UNIVERSITY OF CALIFORNIA AT SAN FRANCISCO

Curriculum vitæ

Name: Andrej Sali

Position: Professor, Step VIII
Department of Bioengineering and Therapeutic Sciences
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-now	Director, California Institute for Quantitative Biosciences (QB3) at UCSF
2003-now	Vice Chair, Department of Bioengineering and Therapeutic Sciences
2003-now	Faculty, California Institute for Quantitative Biosciences (QB3)
2003-now	Faculty, Pharmaceutical Sciences and Pharmacogenomics Graduate Program
2003-now	Faculty, Biophysics Graduate Program
2003-now	Faculty, Bioinformatics and Medical Informatics Graduate Program
2003-now	Faculty, 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 Chancelors, 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	Scientific Advisory Committee

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	Organizer, Keystone Conference on Frontiers in Structural Biology

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 6^{th} 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. Speaker at the Institute of Structural Molecular Biology, Birkbeck Institute, London, England, June 17-18, 2010

NATIONAL, REGIONAL AND OTHER INVITED PRESENTATIONS

48. Second International Georgia Tech Conference in Bioinformatics, Atlanta, Georgia, USA. November 12, 1999.
49. Structural Genomics Targets Workshop, NIH, Washington DC, USA. February 11, 1999.
50. Advances & Opportunities at the Biology/Math/Computational/Physical Sciences Interface, Rutgers University, New Brunswick, NJ, USA. March 6, 1999.
51. Mount Sinai School of Medicine, New York, NY, USA. March 19, 1999.
52. New York Structural Biology Group, New York Academy of Sciences, New York, NY, USA. March 24, 1999.
53. Columbia University, New York, NY, USA, 1999.
54. Chemistry Dept., New York University, New York, NY, USA, 1999.
55. Protein Sequence Structure Function Meeting, UCSF, San Francisco, CA, USA. April 23, 1999.
56. The Scripps Institute, La Jolla, CA, USA. August 13, 1999.
57. Mathematical Problems in the Molecular Sciences, Courant Institute, New York, NY, USA. October 10, 1999.
58. City College of New York, New York, USA. October 20, 1999.
59. Agouron Pharmaceuticals, San Diego, California, USA. October 28, 1999.
60. Structural Genomics Conference, ANL, Chicago, Illinois, USA. November 16, 1999.
61. Structural Genomics and the Pharmaceutical Industry, Princeton, New Jersey, USA. November 18, 1999.
62. Quantitative Challenges in the Post Genomic Sequence Era, La Jolla Interfaces in Science, San Diego,

