

UNIVERSITY OF CALIFORNIA AT SAN FRANCISCO

Curriculum vitae

Name: Andrej Sali

Position: Professor, Step X
 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

Address: Byers Hall, Suite 503B, MC 2552
 University of California at San Francisco
 1700 4th Street
 San Francisco, CA 94158-
 2330 Voice: +1-415-514 4227
 Fax: +1-415-514 4231
 Email: sali@salilab.org
 Web: <http://salilab.org>

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
 2003-2013 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.
 2014 Fellow, International Society for Computational Biology (ISCB)

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:**

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
2009-2013	PROSPECTS (Proteomics Specification in Time and Space) consortium	Scientific Advisory Committee
2010	Keystone Symposia	Scientific Advisory Board (<i>ad hoc</i>)
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
2014-now	Protein Data Bank	Hybrid Methods 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
2007 Program Committee, 4th Conference on Modeling of Protein Interactions (MPI)
2008 Organizer, Workshop on Applications of Protein Structure Models in Biomedical Research,

	UCSF, CA
2010	Program Committee, 3DSIG symposium at ISMB conference, Boston
2010	Co-Organizer, Keystone Symposia on Frontiers in Structural Biology
2012	Co-Organizer, Keystone Symposia on High-Throughput Structural Biology
2012	Co-Organizer, Conference on Structural Analysis of Supramolecular Assemblies by Hybrid Methods, Lake Tahoe
2013	Organizer, Keystone Symposia on Structural Analysis of Supramolecular Assemblies by Hybrid Methods, Lake Tahoe
2014	Organizer, Martin Karplus Celebration Symposium
2006-now	Organizer, World Molecular Engineering Network, annual TSRI & UCSF meeting in San Jose del Cabo, Mexico

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. Plenary Speaker at the Molecular Modeling Meeting, Queenstown, New Zealand, August 30-September 1, 2012.
60. Speaker at the IISc Conference, Bangalore, India, January 8-11, 2013.
61. Speaker at the Swiss Federal Institute of Technology, Lausanne, Switzerland, January 14, 2013.
62. Speaker at the Biozentrum Lecture, Basel, Switzerland, January 15, 2013.

63. Organizer and Speaker at the 23rd World Molecular Engineering Network Conference, Cabo San Lucas, Mexico, May 5-8, 2013.
64. Speaker at the Bioinformatics Meeting, Recife, Brazil, November 3-7, 2013.
65. Speaker at the Lorne Conference, Victoria, Australia, February 9-13, 2014.
66. Speaker at Shanghai Tech University, Shanghai, China, March 14-18, 2014.
67. Organizer and Speaker at the 24th World Molecular Engineering Network Conference, Cabo San Lucas, Mexico, May 4-7, 2014.
68. Keynote speaker at the Emerging Trends in Computational Biology Conference, Singapore, June 20-21, 2014.
69. Speaker at the PDB Hybrid Methods Task Force Meeting, EMBL-EBI, Hinxton, UK, October 6-7, 2014.
70. Seminar at A*Star BII, Singapore, March 12-14, 2015.
71. Organizer and Speaker at the 25th World Molecular Engineering Network Conference, Cabo San Lucas, Mexico, May 3-6, 2015.
72. Speaker at the GRC on Computational Aspects of Biomolecular NMC, Il Ciocco, Italy, June 7-12, 2015.
73. Speaker at the 29th Annual Symposium of the Protein Society, Barcelona, Spain, July 22-25, 2015.
74. Speaker at iHuman Institute, Shanghai Tech University, Shanghai, China, July 27-31, 2015.
75. Speaker at the Hybrid Methods Meeting, Osaka, Japan, October 2-4, 2015.

NATIONAL, REGIONAL AND OTHER INVITED PRESENTATIONS

1. Second International Georgia Tech Conference in Bioinformatics, Atlanta, Georgia, USA. November 12, 1999.
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. NCCR 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 on 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, Savannah, 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. NCM 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.
- 166.Speaker at the NRAMM Workshop, Scripps Research Institute, San Diego, CA, USA, November 16, 2012.
- 167.Seminar at NIH, Bethesda, MD, USA, January 17, 2013.
- 168.Speaker at the Herron Lecture, Florida State University, Tallahassee, FL, USA, February 15, 2013.
- 169.Speaker at the Hauptman-Woodward Medical Research Institute, Buffalo, NY, USA, March 28, 2013.
- 170.Seminar at Harvard University, Cambridge, MA, USA, February 3, 2014.

