Denmark. April 28, 2000.
9. University of Zuerich, Zuerich, Switzerland. December 5, 2001.
10. Bioinformatics & Proteomics: From Sequence to Function, Lausanne, Switzerland. December 6, 2001.
11. Structural Genomics and Bioinformatics, Instituto Juan March, Madrid, Spain. March 12-14, 2001.
12. Annual meeting of the Canadian Society for Biochemistry and Molecular and Cellular Biology (CSBMCB), Toronto, Canada. May 31-June 3, 2001.
13. Math/Chem/Comp 2001, Dubrovnik, Croatia. June 25-30, 2001.
14. 4th International Conference on Biological Physics, ICBP2001, Kyoto, Japan. July 30-August 3, 2001.
15. 4th International Conference on Molecular Structural Biology, ICMSB2001, Vienna, Austria. September 5-9, 2001.
16. Genomics & Proteomics meeting, Barcelona, Spain. October 19, 2001.
17. University of Barcelona, Barcelona, Spain. May 21, 2002.
18. Genomics & Proteomics meeting, Barcelona, Spain. May 22, 2002.
19. Samuel Lunenfeld Research Institute, Toronto, Canada. May 29, 2002.
20. The 19th Congress and General Assembly of the International Union of Crystallography IUCR, Geneva, Switzerland. August 6-15, 2002.
21. Genomics and Bioinformatics Center Inaugural Symposium, Pontificia Universidad Catolica, Santiago, Chile. November 18-20, 2002.
22. Fourteenth Annual World Molecular Engineering Network (WMEN) Conference, San Jose del Cabo, Baja California Sur, Mexico. May 4-8, 2003.
23. 5th Meeting of the Slovenian Biochemical Society, Ljubljana, Slovenia. September 24-28, 2003.
24. University of Cologne, Cologne, Germany. January 19, 2004.
25. Ringberg meeting, Schloss Ringberg, Germany. January 21-23, 2004.
26. Fourteenth Annual World Molecular Engineering Network (WMEN) Conference (2004), San Jose del Cabo, Baja California Sur, Mexico. May 2-6, 2004.
27. EMBO conference on Structures in Biology, EMBL, Heidelberg, Germany. November 10-13, 2004.
28. The 7th World Congress of the World Association of Theoretically Oriented Chemists (WATOC), Capetown, South Africa. January 16-21, 2005.
29. Keynote Speaker in XX IUCr Congress in Firenze, Italy. August 23-31, 2005.

30. Speaker at the International Workshop M2CELL, The Royal Abbey of Fontevraud, Paris, France. December 4-6, 2005.
31. Organizer and Speaker at the World Molecular Engineering Network Conference. Cabo San Lucas, Mexico. April 30-May 2nd, 2006.
32. Plenary Speaker at the 11th Symposium on Recent Advances in Biophysics, National Taiwan University, Taipei, Taiwan. May 23-26, 2006
33. 2006 Keystone Symposium on Multi-Protein Complexes Involved in Cell Regulation, St. John's College, Cambridge, UK. August 18-23, 2006.
34. Organizer and Speaker at the World Molecular Engineering Network Conference. Cabo San Lucas, Mexico. April 29-May 2nd, 2007.
35. Protein Complexes and Protein Networks Symposium in Martinsried, Germany, May 21-22, 2007.
36. Symposium on Structural Biology and its Application to Drug Development at the University of Tokyo, Tokyo, Japan, 28 January 2007.
37. Invited Speaker at the Basel Computational Biology Conference [BC]2 , Basel, Switzerland, March 13-14, 2008.
38. Organizer and Speaker of the World Molecular Engineering Network Conferenc. Cabo San Lucas, Mexico. May 4-8, 2008.
39. University of Toronto, Canada, 26 July, 2008.
40. Speaker at the 40th Course: From Molecules to Medicines Integrating Crystallography in Drug Discovery, Erice, Italy. May 29 - June 8, 2008.
41. Speaker at the Gordon Research Conference on Macromolecular Organization & Cell Function: Systems Cell Biology, Oxford, England, July 27 to August 2, 2008.
42. Speaker at the 6th National NCCR Symposium on New Trends in Structural Biology, Zurich, Switzerland, September 8-9 2008.
43. Speaker at the Max Planck Institute, Student Workshop, Goettingen, Germany. September 10-13 2008.
44. Speaker at the Max Planck Institute of Biochemistry, INSTRUCT Open Meeting, in Martinsried, Germany, October 16-17 2008.
45. Speaker at the NoE 3DEM final Meeting, Brdo, Slovenia, February 9-13, 2009.
46. McDowell Lecture at the University of British Columbia, Vancouver, BC, Canada, March 10, 2009.
47. Seminar at the University of Ljubljana, Ljubljana, Slovenia, December 17, 2009.
48. Organizer and Speaker at the 20th World Molecular Engineering Network Conference, Cabo San Lucas, Mexico, May 2-5, 2010.
49. Speaker at the Institute of Structural Molecular Biology, Birkbeck Institute, London, England, June 17-18, 2010
50. Speaker at the MPIMP Dahlem Colloquia in Molecular Genetics, Max Planck Institute, Berlin, Germany, August 22-24, 2010.
51. Speaker at Exeter College, Oxford University, England, October 4, 2010.
52. Speaker at the PROteomics SPECification in Time and Space – PROSPECTS Meeting, Taormina, Sicily, Italy, November 2-4, 2010.
53. Speaker at the 6th International Conference on Structural Biology and Functional Genomics, National University of Singapore, Singapore, December 6-8, 2010.
54. Organizer and Speaker at the 21st World Molecular Engineering Network Conference, Cabo San Lucas, Mexico, May 1-4, 2011.
55. Speaker at the International Conference on Structural Genomics, University of Toronto, Toronto, Ontario, Canada, May 10-14, 2011.
56. Speaker at IGBMC, Strasbourg, France, July 17-18, 2011.
57. Speaker at Max Planck Institute, Munich, Germany, July 20-21, 2011.
58. Plenary Speaker at the ComBio 2011, Cairns Convention Centre, Cairns, Australia, September 26-29, 2011.
59. Organizer and Speaker at the 22nd World Molecular Engineering Network Conference, Cabo San Lucas, Mexico, May 6-9, 2012.
60. Speaker at the PROteomics SPECification in Time and Space – PROSPECTS Meeting, Sissi, Crete, Greece, May 29-June 1, 2012.