California, USA. January 12, 2000.
63. UCSD, Dept of Physics, San Diego, California, USA. January 19, 2000.
64. UCSF, San Francisco, California, USA. January 20, 2000.
65. Center for Physics and Biology, Rockefeller University,New York, New York, USA. January 24, 2000.
66. Biological Chemistry Seminar Series, University of Penn, Philadelphia, Pennsylvania, USA. February 17, 2000.
67. ABRF 2000 ``From Singular to Global Analyses of Biological Systems", Bellevue, Washington, USA. February 22, 2000.
68. AAAS conference, Washington DC, USA. March 20, 2000.
69. Keystone Symposium on Macromolecular Assemblies at Work: Application of Physics, Chemistry, and Mathematics to Biology, Durango, Colorado, USA. March 25, 2000.
70. Bio2000, Boston, Massachusetts, USA. March 28, 2000.
71. Computational Challenges of the Post Genomic Age, SUN, San Francisco, California, USA. May 12, 2000.
72. Biopolymers Gordon Conference, Newport, Rhode Island, USA. June 18-22, 2000.
73. 2000 FASEB Summer Research Conference on Protein Folding in the Cell, Saxton River, Vermont, USA. July 22-27, 2000.
74. Monsanto/Pharmacia lectureship series, Univ. of Saint Louis, Missouri, USA. September 28, 2000.
75. Workshop on Structural Genomics. NIGMS, Washington DC, USA. October 23, 2000.
76. Genomics and Bioinformatics, UMD, New Brunswick, New Jersey, USA. November 2, 2000.
77. University of Minnesota, Minneapolis, Minnesota, USA. November 27, 2000.
78. Oncogenomics: Dissecting Cancer Through Genome Research, Nature Genetics, Tuscon, Arizona, USA. January 25-27, 2001.
79. UAB, Birmingham, Alabama, USA. February 26, 2001.
80. Bard College, New York, USA. April 18, 2001.
81. Physics/Chemistry. CSUN, Northridge, California, USA. May 2, 2001.
82. ACS Meeting, Chicago, Illinois, USA. August 26-30, 2001.
83. University of Maryland, Maryland, USA. October 2, 2001.
84. Columbia University, New York, New York, USA. October 15, 2001.
85. Mast Cell Workshop, Bethesda, Maryland, USA. November 26-30, 2001.
86. Genomics Seminar Series, Skirball Institute, New York, New York, USA. February 6, 2002.
87. Mining the Human Genome for New Drug Discovery - New Ways of Handling Orphan Targets. NYAS, New York, New York, USA. February 26, 2002.
88. Biological Processes for New and Innovative Engineering Systems and Applications, ARO workshop, Research Triangle Park, North Carolina, USA. February 26-27, 2002.
89. New York City Blood Centre, New York, New York, USA. March 7, 2002.
90. Proteomics - The New Frontiers: Discovery, Separation, Prediction & Modeling, University of Delaware, Newark, Delaware, USA. March 14-15, 2002.
91. Harvard University, Cambridge, Massachusetts, USA, March 28, 2002.
92. Molecular Cell Biology and Biochemistry Seminar Series, Virginia Tech, Blacksburg, Virginia, USA. April 5, 2002.
93. UCSF, San Francisco, California, USA, April 15, 2002.
94. A Workshop on large biological structures, Asilomar, California, USA. April 20-22, 2002.
95. SCBMB Program, Baylor College of Medicine, Houston, Texas, USA. May 15, 2002.
96. 50th ASMS conference American Society of Mass Spectrometry, Orlando, Florida, USA. June 2-6, 2002.