- 171.Seminar at Columbia University, New York, NY, USA, February 5, 2014.
 172.Seminar at the Scripps Research Institute, San Diego, CA, USA, February 24-25, 2014.
 173.Seminar at UC Berkeley, Berkeley, CA, USA, March 10, 2014.
 174.Keynote Speaker at the 2014 Biopolymers Gordon Research Conference, Salve Regina University, Newport, RI, USA, June 1-6, 2014.
 175.Keynote Speaker at the 2014 Annual RosettaCon, Leavenworth, WA, USA, July 30-August 1, 2014.
 176.Speaker at the Peter Wright Symposium, University of California, San Francisco, CA, USA, September 15, 2014.
 177.Speaker at the NCI Workshop at the Houston Methodist Research Institute at Texas Medical Center, Houston, TX, USA, September 18-19, 2014.
 178.Organizer of the Martin Karplus Celebration Symposium, San Francisco, CA, USA, October 1, 2014.
 179.Speaker at the International Society for the Study of Xenobiotics meeting, San Francisco, CA, USA, October 19-23, 2014.
 180.Seminar at Rutgers University, New Brunswick, NJ, USA, October 29, 2014.
 181.Seminar and Biophysics Course at the Scripps Research Institute, San Diego, CA, USA, February 26-27, 2015.
 182.Speaker at the U.S. Human Proteome Organization (US-HUPO) Annual Meeting, Tempe, AZ, USA, March 15-18, 2015.
 183.Speaker at the American Chemical Society National Meeting, Denver, CO, USA, March 22-26, 2015.
 184.Seminar at the University of Florida Genetics Institute, Gainesville, FL, USA, April 14, 2015.
 185.Seminar at the Oregon Health and Science University, Portland, OR, USA, May 19, 2015.

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	<i>ad hoc</i> Grant Reviews

UNIVERSITY AND PUBLIC SERVICE:

UNIVERSITY SERVICE:

UCSF

2003-now	<i>Ad hoc</i> Faculty reviews (~30)
2003	Future of Computing at UCSF Committee
2003-2007	MD/PhD Scientist in QB3 Search Committee
2003-2005	Byers Hall (QB3) Building Committee Pharmaceutical Sciences and Pharmacogenomics Graduate Program
2003-2005	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

4/8/15

Andrej Sali

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
2011-now IT Governance Committee on Research Technology
2012-now Enabling Technologies Advisory Committee
2012 Gladstone Institute Faculty Search Committee
2012-now Institute for Computational and Health Sciences Infrastructure Committee
2012-now Institute for Computational and Health Sciences Executive Committee
2012-now Funding Shared Equipment Awards Committee
2012-now Bioimaging Faculty Search Committee
2013-now Data Center Services Advisory Board
2013-now 2.0-Ideation for the Future of UCSF Committee
2013-now Shared Research Facilities Roadmap Steering Committee
2014-now Institute for Neurodegenerative Diseases 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
2010-2011 SOP Faculty Awards Committee
2012-2014 SOP Educational Policy Committee
2014-now SOP Frontiers in Science and Practice of Therapeutics Committee

DEPARTMENTAL SERVICE

2003-now BTS Internal Advisory Committee

2013-now PSPG Graduate Program Admissions 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
F	2010	Bioinformatics BMI-206	Organizer, Lecturer	3	15
F	2012	Bioinformatics BMI-206	Lecturer	3	15
F	2013	Bioinformatics BMI-206	Lecturer	3	15
W	2013	BPS 134	Lecturer	3	6
F	2013	NSF proposal course	Lecturer		
F	2014	NSF proposal course	Lecturer		
F	2014	Bioinformatics BMI-206	Lecturer	3	15
W	2014	BPS 134	Lecturer	3	6
W	2003-now	Macromolecular Interactions BP-204	Occasional Guest Lecturer	4	20
W	2011-now	Chem 204	Guest Lecturer	2	3
W	2015-now	Systems Pharmacology, Pharmacogenomics 245B	Guest Lecturer	4	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).
- Annual guest lecturer at the structural biology course at Scripps Institute, organized by Ian Wilson, since 2007.