61. Speaker at the XXVth ICMRBS Conference, Lyon, France, August 19-24, 2012.
62. Plenary Speaker at the Molecular Modeling Meeting, Queenstown, New Zealand, August 30-September 1, 2012.
63. Speaker at the IISc Conference, Bangalore, India, January 8-11, 2013.

NATIONAL, REGIONAL AND OTHER INVITED PRESENTATIONS

1. Second International Georgia Tech Conference in Bioinformatics, Atlanta, Georgia, USA. November 12, 1999.
2. 2.Structural Genomics Targets Workshop, NIH, Washington DC, USA. February 11, 1999.
3. Advances & Opportunities at the Biology/Math/Computational/Physical Sciences Interface, Rutgers University, New Brunswick, NJ, USA. March 6, 1999.
4. Mount Sinai School of Medicine, New York, NY, USA. March 19, 1999.
5. New York Structural Biology Group, New York Academy of Sciences, New York, NY, USA. March 24, 1999.
6. Columbia University, New York, NY, USA, 1999.
7. Chemistry Dept., New York University, New York, NY, USA, 1999.
8. Protein Sequence Structure Function Meeting, UCSF, San Francisco, CA, USA. April 23, 1999.
9. The Scripps Institute, La Jolla, CA, USA. August 13, 1999.
10. Mathematical Problems in the Molecular Sciences, Courant Institute, New York, NY, USA. October 10, 1999.
11. City College of New York, New York, USA. October 20, 1999.
12. Agouron Pharmaceuticals, San Diego, California, USA. October 28, 1999.
13. Structural Genomics Conference, ANL, Chicago, Illinois, USA. November 16, 1999.
14. Structural Genomics and the Pharmaceutical Industry, Princeton, New Jersey, USA. November 18, 1999.
15. Quantitative Challenges in the Post Genomic Sequence Era, La Jolla Interfaces in Science, San Diego, California, USA. January 12, 2000.
16. UCSD, Dept of Physics, San Diego, California, USA. January 19, 2000
17. UCSF, San Francisco, California, USA. January 20, 2000.
18. Center for Physics and Biology, Rockefeller University,New York, New York, USA. January 24, 2000.
19. Biological Chemistry Seminar Series, University of Penn, Philadelphia, Pennsylvania, USA. February 17, 2000.
20. ABRF 2000 ``From Singular to Global Analyses of Biological Systems'', Bellevue, Washington, USA. February 22, 2000.
21. AAAS conference, Washington DC, USA. March 20, 2000.
22. Keystone Symposium on Macromolecular Assemblies at Work: Application of Physics, Chemistry, and Mathematics to Biology, Durango, Colorado, USA. March 25, 2000.
23. Bio2000, Boston, Massachusetts, USA. March 28, 2000
24. Computational Challenges of the Post Genomic Age, SUN, San Francisco, California, USA. May 12, 2000.
25. Biopolymers Gordon Conference, Newport, Rhode Island, USA. June 18-22, 2000.
26. 2000 FASEB Summer Research Conference on Protein Folding in the Cell, Saxton River, Vermont, USA. July 22-27, 2000.
27. Monsanto/Pharmacia lectureship series, Univ. of Saint Louis, Missouri, USA. September 28, 2000.
28. Workshop on Structural Genomics. NIGMS, Washington DC, USA. October 23, 2000.
29. Genomics and Bioinformatics, UMD, New Brunswick, New Jersey, USA. November 2, 2000.
30. University of Minnesota, Minneapolis, Minnesota, USA. November 27, 2000.
31. Oncogenomics: Dissecting Cancer Through Genome Research, Nature Genetics, Tuscon, Arizona, USA. January 25-27, 2001.
32. UAB, Birmingham, Alabama, USA. February 26, 2001.
33. Bard College, New York, USA. April 18, 2001.