97. The 5th Summer Session of the New York Structural Biology Discussion Group , Cold Spring Harbor Laboratory, New York, USA. June 26, 2002.
98. Berkeley-Stanford summer school for protein crystallography, SSRL, Stanford, California, USA. July 8-12, 2002.
99. Gordon Conference on Diffraction Methods in Structural Biology, Connecticut College, New London, Connecticut, USA. July 14-19, 2002.
100. NYCBS New York Computational Biology Society seminar, NAS, New York, New York, USA. September 18, 2002.
101. Center for Biological Modeling, Michigan State University, East Lansing, Michigan, USA. September 27, 2002.
102. Bioinformatics seminar, Texas A&M University, Tamu, TX, USA. November 7, 2002.
103. Structure and Function of the Proteome, Argonne National Laboratory, Argonne, Illinois, USA. November 23-24, 2002.
104. Keystone Symposium in Proteomics: Technologies and Applications, Keystone Resort in Keystone, Colorado, USA. March 25-30, 2003.
105. NCRR sponsored Workshop on Structural Proteomics of Complexes, Bethesda, Maryland, USA. April 7-8, 2003.
106. American Society for Biochemistry and Molecular Biology meeting, San Diego, California, USA. April 11-15, 2003.
107. St. Jude Children's Research Hospital, Memphis, TN, USA. April 22, 2003.
108. Genentech, Inc., South San Francisco, CA, USA. April 29, 2003.
109. Structure and Function of Proteome, SBC, Argonne National Laboratory, Argonne, Illinois, USA. Spring, 2003.
110. "Frontiers of Bioinformatics" symposium, Center of Excellence in Bioinformatics, University at Buffalo, Buffalo, New York, USA. June 6-8, 2003.
111. IBM Thomas J. Watson Research Center, New York, New York, USA. June 11, 2003.
112. 2003 Gordon Research Conference on 3D Electron Microscopy of Macromolecules, Colby Sawyer College, New London, New Hampshire, USA. June 22-26, 2003.
113. PSI workshop ond data management, NIH Campus, Bethesda, MD, USA. July 10-11, 2003.
114. GTL and Beyond: Data and Computational Needs Workshop, San Francisco, CA, USA. September 10-11, 2003.
115. 2003 Pharmaceutical Sciences and Pharmacogenomics Retreat, Marshall, CA, USA. September 11-13, 2003.
116. Structure and Chemistry Seminar at Scripps, San Diego, CA, USA. September 18, 2003.
117. Seminar at Northeastern University, Boston, MA, USA. October 6, 2003
118. Workshop on Visualization of Biological Complexes, Four Points Sheraton Hotel, Emeryville, San Francisco Bay Bridge, CA, USA. October 11-12, 2003
119. Seminar at PARC, Palo Alto, CA, USA. October 15, 2003.
120. NIGMS Homology Modeling Workshop, Bethesda, MD, USA. October 21-22, 2003.
121. Seminar at Purdue University, West Lafayette, IN, USA. October 24-25, 2003.
122. PSI Target Selection Workshop, Bethesda, MD, USA. November 13-14, 2003.
123. Biophysics/CCB Retreat, Asilomar Conference Center, Pacific Grove, CA, USA. December 7-9, 2003.
124. Licensing Executives Society meeting, San Francisco, CA, USA. February 12, 2004.
125. The Structural, Functional and Evolutionary Gordon Conference, Four Points Sheraton Harbortown, Ventura, CA, USA. February 15-20, 2004.
126. Seminar at Berkeley, Berkeley, CA, USA. March 8, 2004.

127. Seminar at UCSC, Santa Cruz, CA, USA. March 11, 2004.
128. Workshop on Structure Determination of Macromolecular Machines and Assemblies by Hybrid Methods, Granlibakken/Lake Tahoe Conference Center, CA, USA. March 17-20, 2004.
129. 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.
130. 2004 Keystone Symposium on Structural Genomics, Snowbird Resort, Snowbird, Utah, USA April 13-19, 2004.
131. BayGenomics PGA, San Francisco, CA, USA. April 27, 2004.
132. Gladstone Scientific Retreat, Asilomar in Monterey County, CA, USA. May 18-20. 2004.
133. Seminar at Caltech, Pasadena, CA, USA. October 12, 2004.
134. ICSG 2004 Meeting, Washington, DC, USA. November 17-24, 2004.
135. Workshop of the Center of Protein Folding Machinery, Stanford University, CA, USA. December 4-5, 2004.
136. Biological and Medical Informatics/Biophysics/Chemistry and Chemical Biology graduate groups retreat, Asilomar Conference Center, Pacific Grove, CA, USA. December 5-7, 2004.
137. ABRF meeting, Biomolecular Technologies:Discovery to Hypothesis, Savanah, Georgia, USA. February 5-8, 2005.
138. Frontiers in Computational Biophysics Symposium, NIH campus in Bethesda, MD, USA. April 29-30, 2005.
139. NIH Symposium on Structural Analysis of Large Assemblies: Sizing up the Challenges, NIH campus in Bethesda, MD, USA. June 2-3, 2005.
140. SRI's Computational Biology series, SRI International, Menlo Park, CA, USA. June 29, 2005.
141. 19th Annual Symposium of the Protein Society, Boston, MA, USA. July 30 - August 3, 2005.
142. GRC 2005 Computer-aided design meeting, Tilton School, NH, USA. July 31 - August 5, 2005.
143. Seminar at the Biochemical and Biophysical Methods Course Fall 2005, The Rockefeller University, New York, NY, USA. October 11, 2005.
144. Seminar at the Novartis Institutes for BioMedical Research, Cambridge, MA, USA. November 9, 2005.
145. Workshop on Biological Macromolecular Structure Models, The State University of New Jersey, Piscataway, NJ, USA. November 19-20, 2005.
146. Organizer and Speaker of the Theme "Macromolecular Structure and Dynamics" with 4 Symposia. ASBMB 2006 meeting, San Francisco, CA, USA. April 1-5, 2006.
147. Seminar at UC Davis, CA. June 1, 2006.
148. Symposium at Wyeth Research, Cambridge, MA, USA. October 16, 2006.
149. Seminar at the University of Massachusetts, Dept. of Biochemistry and Molecular Pharmacology, Worcester, MA, USA. October 18, 2006.
150. Seminar at the Fifth Annual Systems Biology Course at the Institute for Systems Biology, Seattle, WA, USA. 9 November 2006.
151. Seminar at UC Merced Center for Computational Biology, Merced, CA, USA. 30 November 2006.
152. TDR/WHO Drug Target Selection Meeting in Seattle, OR, USA. 1 December, 2006.
153. Biological and Medical Informatics/Biophysics/Chemistry and Chemical Biology Graduate Groups Retreat, Monterey, CA, USA. 3-5 December, 2006.
154. Collaborative Drug Discovery meeting, UCSF, San Francisco, USA. 1 March 2007
155. The Protein Folding Center Annual Retreat, Stanford, CA, USA. 27-29 May 2007.
156. Seminar at the Center for Theoretical Biological Physics. UCSD,San Diego USA. 1 June, 2007.
157. Institute for Systems Biology, Seattle, WA, 12 July 2007.