PREDOCTORAL STUDENTS SUPERVISED OR MENTORED:

Dates	Name	Program or School	Role	Current Position
1995-00	Roberto Sanchez	Rockefeller University	PhD Advisor	Associate Professor, Mount Sinai School of Medicine, NY
1999-01	Eric Feyfant	Rockefeller University	PhD Advisor	Senior Scientist, Wyeth Inc. Cambridge, MA.
1999-03	Nebojsa Mirkovic	Rockefeller University	PhD Advisor	Postdoctoral fellow with Diana Murray at Weill Medical College of Cornell University, NY
2000-03	Bino John	Rockefeller University	PhD Advisor	Assistant Professor, University of Pittsburg
2002-08	Ranyee Chiang	BMI	PhD Advisor	Postdoc at New York University
2003-07	Fred Davis	Biophysics	PhD Advisor	Postdoc at Janelia Farm, HHMI
2003-08	Michael Kim	BMI	PhD Advisor	The Mechanical Zoo
2003-08	Libusha Kelly	BMI	PhD Advisor	Postdoc at MIT, with Penny Chisholm
2004-08	David Eramian	Biophysics	PhD Advisor	Patent Counsel, eBay Inc.
2005-08	Mark Peterson	BMI	PhD Advisor	The Boston Consulting Group
2006-11	David Barkan	BMI	PhD Advisor	Staff Scientist, Protagonist Therapeutics
2006-11	Keren Lasker	Tel-Aviv University	PhD Advisor	Postdoctoral Fellow, Stanford University
2007-09	Adam Marko	BMI	MSc Advisor	Asuragen, Inc., Austin, TX Bioinformatics Developer
2007-12	Jeremy Phillips	BMI	PhD Advisor	Genome Institute/LBL Bioinformatics Analyst
2009-14	Peter Cimermanic	BMI	PhD Advisor	UCSF Specialist
2010-14	Natalia Khuri	Biophysics	PhD Advisor	Graduate Student
2010-now	Charles Greenberg	BMI	PhD Advisor	Graduate Student
2012-now	Adrian Stecula	PSPG	PhD Advisor	Graduate Student
2012-now	Sara Calhoun	Biophysics	PhD Advisor	Graduate Student
2014-now	Ilan Chemmama	Biophysics	PhD Advisor	Graduate Student

POSTDOCTORAL FELLOWS DIRECTLY SUPERVISED OR MENTORED:

Dates	Name	Fellow	Role	Current Position
1995-97	Ilya Vakser	Postdoc researcher	Research supervision	Professor, University of Kansas, Lawrence, KS
1996-99	Azat Badretdinov	Postdoc researcher	Research supervision	Senior scientific programmer at Accelrys Inc., San Diego
1997-02	Andras Fiser	Postdoc researcher	Research supervision	Associate Professor, Albert Einstein College of Medicine, Bronx, NY
1998-01	Francisco Melo	Postdoc researcher	Research supervision	Associate Professor, Pontificia Universidad Catolica de Chile
1999-03	Ash Stuart	Postdoc researcher	Research supervision	Assistant Professor, Ramapo College, Mahwah, NJ
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
2000-06	Andrea Rossi	Postdoc researcher	Research supervision	Senior Scientist, Rinat Laboratories, Pfizer Inc.
2000-2007	M.S. Madhusudhan	Postdoc researcher	Research supervision	Assistant Professor, Bioinformatics Institute, Singapore
2000-2008	Narayanan Eswar	Scientific Programmer	Research supervision	Group Leader, Du Pont Inc.
2000-2014	Ursula Pieper	Scientific Programmer	Research supervision	Web Applications Specialist, National Agricultural Library
2001-2007	Frank Alber	Postdoc researcher	Research supervision	Assistant Professor, University of Southern California
2002-03	Bozidar Yerkovich	Scientific Programmer	Research supervision	Head of Structural Bioinformatics at Rosetta Inpharmatics Inc., Seattle
2002-06	Damien Devos	Postdoc researcher	Research supervision	Senior postdoc with Rob Russell, EMBL, Heidelberg
2002-2007	Dmitry Korkin	Postdoc researcher	Research supervision	Assistant Professor, University of Missouri at Columbia
2003-04	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
2003-06	Rachel Karchin	Postdoc researcher	Research supervision	Assistant Professor, Johns Hopkins University