34. Physics/Chemistry. CSUN, Northridge, California, USA. May 2, 2001.
35. ACS Meeting, Chicago, Illinois, USA. August 26-30, 2001.
36. University of Maryland, Maryland, USA. October 2, 2001.
37. Columbia University, New York, New York, USA. October 15, 2001.
38. Mast Cell Workshop, Bethesda, Maryland, USA. November 26-30, 2001.
39. Genomics Seminar Series, Skirball Institute, New York, New York, USA. February 6, 2002.
40. Mining the Human Genome for New Drug Discovery – New Ways of Handling Orphan Targets. NYAS, New York, New York, USA. February 26, 2002.
41. Biological Processes for New and Innovative Engineering Systems and Applications, ARO workshop, Research Triangle Park, North Carolina, USA. February 26-27, 2002.
42. New York City Blood Centre, New York, New York, USA. March 7, 2002.
43. Proteomics – The New Frontiers: Discovery, Separation, Prediction & Modeling, University of Delaware, Newark, Delaware, USA. March 14-15, 2002.
44. Harvard University, Cambridge, Massachusetts, USA, March 28, 2002.
45. Molecular Cell Biology and Biochemistry Seminar Series, Virginia Tech, Blacksburg, Virginia, USA. April 5, 2002.
46. UCSF, San Francisco, California, USA, April 15, 2002.
47. A Workshop on large biological structures, Asilomar, California, USA. April 20-22, 2002.
48. SCBMB Program, Baylor College of Medicine, Houston, Texas, USA. May 15, 2002.
49. 50th ASMS conference American Society of Mass Spectrometry, Orlando, Florida, USA. June 2-6, 2002.
50. The 5th Summer Session of the New York Structural Biology Discussion Group , Cold Spring Harbor Laboratory, New York, USA. June 26, 2002
51. Berkeley-Stanford summer school for protein crystallography, SSRL, Stanford, California, USA. July 8-12, 2002.
52. Gordon Conference on Diffraction Methods in Structural Biology, Connecticut College, New London, Connecticut, USA. July 14-19, 2002.
53. NYCBS New York Computational Biology Society seminar, NAS, New York, New York, USA. September 18, 2002.
54. Center for Biological Modeling, Michigan State University, East Lansing, Michigan, USA. September 27, 2002.
55. Bioinformatics seminar, Texas A&M University, Tamu, TX, USA. November 7, 2002.
56. Structure and Function of the Proteome, Argonne National Laboratory, Argonne, Illinois, USA. November 23-24, 2002.
57. Keystone Symposium in Proteomics: Technologies and Applications, Keystone Resort in Keystone, Colorado, USA. March 25-30, 2003.
58. NCRR sponsored Workshop on Structural Proteomics of Complexes, Bethesda, Maryland, USA. April 7-8, 2003.
59. American Society for Biochemistry and Molecular Biology meeting, San Diego, California, USA. April 11-15, 2003.
60. St. Jude Children's Research Hospital, Memphis, TN, USA. April 22, 2003.
61. Genentech, Inc., South San Francisco, CA, USA. April 29, 2003.
62. Structure and Function of Proteome, SBC, Argonne National Laboratory, Argonne, Illinois, USA. Spring, 2003.
63. "Frontiers of Bioinformatics" symposium, Center of Excellence in Bioinformatics, University at Buffalo, Buffalo, New York, USA. June 6-8, 2003.
64. IBM Thomas J. Watson Research Center, New York, New York, USA. June 11, 2003.
65. 2003 Gordon Research Conference on 3D Electron Microscopy of Macromolecules, Colby Sawyer College, New London, New Hampshire, USA. June 22-26, 2003.
66. PSI workshop ond data management, NIH Campus, Bethesda, MD, USA. July 10-11, 2003.
67. GTL and Beyond: Data and Computational Needs Workshop, San Francisco, CA, USA. September 10-11, 2003.
68. 2003 Pharmaceutical Sciences and Pharmacogenomics Retreat, Marshall, CA, USA. September 11-13, 2003.
69. Structure and Chemistry Seminar at Scripps, San Diego, CA, USA. September 18, 2003.

70. Seminar at Northeastern University, Boston, MA, USA. October 6, 2003
71. Workshop on Visualization of Biological Complexes, Four Points Sheraton Hotel, Emeryville, San Francisco Bay Bridge, CA, USA. October 11-12, 2003
72. Seminar at PARC, Palo Alto, CA, USA. October 15, 2003.
73. NIGMS Homology Modeling Workshop, Bethesda, MD, USA. October 21-22, 2003.
74. Seminar at Purdue University, West Lafayette, IN, USA. October 24-25, 2003.
75. PSI Target Selection Workshop, Bethesda, MD, USA. November 13-14, 2003.
76. Biophysics/CCB Retreat, Asilomar Conference Center, Pacific Grove, CA, USA. December 7-9, 2003.
77. Licensing Executives Society meeting, San Francisco, CA, USA. February 12, 2004.
78. The Structural, Functional and Evolutionary Gordon Conference, Four Points Sheraton Harbortown, Ventura, CA, USA. February 15-20, 2004.
79. Seminar at Berkeley, Berkeley, CA, USA. March 8, 2004.
80. Seminar at UCSC, Santa Cruz, CA, USA. March 11, 2004.
81. Workshop on Structure Determination of Macromolecular Machines and Assemblies by Hybrid Methods, Granlibakken/Lake Tahoe Conference Center, CA, USA. March 17-20, 2004.
82. 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.
83. 2004 Keystone Symposium on Structural Genomics, Snowbird Resort, Snowbird, Utah, USA April 13-19, 2004.
84. BayGenomics PGA, San Francisco, CA, USA. April 27, 2004.
85. Gladstone Scientific Retreat, Asilomar in Monterey County, CA, USA. May 18-20. 2004.
86. Seminar at Caltech, Pasadena, CA, USA. October 12, 2004.
87. ICSG 2004 Meeting, Washington, DC, USA. November 17-24, 2004.
88. Workshop of the Center of Protein Folding Machinery, Stanford University, CA, USA. December 4-5, 2004.
89. Biological and Medical Informatics/Biophysics/Chemistry and Chemical Biology graduate groups retreat, Asilomar Conference Center, Pacific Grove, CA, USA. December 5-7, 2004.
90. ABRF meeting, Biomolecular Technologies:Discovery to Hypothesis, Savanah, Georgia, USA. February 5-8, 2005.
91. Frontiers in Computational Biophysics Symposium, NIH campus in Bethesda, MD, USA. April 29-30, 2005.
92. NIH Symposium on Structural Analysis of Large Assemblies: Sizing up the Challenges, NIH campus in Bethesda, MD, USA. June 2-3, 2005.
93. SRI's Computational Biology series, SRI International, Menlo Park, CA, USA. June 29, 2005.
94. 19th Annual Symposium of the Protein Society, Boston, MA, USA. July 30 – August 3, 2005.
95. GRC 2005 Computer-aided design meeting, Tilton School, NH, USA. July 31 – August 5, 2005.
96. Seminar at the Biochemical and Biophysical Methods Course Fall 2005, The Rockefeller University, New York, NY, USA. October 11, 2005.
97. Seminar at the Novartis Institutes for BioMedical Research, Cambridge, MA, USA. November 9, 2005.
98. Workshop on Biological Macromolecular Structure Models, The State University of New Jersey, Piscataway, NJ, USA. November 19-20, 2005.
99. Organizer and Speaker of the Theme "Macromolecular Structure and Dynamics" with 4 Symposia. ASBMB 2006 meeting, San Francisco, CA, USA. April 1-5, 2006.
100. Seminar at UC Davis, CA. June 1, 2006.
101. Symposium at Wyeth Research, Cambridge, MA, USA. October 16, 2006.
102. Seminar at the University of Massachusetts, Dept. of Biochemistry and Molecular Pharmacology, Worcester, MA, USA. October 18, 2006.
103. Seminar at the Fifth Annual Systems Biology Course at the Institute for Systems Biology, Seattle, WA, USA. 9 November 2006.
104. Seminar at UC Merced Center for Computational Biology, Merced, CA, USA. 30 November 2006.
105. TDR/WHO Drug Target Selection Meeting in Seattle, OR, USA. 1 December, 2006.