158. Seminar at Genentech, San Francisco, CA, 25 September 2007.
159. Seminar at the SCRIPPS Institute, La Jolla, CA, USA. September 27-28
160. Speaker and Organizer of the Modeling of Protein Interactions Meeting, MPI-2007, Lawrence, KA, USA, September 30 - October 2, 2007.
161. Seminar at the Albert Einstein College of Medicine, New-York, NY. 16 October 2007.
162. Seminar at University of California Berkeley, New-York, NY. 25 October 2007.
163. Seminar at the Carolina Center for Genomic Sciences colloquium, UNC, Chapel Hill, NC, USA. 9 November 2007.
164. Seminar at the Duke University Computational Biology Series, Durham, NC, USA. 12 November 2007.
165. Keystone Symposium on Structural Genomics and Its Applications to Chemistry, Biology and Medicine, Steamboat Springs, Colorado, CO, USA, 6-11 January 2008.
166. Seminar for the Biochemical and Biophysical Methods Course at the Rockefeller University, New York, NY. 30 January 2008.
167. Seminar at the University of Utah, February 25 2008.
168. Seminar at The Buck Institute for Age Research, Novato, CA, USA, July 1 2008.
169. Speaker and Organizer of the Protein Modeling Workshop, University of California, San Francisco, CA, USA, July 11-12 2008.
170. Speaker at the 2008 Senior Vice Chancellor's Laureate Lecture Series at the University of Pittsburgh, July 18 2008.
171. Protein Structure Initiative (PSI3), Washington DC, USA, October 29-30, 2008.
172. Seminar at UT Southwestern Medical Center, 5-6 Nov 2008.
173. Biology and Mathematics in the Bay Area (BaMBA), University of California, Davis, CA,USA, November 15, 2008.
174. Biological and Medical Informatics/Biophysics/Chemistry and Chemical Biology Graduate Groups Retreat, Monterey, CA, USA. 7-9 December, 2008.
175. NCMI Single Particle Reconstruction Workshop, Baylor College of Medicine, Houston, TX, USA, December 10-13, 2008**.**
176. Seminar at the University of Pennsylvania School of Medicine, Philadelphia, PA, USA, January 29, 2009.
177. Mesilla Chemistry Workshop Multi-Scale Modeling of Biological Molecules, Mesilla, TX, USA, February 1-4, 2009.
178. Technology Centers for Networks and Pathways Annual All Hands Meeting, Washington DC, USA, March 12-13, 2009
179. 2009 Symposium on Molecular Systems Biology of the Cell, Seattle, WA, USA, April 19, 2009.
180. Seminar at the University of Minnesota, Minneapolis, MN, USA, April 22, 2009.
181. Seminar at the University of Washington, Seattle, WA, USA, May 14, 2009.
182. Seminar at Indiana University, Indianapolis, IN, USA, May 18, 2009.
183. Seminar at University of Texas Southwestern, Dallas, TX, USA, May 20-21, 2009.
184. 23rd Annual Symposium of the Protein Society, Boston, MA, USA, July 25-29, 2009.
185. Beckman Institute 20th Anniversary Symposium, University of Illinois at Urbana-Champaign, Urbana, IL, USA, September 20-23, 2009.
186. Speaker and Co-Organizer of the Keystone Symposia on Structural Biology/Structural Genomics, Steamboat Springs, CO, USA, January 8-13, 2010.
187. Speaker at the Hybrid Methods Symposium, Lake Tahoe, CA, USA, March 10-14, 2010