2003-2008	Min-yi Shen	Postdoc researcher	Research supervision	Postdoc researcher
2003-now	Ben Webb	Scientific Programmer	Research supervision	Scientific Programmer
2005-2008	Friedrich Foerster	Postdoc researcher	Research supervision	MPI Martinsried, Germany Group leader
2006-2013	Javier Velazquez	Postdoc researcher	Research supervision	Cypher Genomics Bioinformatics Analyst
2006-2014	Hao Fan	Postdoc researcher	Research supervision	A*STAR, Singapore Principal Investigator
2007-2014	Daniel Russel	Postdoc researcher	Research supervision	AltSchool Senior Research Engineer
2008-12	Avner Schlessinger	Postdoc researcher	Research supervision	Mount Sinai School of Medicine Assistant Professor
2008-now	Dina Schneidman	Postdoc researcher	Research supervision	Specialist
2008-now	Seung-Joong Kim	Postdoc researcher	Research supervision	Specialist
2009-2010	Sebnem Essiz	Postdoc researcher	Research supervision	Assistant Professor, Kadir Has University, Istanbul
2009-2014	Guangqiang Dong	Postdoc researcher	Research supervision	Data Scientist, Facebook
2009-2014	Patrick Weinkam	Postdoc researcher	Research supervision	Lead Engineer, Data Science, Baselayr
2009-now	Elina Tjioe	Scientific Programmer	Research supervision	Scientific Programmer
2010-11	Backy Chen	Postdoc researcher	Research Supervision	Institute of Biomedical Science, Academia Sinica, Taiwan, Postdoc Researcher
2010-2013	Massimiliano Bonomi	Postdoc researcher	Research Supervision	Postdoc researcher
2010-now	Riccardo Pellarin	Postdoc researcher	Research Supervision	Postdoctoral Fellow, Institut Pasteur
2011-12	Lan Hua	Postdoc researcher	Research Supervision, jointly with Matt Jacobson	Postdoc researcher
2012-13	Miriam Sgobba	Postdoc researcher	Research Supervision	Postdoc researcher
2012-now	Barak Raveh	Postdoc researcher	Research Supervision	Postdoc researcher
2014-now	Peter Cimeranic	Postdoc Researcher	Research Supervision	Specialist
2014-now	Shruthi Viswanath	Postdoc Researcher	Research Supervision	Postdoc researcher
2014-now	Daniel Saltzberg	Postdoc researcher	Research Supervision	Postdoc researcher
2014-now	Kate Stafford	Postdoc researcher	Research Supervision	Postdoc researcher

FACULTY MENTORED:

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

OTHER MENTORING:

2004-now Coaching of iPQB student journal club presentations (approx. 3 students each year). 2006-now The Academic Advisor for approximately one third of students in BMI.

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

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

2007-now	Colin A. Smith	BMI	Orals Committee member
2005-08	Greg Friedland	Biophysics	Orals, Thesis Committee member
2007	Rafaela Ferreira	BMI	Orals Committee member
2007	Michelle Dimon	BMI	Orals Committee member
2007	Michael Hicks	PSPG	Orals Committee member
2008	Matt Eames	Biophysics	Thesis Committee member
2008	Jason Fernandez	PSPG	Orals Committee member
2008	Leonard Apeltsin	BMI	Orals, Thesis Committee member
2009	Alan Barber	PSPG	Orals Committee member
2009	Hannes Braberg	Biophysics	Orals Committee member
2009	Noah Ollikainen	BMI	Orals, Thesis Committee member
2009	Peter Skewes-Cox	BMI	Orals Committee member
2009	Monica Tremont	Biophysics	Orals Committee member
2009	Kiyoshi Egami	Biophysics	Orals Committee member
2009	Martin Turk		Visiting Scholar
2010	Rocco Varela	BMI	Thesis Committee member
2010	Russell Spitzer	BMI	Orals Committee member
2010	Henry Lin	BMI	Orals Committee member
2010	Jeremy Phillips	BMI	Thesis Committee member
2010	Geoff Rollins	Biophysics	Orals Committee member
2010	Laurens Kraal	BMI	Orals Committee member
2010	Ethan Geier	PSPG	Orals Committee member
2010	Davide Bau		Visiting Scholar
2010	Benjamin Schwartz		Visiting Scholar
2010	Yannick Spill		Visiting Scholar
2011	Brittany Fotsch	CCB	Supervised Graduate Rotation
2011	Zac Apte	Biophysics	Orals Committee member
2011	Yi Song	BMI	Supervised Graduate Rotation
2011	Argyris Politis		Visiting Scholar
2011	Amrita Choudhury		Visiting Scholar
2011	Javona White Bear	BMI	Supervised Graduate Rotation
2011	Natalia Khuri	Biophysics	Supervised Graduate Rotation
2011	Pia Unverdorben		Visiting Scholar
2011	Bart Lenselink		Visiting Scholar
2011	Yannick Spill		Visiting Scholar
2012	Sara Calhoun	Biophysics	Supervised Graduate Rotation
2012	Diego Garrido Ruiz	Biophysics	Supervised Graduate Rotation
2012	Kale Kundert	Biophysics	Supervised Graduate Rotation
2012	Adrian Stecula	PSPG	Supervised Graduate Rotation
2012	Miriam Sgobba		Visiting Scholar
2012	Jeff Yunes	Bioengineering	Orals Committee member
2012	James Webber	BMI	Orals Committee member
2013	Kyle Barlow	iPQB	Orals Committee member
2013	Joel Karpiak	CCB	Orals Committee member
2013	Rahel Woldeyes	CCB	Orals Committee member
2013	Andrew Vanbenschoten	Biophysics	Thesis Committee member
2013	Daniel Himmelstein	BMI	Orals Committee member
2014	Dorota Latek		Visiting Scholar
2014	Ilan Chemmama	Biophysics	Supervised Graduate Rotation
2014	Melissa Lemke		Visiting Scholar