106. Biological and Medical Informatics/Biophysics/Chemistry and Chemical Biology Graduate Groups Retreat, Monterey, CA, USA. 3-5 December, 2006.
107. Collaborative Drug Discovery meeting, UCSF, San Francisco, USA. 1 March 2007
108. The Protein Folding Center Annual Retreat, Stanford, CA, USA. 27-29 May 2007.
109. Seminar at the Center for Theoretical Biological Physics. UCSD,San Diego USA. 1 June, 2007.
110. Institute for Systems Biology, Seattle, WA, 12 July 2007.
111. Seminar at Genentech, San Francisco, CA, 25 September 2007.
112. Seminar at the SCRIPPS Institute, La Jolla, CA, USA. September 27-28
113. Speaker and Organizer of the Modeling of Protein Interactions Meeting, MPI-2007, Lawrence, KA, USA, September 30 – October 2, 2007.
114. Seminar at the Albert Einstein College of Medicine, New-York, NY. 16 October 2007.
115. Seminar at University of California Berkeley, New-York, NY. 25 October 2007.
116. Seminar at the Carolina Center for Genomic Sciences colloquium, UNC, Chapel Hill, NC, USA. 9 November 2007.
117. Seminar at the Duke University Computational Biology Series, Durham, NC, USA. 12 November 2007.
118. Keystone Symposium on Structural Genomics and Its Applications to Chemistry, Biology and Medicine, Steamboat Springs, Colorado, CO, USA, 6-11 January 2008.
119. Seminar for the Biochemical and Biophysical Methods Course at the Rockefeller University, New York, NY. 30 January 2008.
120. Seminar at the University of Utah, February 25 2008.
121. Seminar at The Buck Institute for Age Research, Novato, CA, USA, July 1 2008.
122. Speaker and Organizer of the Protein Modeling Workshop, University of California, San Francisco, CA, USA, July 11-12 2008.
123. Speaker at the 2008 Senior Vice Chancellor’s Laureate Lecture Series at the University of Pittsburgh, July 18 2008.
124. Protein Structure Initiative (PSI3), Washington DC, USA, October 29-30, 2008.
125. Seminar at UT Southwestern Medical Center, 5-6 Nov 2008.
126. Biology and Mathematics in the Bay Area (BaMBA), University of California, Davis, CA,USA, November 15, 2008.
127. Biological and Medical Informatics/Biophysics/Chemistry and Chemical Biology Graduate Groups Retreat, Monterey, CA, USA. 7-9 December, 2008.
128. NCMI Single Particle Reconstruction Workshop, Baylor College of Medicine, Houston, TX, USA, December 10-13, 2008.
129. Seminar at the University of Pennsylvania School of Medicine, Philadelphia, PA, USA, January 29, 2009.
130. Mesilla Chemistry Workshop Multi-Scale Modeling of Biological Molecules, Mesilla, TX, USA, February 1-4, 2009.
131. Technology Centers for Networks and Pathways Annual All Hands Meeting, Washington DC, USA, March 12-13, 2009
132. 2009 Symposium on Molecular Systems Biology of the Cell, Seattle, WA, USA, April 19, 2009.
133. Seminar at the University of Minnesota, Minneapolis, MN, USA, April 22, 2009.
134. Seminar at the University of Washington, Seattle, WA, USA, May 14, 2009.
135. Seminar at Indiana University, Indianapolis, IN, USA, May 18, 2009.
136. Seminar at University of Texas Southwestern, Dallas, TX, USA, May 20-21, 2009.
137. 23rd Annual Symposium of the Protein Society, Boston, MA, USA, July 25-29, 2009.
138. Speaker at the Pharmaceutical Sciences and Pharmacogenomics Retreat, Tomales Bay, CA, USA, September 9-10, 2009.
139. Beckman Institute 20th Anniversary Symposium, University of Illinois at Urbana-Champaign, Urbana, IL, USA, September 20-23, 2009.
140. Seminar at University of Southern California, Los Angeles, CA, USA, November 19, 2009.
141. Speaker at the Annual Computational and Theoretical Biology Symposium, Houston, TX, USA, December 4-6, 2009.
142. Speaker and Co-Organizer of the Keystone Symposia on Structural Biology/Structural Genomics, Steamboat Springs, CO, USA, January 8-13, 2010.