GOVERNMENT AND OTHER PROFESSIONAL SERVICES:

2004-09	National Institutes of Health	MSF-B Study Section (successor of BBCA)
1995-now	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 at 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-now	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-now	Rock Hall Governance Committee
2005-now	QB3 Governance/Community Committee, Chair
2005-now	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-now	Systems Biology Faculty Search Committee
2005-now	Systems Biology HHMI/NIBIB Training Grant Leadership Committee
2007-now	BMI Training Grant Leadership Committee
2007-now	Quantitative Imaging Faculty Search Committee
2008-now	Human Genetics Faculty Search Committee, Co-Chair

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

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
	2003-now	Bioengineering, Macromolecules	Occasional Guest Lecturer		

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
2007-now	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	Assistant Professor, Mount Sinai School of Medicine, NY

POSTDOCTORAL FELLOWS DIRECTLY SUPERVISED OR MENTORED:

Dates	Name	Fellow	Role	Current Position
2009-now	Sebnem Essiz	Postdoc researcher	Research supervision	Postdoc researcher
2009-now	Elina Tijoe	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**
2004-now	Tanja Kortemme	Assistant Professor	Mentor	Assistant 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	Allan 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

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.

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

1. R01 GM54762 (PI)	7/1/96 - 6/30/09
NIH/NIGMS	$200,000 direct/yr 1
Protein Modeling by Satisfaction of Spatial Restraints	$2,500,000 direct/yrs 1-13
2. U54 RR022220 (co-PI)	09/01/06 – 08/31/10
NIH	$280,809 direct/yr 1
Nuclear Information Pathway Center	$1,311,851 direct/yrs 1-5
3. IIS-0705196 (PI)	08/01/07 - 07/31/09
NSF	$101,694 direct/yr 1
Integrated modeling of biological nanomachines	direct/yrs 1-2
4. U54 GM074945 (co-PI)	09/30/00 – 08/31/10
SGX/NIH	$261,032 direct/yr 1
NYSGXRC: A Large Scale Center for the Protein Structure Initiative	$2,700,000 direct/yrs 1-10
5. U01 GM61390 (collaborator)	4/1/03-3/31/10
NIH/NIGMS	$63,203 direct/yr 1
Pharmacogenetics of Membrane Transporters	$600,000 direct/yrs 1-9
6. P01 AI035707 (core PI)	7/1/04 - 6/31/09
NIH/AI	$20,000 direct/yr 1
Targeting Cysteine Proteases—Antiparasitic Chemotherapy	$80,000 direct/yrs 1-4