2014	Reed Stein	PSPG	Supervised Summer Rotation
2014	Leo Gendele	Biophysics	Orals Committee member
2014	Ibai Irastorza		Visiting Scholar
2015	Yiran Wu		Visiting Scholar
2015	Seth Axen	Bioinformatics	Supervised Graduate Rotation
2015	Leon Bichman		Visiting Scholar
2015	Sam Ivry	PSPG	Quals Committee Member
2015	Rebecca Davidson	BMI	Quals Committee Member
2015	Neville Bethel	Biophysics	Quals Committee Member

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

2011-12: 10 hours of teaching (including preparation)
 Formal class or course teaching hours: 3 hours
 Informal teaching hours: 10 hours
 Mentoring hours: 500 hours

2012-13: 25 hours of teaching (including preparation)
 Formal class or course teaching hours: 8 hours
 Informal teaching hours: 10 hours
 Mentoring hours: 500 hours

2013-14: 50 hours of teaching (including preparation)

4/8/15

Andrej Sali

Formal class or course teaching hours: 20 hours

Informal teaching hours: 10 hours

Mentoring hours: 500 hours

2014-15: 70 hours of teaching (including preparation)

Formal class or course teaching hours: 26 hours

Informal teaching hours: 20 hours

Mentoring hours: 500 hours

2015-16: 70 hours of teaching (including preparation)

Formal class or course teaching hours: 26 hours

Informal teaching hours: 20 hours

Mentoring hours: 500 hours

TEACHING NARRATIVE:

When I arrived to UCSF in January 2003, I joined Prof. Patsy Babbit in leading the graduate and professional students' courses in Bioinformatics (BMI-206 and BPS-114). In 2008-09, I took the primary responsibility for these two courses. I also gave many of the lectures and supervised student activity associated with the courses (eg, student seminars, exercise sets). Since 2010, I contribute several lectures to BMI-206, but the course is led by others (BPS-114 does not exist anymore). I also participate as a guest lecturer in a number of other courses, such as Macromolecules and Chem 204. Since 2014, I began to be increasingly involved in BPS-134, a course for pharmacy students, led by Nancy Sambol. Finally, I am involved in the shaping of the curriculum for the graduate programs in the iPQB umbrella program, as a member of the iPQB curriculum committee and a contributor to the three training grant re-submissions in 2007 (BMI and Biophysics) and 2008 (Complex Biological Systems).