143.Speaker at the Modeling of Cryo-EM Map Workshop, Baylor College of Medicine, Houston, TX, USA, January 14-17, 2010.
144.Chair and Speaker at the Biophysical Society 54th Annual Meeting, San Francisco, CA, USA, February 20-24, 2010.
145.Speaker at the Hybrid Methods Symposium, Lake Tahoe, CA, USA, March 10-14, 2010.
146.Speaker at the Structural Biology Symposium, Case Western Reserve University, Cleveland, OH, USA, May 19, 2010.
147.Keynote Speaker at the 3Dsig Satellite Meeting, Boston, MA, USA, July 9-10, 2010.
148.Speaker at the 18th International Conference on Intelligent Systems for Molecular Biology (ISMB 2010), Boston, MA, USA, July 11-13, 2010.
149.Seminar at Vanderbilt University, Nashville, TN, USA, October 12, 2010.
150.Seminar at Ohio State University, Columbus, OH, USA, October 26, 2010.
151.Speaker at the MPI Meeting, University of Kansas, Lawrence, KS, USA, October 28-30, 2010.
152.Seminar at the University of California, San Diego, CA, USA, December 12, 2010.
153.Speaker at the Design of Drugs and Chemicals that Influence Biology Workshop, University of California, Los Angeles, CA, USA, April 4-8, 2011.
154.Keynote Speaker at the Sanford-Burnham Structural Systems Biology Symposium, La Jolla, CA, USA, June 7, 2011.
155.Speaker at the Institute for Systems Biology Symposium and Workshop, University of Washington, Seattle, WA, USA, July 24-27, 2011.
156.Speaker at the Accelerating Predictive Drug Development Through Quantitative Pharmacology Symposium University of California, San Francisco, California, USA, September 22-23, 2011.
157.Speaker at the Worldwide Protein Data Bank (wwPDB) Symposium, Cold Spring Harbor, NY, USA, October 28-30, 2011.
158.Seminar at St. Jude Children's Research Hospital, Memphis, TN, USA, November 15, 2011.
159.Seminar at Duke University, Durham, NC, USA, November 18, 2011.
160.Speaker and Co-organizer of the Keystone Symposia on High Throughput and Hybrid Approaches to Structural Biology, Keystone, CO, USA, January 22-27, 2012.
161.Speaker at Eli Lilly Symposium, Indianapolis, IN, USA, February 13-14, 2012.
162.Seminar at the University of Michigan, Ann Arbor, MI, USA, February 15, 2012.
163.Seminar at the Scripps Research Institute, San Diego, CA, USA, March 1-2, 2012.
164.Co-organizer of the 6th International Conference on Structural Analysis of Supramolecular Assemblies by Hybrid Methods, Lake Tahoe, CA, USA, March 14-18, 2012.
165.Keynote Speaker at the ISMB, Long Beach, CA, USA, July 14-17, 2012.

GOVERNMENT AND OTHER PROFESSIONAL SERVICES:

2004-09	National Institutes of Health	MSF-B Study Section (successor of BBCA)
1995-now	NIH, National Science Foundation, DOE, European Community, Burroughs Wellcome Fund, Binational Science Foundation	*ad hoc* Grant Reviews

UNIVERSITY AND PUBLIC SERVICE:

UNIVERSITY SERVICE:

UCSF

2003-now	*Ad hoc* Faculty reviews (~20)

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-now	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-now	iPQB Curriculum committee
2005-now	iPQB Executive Committee
2005-2009	iPQB Admissions Committee
2004	Chancellor's Council committee
2004	Academic Information Technology Coordinator search committee
2004-now	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-now	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-now	BMI Training Grant Leadership Committee
2007	Quantitative Imaging Faculty Search Committee
2008	Human Genetics Faculty Search Committee, Co-Chair
2011	Pharmacometrics Faculty Search Committee
2011-now	Bioinformatics Task Force
2012	Enabling Technologies Advisory Committee
2012	Gladstone Institute Faculty Search Committee

SCHOOL OF PHARMACY

2003-08	SOP Information Technology Committee
2005	SOP Strategic Planning Committee
2007	SOP Advisory committee for sharing software royalties
2007	SOP Advisory committee for developing the SOP price / performance metric
2007	SOP Space allocation committee
2009-now	SOP Outreach to industry program
2010-2011	SOP Faculty Awards Committee

DEPARTMENTAL SERVICE

2003-now	BTS Internal Advisory Committee

ROCKEFELLER UNIVERSITY

1995-2000	Chemistry Search Committee
2000	Computer Security Committee, Chair
2000-2002	Dean's Graduate Studies Admissions Committee
2000-2002	Faculty Awards Nominations Committee
2000-2002	Bioinformatics Search Committee
2002-2003	Bioinformatics and Computational Biology Faculty Search Committee

TEACHING AND MENTORING

FORMAL SCHEDULED CLASSES FOR UCSF STUDENTS:

Qtr	Academic Yr	Course No & Title	Teaching Contribution	Units	Class Size
S	2004	Bioinformatics BMI-206	Co-Organizer, Lecturer	3	15
S	2005	Bioinformatics BMI-206	Co-Organizer, Lecturer	3	15
S	2005	Bioinformatics BPS-114	Co-Organizer, Lecturer	3	130
S	2006	Bioinformatics BMI-206	Co-Organizer, Lecturer	3	15
S	2006	Bioinformatics BPS-114	Co-Organizer, Lecturer	3	130
S	2007	Bioinformatics BMI-206	Co-Organizer, Lecturer	3	15
S	2007	Bioinformatics BPS-114	Co-Organizer, Lecturer	3	130
S	2007	Bioinformatics BMI-206	Co-Organizer, Lecturer	3	15
S	2007	Bioinformatics BPS-114	Co-Organizer, Lecturer	3	130
S	2008	Bioinformatics BMI-206	Organizer, Lecturer	3	15
S	2008	Bioinformatics BPS-114	Organizer, Lecturer	3	130
F	2009	Bioinformatics BMI-206	Organizer, Lecturer	3	15
S	2009	Bioinformatics BPS-114	Lecturer	3	130
	2003-now	Bioengineering, Macromolecules	Occasional Guest Lecturer		
F	2010	Bioinformatics BMI-206	Organizer, Lecturer	3	15

FORMAL COURSES ELSEWHERE:

- Instructor for a one semester graduate course "Analysis and prediction of protein structures" at The Rockefeller University, in 1998 and 2000.
- Guest lecturer at courses and workshops at Rockefeller University (1995-2008), Weill Medical College of Cornell University (1999-2002), New York University (2000-2002), Crystallography School in Erice, Italy (1999, 2008), FEBS course in Barcelona, Spain (1990), Stanford University (2002), and Institute for Systems Biology (2006 and 2007).