7. P01 GM71790 (collaborator) 7/1/04 - 6/30/09
NIH/NIGMS $80,000 direct/yr 1
Deciphering Enzyme specificity $400,000 direct/yrs 1-5

8. U54 GM074929 (co-PI) 7/1/05 – 6/30/10
NIH/NIGMS $65,000 direct/yr 1
Specialized Center for the Protein Structure Initiative $325,000 direct/yrs 1-5

9. PN2 EY016525 (co-PI) 09/30/05 – 09/29/10
NIH $70,780 direct/yr 1
Center for Protein Folding Machinery $325,534 direct/yrs 1-5

10. EF 0626651 (collaborator) 1/1/08 -12/31/11
NSF $11,197 direct/yr 1
The PhyloFacts phylogenomic encyclopedia of microbial protein families $35,587 direct/yrs 1-2

11. R01 GM083960 (PI) 04/01/08 - 03/31/12
NIH/NIGMS $180,000 direct/yr 1
IMP: Software for Hybrid Determination of Macromolecular Assembly Structures $720,000 direct/yrs 1-4

12. Pfizer / QB3 Award (PI) 09/01/08 - 08/31/09
Pfizer Inc. $185,000 direct/yr 1
Epitope mapping by combining protein-protein docking and varied low-resolution structural data

13. Sandler Center for Basic Research in Parasitic Diseases (collaborator) 07/01/08 – 06/30/10
Sandler Family Supporting Foundation $20,000 direct/yr 2
Bioinformatics of host-pathogen interactions

PENDING

1. P01 GM71790 (collaborator) 7/1/10 - 6/30/15
NIH/NIGMS $100,000 direct/yr 1
Deciphering Enzyme specificity $500,000 direct/yrs 1-5

2. U54 RR022220 (co-PI) 09/01/10 – 08/31/14
NIH $290,000 direct/yr 1
Nuclear Information Pathway Center $1,000,000 direct/yrs 1-4

3. TBD (PI) 04/01/11 – 03/31/12
NIH $499,512 direct/yr 1
High Performance Computing Cluster for Bioimaging & Computational Biology $499,512 direct/yr 1

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
3D-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

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)

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.." *Biological Chemistry 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.." *Journal of Molecular Biology* **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 in Biochemical Sciences* **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.." *Journal of Molecular Biology* **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.." *Current Science* **59**, 867-874, 1990.

16. M.S. Johnson, A. Sali, T.L. Blundell. "Phylogenetic relationships from three-dimensional protein structures.." *Methods in Enzymology* **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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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.

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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 Science* **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 Engineering* **5**, 43-51, 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.." *Journal of Biological Chemistry* **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.

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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.." *Journal of Chemical Physics* **101**, 1444-1451, 1994.

36. M. Karplus, A. Sali. "Theoretical studies of protein folding and unfolding.." *Current Opinion in Structural Biology* **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.

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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.." *Journal of Biological Chemistry* **270**, 19524-19531, 1995.

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44. A. Sali, L. Potterton, F. Yuan, H. van Vlijmen, M. Karplus. "Evaluation of comparative protein modeling by MODELLER.." *Proteins* **23**, 318-326, 1995.

45. A. Sali. "Modeling mutations and homologous proteins.." *Current Opinion in Biotechnology* **6**, 437-451, 1995.

46. M. Karplus, A. Sali, E. Shakhnovich. "Kinetics of protein folding.." *Nature* **373**, 664-665, 1995.

47. Y. Sheng, A. Sali, H. Herzog, J. Lahnstein, S.A. Krilis. "Site-directed mutagenesis of recombinant human beta 2-glycoprotein I identifies a cluster of lysine residues that are critical for phospholipid binding and anti-cardiolipin antibody activity.." *Journal of Immunology* **157**, 3744-3751, 1996.

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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).

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.