RESEARCH AND CREATIVE ACTIVITIES	
RESEARCH AWARDS AND GRANTS:	
<i>CURRENT</i>	
U54 GM094662 (co-PI)	07/01/10 – 06/30/15
NIH/NIGMS	\$144,175 direct/yr 2
<i>New York Structural Genomics Research Consortium</i>	\$750,000 direct/yrs 1-5
U01 GM61390 (collaborator)	4/1/03-6/30/15
NIH/NIGMS	\$30,000 direct/yr 13

<i>Pharmacogenetics of Membrane Transporters</i>	\$600,000 direct/yrs 1-12
U54 GM094625 (co-PI)	7/1/05 – 6/30/15
NIH/NIGMS	\$65,000 direct/yr 6
<i>CSMP: Centers for Membrane Protein Structure Determination</i>	\$650,000 direct/yrs 1-10
R01 GM083960 (PI)	04/01/12 - 03/31/16
NIH/NIGMS	\$200,000 direct/yr 1
<i>IMP: Software for Hybrid Determination of Macromolecular Assembly Structures</i>	\$720,000 direct/yrs 1-4
U54 GM093342 (co-PI)	05/20/10 – 4/30/15
NIH/NIGMS	\$140,000 direct/yr 4
<i>Collaborative Center for Enzyme Function Initiative</i>	\$850,000 direct/yrs 1-5
P01 AI091575-01 (co-PI)	07/13/11 – 06/30/16
NIH/NIGMS	\$197,424 direct/yr 2
<i>Protein Homeostasis Mechanism Underlying Enterovirus Replication and Evolution</i>	\$650,000 direct/yrs 1-5
U01 GM098256 (co-PI)	09/01/11 – 07/31/15
NIH/NIGMS	\$51,219 direct/yr 2
<i>Nucleocytoplasmic Transport: A Target for Cellular Control</i>	\$200,000 direct/yrs 1-4
P01 GM105537 (co-PI)	7/1/14 – 6/30/19
NIH	\$150,000 direct/yr 1
<i>The Yeast Centrosome-Structure, Assembly & Function</i>	
P41 GM109824 (co-PI)	08/01/14 – 07/31/19
NIH	\$199,000 direct/yr 1
<i>National Center for Dynamic Interactome Research</i>	
R01 GM112108 (co-PI)	03/01/15 – 02/28/19
NIH/NIGMS	\$48,843 direct/yr 1
<i>Structure-function Mapping of the Nuclear Pore Complex</i>	
<i>PENDING</i>	
P01 (co-PI)	
NIH	\$170,000 direct/yr 1
Degenerative and Dementing Diseases of Aging	\$850,000 entire period
P01 (co-PI)	
NIH	\$200,000 direct/yr 1
Mapping the conformational cycle of transmembrane transporters	\$1,000,000 entire period
P50 (co-PI)	
NIH/NIGMS	\$120,000 direct/yr 1
Center for Metformin Action in Pharmacogenomics and Precision Medicine	\$480,000 entire period

U54 (co-PI)	
NIH/NIGMS	\$79,701 direct/yr 1
Mapping the 3D Genome Landscape	\$398,505 entire period
(PI)	
NSF	\$459,112 direct/yr 1
MRI: Acquisition of a High-Performance Computer for Computational Biosciences	\$459,112 entire period
<i>PAST</i>	
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	
U54 GM103511 (co-PI)	06/10/05 – 07/31/14
NIH/NIGMS	\$273,439 direct/yr 8
<i>Nuclear Information Pathway Center</i>	\$2,100,000 direct/yrs 1-9
P01 GM71790 (collaborator)	7/1/04 - 6/30/14
NIH/NIGMS	\$96,350 direct/yr 9
<i>Deciphering Enzyme specificity</i>	\$800,000 direct/yrs 1-10
Pfizer Inc. (PI)	10/1/13 – 09/30/14
QB3	\$55,000 direct/yr 1
<i>A Computational Model of Allostery with Application to Antibody Design</i>	