PREDOCTORAL STUDENTS SUPERVISED OR MENTORED:

Dates	Name	Program or School	Role	Current Position
2010-now	Peter Cimermancic	BMI	PhD Advisor	Graduate Student
2010-now	Charles Greenberg	BMI	PhD Advisor	Graduate Student
2007-09	Adam Marko	BMI	MSc Advisor	MSc student

2006-now	David Barkan	BMI	PhD Advisor	Graduate Student
2007-now	Jeremy Phillips	BMI	PhD Advisor	Graduate Student
2006-now	Keren Lasker	Tel-Aviv University	PhD Advisor	Graduate Student, jointly with Haim Wolfson
2004-08	David Eramian	Biophysics	PhD Advisor	UCSF Tech Transfer Office
2003-08	Michael Kim	BMI	PhD Advisor	The Mechanical Zoo
2003-08	Libusha Kelly	BMI	PhD Advisor	Postdoc at MIT, with Penny Chisholm
2005-08	Mark Peterson	BMI	PhD Advisor	The Boston Consulting Group
2002-08	Ranyee Chiang	BMI	PhD Advisor	Postdoc at New York University
2003-07	Fred Davis	Biophysics	PhD Advisor	Postdoc at Janelia Farm, HHMI
2000-03	Bino John	Rockefeller University	PhD Advisor	Assistant Professor, University of Pittsburg
1999-03	Nebojsa Mirkovic	Rockefeller University	PhD Advisor	Postdoctoral fellow with Diana Murray at Weill Medical College of Cornell University, NY
1999-01	Eric Feyfant	Rockefeller University	PhD Advisor	Senior Scientist, Wyeth Inc. Cambridge, MA.
1995-00	Roberto Sanchez	Rockefeller University	PhD Advisor	Associate Professor, Mount Sinai School of Medicine, NY

POSTDOCTORAL FELLOWS DIRECTLY SUPERVISED OR MENTORED:

Dates	Name	Fellow	Role	Current Position
2011-now	Lan Hua	Postdoc researcher	Research Supervision, jointly with Matt Jacobson	Postdoc researcher
2012-now	Barak Raveh	Postdoc researcher	Research Supervision	Postdoc researcher
2010-now	Backy Chen	Postdoc researcher	Research Supervision	Postdoc researcher
2010-now	Riccardo Pellarin	Postdoc researcher	Research Supervision	Postdoc research
2010-now	Massimiliano Bonomi	Postdoc researcher	Research Supervision	Postdoc researcher
2009-now	Guangqiang Dong	Postdoc researcher	Research supervision	Postdoc researcher
2009-now	Patrick Weinkam	Postdoc researcher	Research supervision	Postdoc researcher
2009-now	Sebnem Essiz	Postdoc researcher	Research supervision	Postdoc researcher
2009-now	Elina Tjioe	Scientific Programmer	Research supervision	Scientific Programmer
2008-now	Dina Schneidman	Postdoc researcher	Research supervision	Postdoc researcher

2008-now	Seung-Joong Kim	Postdoc researcher	Research supervision	Postdoc researcher
2008-now	Avner Schlessinger	Postdoc researcher	Research supervision	Postdoc researcher
2007-now	Daniel Russel	Postdoc researcher	Research supervision	Postdoc researcher
2006-now	Javier Velazquez	Postdoc researcher	Research supervision	Postdoc researcher
2006-now	Hao Fan	Postdoc researcher	Research supervision	Postdoc researcher
2005-08	Friedrich Foerster	Postdoc researcher	Research supervision	Postdoc researcher
2003-now	Ben Webb	Scientific Programmer	Research supervision	Scientific Programmer
2003-08	Min-yi Shen	Postdoc researcher	Research supervision	Postdoc researcher
2002-07	Dmitry Korkin	Postdoc researcher	Research supervision	Assistant Professor, University of Missouri at Columbia
2001-07	Frank Alber	Postdoc researcher	Research supervision	Assistant Professor, University of Southern California
2000-07	M.S. Madhusudhan	Postdoc researcher	Research supervision	Assistant Professor, Bioinformatics Insitute, Singapore
2000-08	Narayanan Eswar	Scientific Programmer	Research supervision	Group Leader, Du Point Inc.
2000-now	Ursula Pieper	Scientific Programmer	Research supervision	Scientific Programmer
2000-06	Andrea Rossi	Postdoc researcher	Research supervision	Senior Scientist, Rinat Laboratories, Pfizer Inc.
2003-04	Niu Huang	Postdoc researcher	Research supervision	Assistant Professor, Beijing, China
2003-06	Maya Topf	Postdoc researcher	Research supervision	Lecturer, Department of Crystallography, Birkbeck College, London
2002-06	Damien Devos	Postdoc researcher	Research supervision	Senior postdoc with Rob Russell, EMBL, Heidelberg
2003-06	Rachel Karchin	Postdoc researcher	Research supervision	Assistant Professor, Johns Hopkins University
1999-06	Marc Marti-Renom	Adjunct Assistant Professor	Research supervision	Assistant Professor, Prince Felipe Research Center, Valencia, Spain
2000-02	Valya Ilyin	Scientific Programmer	Research supervision	Associate Professor, Northeastern University, Boston
2002-03	Bozidar Yerkovich	Scientific Programmer	Research supervision	Head of Structural Bioinformatics at Rosetta Inpharmatics Inc., Seattle
1998-01	Francisco Melo	Postdoc researcher	Research supervision	Associate Professor, Pontificia Universidad Catolica de Chile
1996-99	Azat Badretdinov	Postdoc researcher	Research supervision	Senior scientific programmer at Accelrys Inc., San Diego

1999-03	Ash Stuart	Postdoc researcher	Research supervision	Assistant Professor, Ramapo College, Mahwah, NJ
1997-02	Andras Fiser	Postdoc researcher	Research supervision	Associate Professor, Albert Einstein College of Medicine, Bronx, NY
1995-97	Ilya Vakser	Postdoc researcher	Research supervision	Professor, University of Kansas, Lawrence, KS

FACULTY MENTORED:

Dates	**Name**	**Position while mentored**	**Mentoring Role**	**Current Position**
2010-now	Ryan Hernandez	Assistant Professor	Mentor	Assistant Professor, BTS
2004-now	Tanja Kortemme	Assistant Professor	Mentor	Associate Professor, BTS
2007-2008	Mats Gustafsson	Assistant Professor	Mentor	Assistant Professor, Physiology

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
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	Natalia Khuri	Biophysics	Thesis Committee member
2012	Sara Calhoun	Biophysics	Supervised Graduate Rotation
2012	Diego Garrido Ruiz	Biophysics	Supervised Graduate Rotation

SUMMARY OF TEACHING HOURS:

2005-06: 50 hours of teaching (including preparation).
Formal class or course teaching hours: 10 hours.
Informal teaching hours: 10 hours.
Mentoring hours: 500 hours.

2006-07: 50 hours of teaching (including preparation).
Formal class or course teaching hours: 10 hours.
Informal teaching hours: 10 hours.
Mentoring hours: 500 hours.

2007-08: 50 hours of teaching (including preparation).
Formal class or course teaching hours: 10 hours.
Informal teaching hours: 10 hours.
Mentoring hours: 500 hours.

2008-09: 50 hours of teaching (including preparation).
Formal class or course teaching hours: 10 hours.
Informal teaching hours: 10 hours.
Mentoring hours: 500 hours.

2009-10: 20 hours of teaching (including preparation).
Formal class or course teaching hours: 6 hours.
Informal teaching hours: 14 hours.
Mentoring hours: 500 hours.

2010-11: 10 hours of teaching (including preparation)
Formal class or course teaching hours: 3 hours
Informal teaching hours: 10 hours
Mentoring hours: 500 hours

TEACHING NARRATIVE:

Since my arrival 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. Patsy and I also give many of the lectures and supervise student activity associated with the courses (*eg*, student seminars, exercise sets). I also participate as a guest lecturer in a number of other courses, such as Macromolecules. And 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 three training grant re-submissions in 2007 (BMI and Biophysics) and 2008 (Complex Biological Systems).

RESEARCH AND CREATIVE ACTIVITIES	
RESEARCH AWARDS AND GRANTS:	
CURRENT	
U54 RR022220 (co-PI)	06/10/05 – 05/31/14
NIH/NIGMS	$279,658 direct/yr 7
Nuclear Information Pathway Center	$2,100,000 direct/yrs 1-9
U54 GM094662 (co-PI)	07/01/10 – 06/30/15
NIH/NIGMS	$150,000 direct/yr 1
New York Structural Genomics Research Consortium	$750,000 direct/yrs 1-5
U01 GM61390 (collaborator)	4/1/03-3/31/15
NIH/NIGMS	$45,000 direct/yr 7
Pharmacogenetics of Membrane Transporters	$600,000 direct/yrs 1-12
P01 GM71790 (collaborator)	7/1/04 - 6/30/14
NIH/NIGMS	$80,000 direct/yr 1
Deciphering Enzyme specificity	$800,000 direct/yrs 1-10
U54 GM074929 (co-PI)	7/1/05 – 6/30/14
NIH/NIGMS	$65,000 direct/yr 6
CSMP: Specialized Center for the Protein Structure Initiative	$650,000 direct/yrs 1-10
PN2 EY016525 (co-PI)	09/30/05 – 09/29/15
NIH	$50,000 direct/yr 6
Center for Protein Folding Machinery	$600,000 direct/yrs 1-10
R01 GM083960 (PI)	04/01/08 - 03/31/12
NIH/NIGMS	$180,000 direct/yr 3
IMP: Software for Hybrid Determination of Macromolecular Assembly Structures	$720,000 direct/yrs 1-4
U54 GM093342 (co-PI)	04/01/10 – 3/31/15
NIH/NIGMS	$170,000 direct/yr 1
Collaborative Center for an Enzyme Function Initiative	$850,000 direct/yrs 1-5
Pfizer Inc. (PI)	07/1/10 – 06/30/11
QB3	$70,000 direct/yr 1
A Computational Model of Allostery with Application to Antibody Design	
P01 AI091575-01 (co-PI)	07/13/11 – 06/30/15
NIH/NIGMS	$130,000 direct/yr 1
Protein Homeostasis Mechanism Underlying Enterovirus Replication and Evolution	$650,000 direct/yrs 1-5
U01 (co-PI)	07/01/11 – 06/30/15
NIH/NIGMS	$50,000 direct/yr 1
Nucleocytoplasmic Transport: A Target for Cellular Control	$200,000 direct/yrs 1-4

PENDING	
PAST	
Sinsheimer Scholar Award (PI)	09/01/96 - 08/31/98
Alexandrine and Alexander L. Sinsheimer Fund	
Knowledge based protein structure modeling for genome projects	
BIR-9601845 (PI)	10/01/96 – 09/30/98
NSF	
Acquisition of a multiprocessor computer for computational physics and structural biology	
Alfred P. Sloan Fellowship (PI)	10/01/98 – 09/30/00
Alfred P. Sloan Foundation	
Gift (PI)	07/01/98
Molecular Simulations Inc.	
R01 HL63284 (collaborator)	09/01/99 – 08/31/03
NIH/NHLBI	
Disruption and expression of mast cell protease genes	
Gift (PI)	07/01/00
Prospect Genomics Inc.	
Career Scientist Award (PI)	01/01/00 – 12/31/04
Irma T. Hirschl Monique Weill-Caulier Trust	
Comparative protein structure modeling for genomics	
Mathers Foundation Award (PI)	01/01/00 – 12/31/02
Mathers Foundation	
Comparative annotation of eukaryotic genomes: From gene detection to protein structure modeling	

R33 CA84699 (co-PI)	02/01/00 – 01/31/03
NIH/NCI	
Target selection for the structural genomics of cancer	
The Merck Genome Research Institute Award (PI)	02/01/00 – 01/31/02
The Merck Genome Research Institute	

Database of comparative protein structure models for genomics	
R33 CA89810 (collaborator)	06/01/01 – 03/31/04
NIH/NCI	
Comprehensive map of cellular protein interactions	
EDUD-7824-020257-US (PI)	07/03/01
Sun Academic Equipment Grant	
Development of an integrated software environment for high-throughput structural biology and automated comparative protein structure modeling	
RGP67/2003 (Co-PI)	07/01/03 – 06/30/06
Human Frontier Science Program Organization	
3-D Reconstruction and Identification of Postsynaptic Molecular Complexes Images by Electron cryotomography	
California Institute for Quantitative Biomedical Research (PI)	08/01/03 – 07/31/05
Towards a comprehensive map of protein-ligand interactions	
SUR Equipment Award (PI)	08/03/03
IBM Inc.	
Large-scale protein structure modeling and ligand docking	
Equipment Award (PI)	09/15/03
Intel Inc.	
Large-scale protein structure modeling and ligand docking	
EIA-0324645 (Co-PI)	11/01/03 – 10/31/06
NSF	
Subnanometer structure based fold determination of biological complexes	
Opportunity Award (PI)	02/15/04 – 02/14/06
Sandler Program in Basics Sciences	
Hierarchical framework for structural biology	
IIS-0705196 (PI)	08/01/07 - 07/31/09
NSF	
Integrated modeling of biological nanomachines	

P01 AI035707 (core PI)	7/1/04 - 6/30/09
NIH/AI	
Targeting Cysteine Proteases—Antiparasitic Chemotherapy	
Pfizer / QB3 Award (PI)	09/01/08 - 08/31/09
Pfizer Inc.	
Epitope mapping by combining protein-protein docking and varied low-resolution structural data	
Sandler Center for Basic Research in Parasitic Diseases (collaborator)	07/01/03 – 06/30/10
Sandler Family Supporting Foundation	
Bioinformatics of host-pathogen interactions	
EF 0626651 (collaborator)	1/1/08 -10/31/10
NSF	$17,261 direct/yr 1
The PhyloFacts phylogenomic encyclopedia of microbial protein families	$35,587 direct/yrs 1-2
S10 RR027100-01 (PI)	04/01/10 – 03/31/11
NIH/NIGMS	$499,512 direct/yr 1
High Performance Computing Cluster for Bioimaging & Computational Biology	
R01 GM54762 (PI)	7/1/96 – 6/30/10
NIH/NIGMS	$200,000 direct/yr 1
Protein Modeling by Satisfaction of Spatial Restraints	$2,500,000 direct/yr 1-13
U54 GM074945 (Co-PI)	09/30/00 – 08/31/10
SGX/NIH	$261,032 direct/yr 1
NYSGRC: A Large Scale Center for the Protein Structure Initiative	$2,700,000 direct/yrs 1-10
SP41RR001081-32S1 (collaborator)	09/15/09 – 09/14/11
NIH	$7,140 direct/yr 1
Resource for Biocomputing, Visualization, and Informatics	$14,500 direct/yr 1-2

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)

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.

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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.

RESEARCH PROGRAM (SEPARATE SUMMARY)

The following five articles represent much of the research of the Sali group. The role of the PI has been to largely conceive and lead the research.

1. NEW METHODS FOR HIGH-RESOLUTION PROTEIN STRUCTURE MODELING

M.-Y. Shen, A. Sali. “Statistical Potential for Assessment and Prediction of Protein Structure” Protein Science 15, 2507 – 2524, 2006.

We are concerned with essentially all aspects of protein structure prediction. In this paper, we addressed the problem of how best to extract information about the sequence-structure relationship from known protein structures. A general and formal statistical theory was developed, resulting in an accurate atomistic distance-dependent statistical potential.

2. NEW METHODS FOR FUNCTIONAL ANNOTATION OF PROTEINS

R. Karchin, A.N.A. Monteiro, S. V. Tavtigian, M. A. Carvalho, A. Sali “Functional impact of missense variants in BRCA1 predicted by supervised learning”. PLoS Computational Biology 3(2): e26, 2007.

We are developing methods for functional annotation of proteins based on their structures, be it experimentally determined or computationally predicted. In this paper, we developed and applied a method for predicting functional consequences of single point mutations in proteins.

3. INTEGRATIVE PLATFORM FOR STRUCTURAL BIOLOGY

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.

We are developing mathematical formalism and 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. 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.

4. APPLICATIONS OF BIOINFORMATICS TO SPECIFIC BIOLOGICAL SYSTEMS

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.

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. In this paper, we describe one such application, resulting in the determination of the molecular architecture of the nuclear pore complex that consists of 456 proteins of 30 different types.

5. A VIEW OF STRUCTURAL BIOLOGY

F. Alber, F. Förster, D. Korkin, M. Topf, A. Sali. “Integrating Diverse Data for Structure Determination of Macromolecular Assemblies.” Annual Review of Biochemistry 77, 443-477, 2008.

Technical advances on several frontiers have expanded the applicability of existing methods in structural biology and helped close the resolution gaps between them. As a result, we are now poised to integrate structural information gathered at multiple levels of the biological hierarchy — from atoms to cells — into a common framework. The goal is a comprehensive description of the multitude of interactions between molecular entities, which in turn is a prerequisite for the discovery of general structural principles that underlie all cellular processes.