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	
<i>The PhyloFacts phylogenomic encyclopedia of microbial protein families</i>	
S10 RR027100-01 (PI)	04/01/10 – 03/31/11
NIH/NIGMS	
<i>High Performance Computing Cluster for Bioimaging & Computational Biology</i>	
R01 GM54762 (PI)	7/1/96 – 6/30/10
NIH/NIGMS	
<i>Protein Modeling by Satisfaction of Spatial Restraints</i>	
U54 GM074945 (Co-PI)	09/30/00 – 08/31/10
SGX/NIH	
<i>NYSGRG: A Large Scale Center for the Protein Structure Initiative</i>	
SP41RR001081-32S1 (collaborator)	09/15/09 – 09/14/11
NIH	
<i>Resource for Biocomputing, Visualization, and Informatics</i>	
PN2 EY016525 (co-PI)	09/30/05 – 09/29/11
NIH	
<i>Center for Protein Folding Machinery</i>	
Bayer A119846 (PI)	12/15/12 – 12/15/14
<i>Modeling of ternary MHCII-peptide-TCR complexes</i>	\$73,877 direct/yr 1
	\$147,755 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)
 NIH Ruth Kirstein Fellowship (K. Stafford)
 Mel Jones Excellence in Graduate Student Research Award (C. Greenberg)
 PhRMA Fellowship in Pharmacology/Toxicology (A. Stecula)
 AFPE Pre-Doctoral Award in Pharmaceutical Science (A. Stecula)
 NSF Fellowship (I. Chemmama)

PUBLICATIONS:

1. M. Renko, **A. Sali**, V. Turk, M. Pokomy, I. Kregar. "A neutral metalloproteinase from *Streptomyces rimosus*." *Vestnik Slovenskega Kemijskega Drustva* **32/2**, 161-173, 1985.
2. B. Lenarcic, A. Ritonja, **A. Sali**, M. Kotnik, V. Turk, W. Machleidt. "Properties and structure of human spleen stefin B - a low molecular weight protein inhibitor of cysteine proteinases." In: *Cysteine Proteinases and Their Inhibitors; First International Symposium, Portoroz, Yugoslavia, September 15-18, 1985*. Xvi+846p. Ed: V. Turk, pp. 473-488, Walter De Gruyter and Co., Berlin, West Germany; New York, New York, USA., 1986.
3. V. Turk, J. Brzin, B. Lenarcic, **A. Sali**, W. Machleidt. "Human stefins and cystatins: their properties and structural relationships." In: *Cysteine Proteinases and Their Inhibitors; First International Symposium, Portoroz, Yugoslavia, September 15-18, 1985*. Xvi+846p. Ed: V. Turk, pp. 429-442, Walter De Gruyter and Co., Berlin, West Germany; New York, New York, USA., 1986.
4. M. Kotnik, **A. Sali**, J. Kos, B. Turk, V. Turk. "Nova metoda za hitro določanje kinetičnih konstant pri interakciji encima s kompetitivnim inhibitorjem (A new method for rapid determination of kinetic constants for competitive inhibition of enzymes)." *Vestnik Slovenskega Kemijskega Drustva* **34**, 369-377, 1987.
5. **A. Sali**, V. Turk. "Prediction of the secondary structures of stefins and cystatins, the low-molecular mass protein inhibitors of cysteine proteinases." *Biol Chem Hoppe Seyler* **368**, 493-499, 1987.
6. T. Lah, I. Kregar, **A. Sali**, B. Lenarcic, M. Kotnik, V. Kostka, V. Turk. "Circular dichroism studies of different aspartyl proteinases and their interactions with pepstatin." *Periodicum Biologorum* **90**, 31-38, 1988.
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, 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, 1989.
11. **A. Sali**, T.L. Blundell. "Definition of general topological equivalence in protein structures. A procedure involving comparison of properties and relationships through simulated annealing and dynamic programming." *J Mol Biol* **212**, 403-428, 1990.
12. **A. Sali**, J.P. Overington, M.S. Johnson, T.L. Blundell. "From Comparisons of protein sequences and structures to protein modelling and design." *Trends Biochem Sci* **15**, 235-240, 1990.
13. B. Veerapandian, J.B. Cooper, **A. Sali**, T.L. Blundell. "X-ray analyses of aspartic proteinases. III Three-dimensional structure of endothiapepsin complexed with a transition-state isostere inhibitor of renin at 1.6 Å resolution." *J Mol Biol* **216**, 1017-1029, 1990.
14. J. Overington, M.S. Johnson, **A. Sali**, T.L. Blundell. "Tertiary structural constraints on protein evolutionary diversity: templates, key residues and structure prediction." *Procedures in Biological Science* **241**, 132-145, 1990.
15. J.P. Overington, M.S. Johnson, C. Topham, A. McLeod, **A. Sali**, Z.Y. Zhu, L. Sibanda, T.L. Blundell. "Applications of environment specific amino acid substitution tables to identification of key residues in protein tertiary structure." *Curr Sci* **59**, 867-874, 1990.
16. M.S. Johnson, **A. Sali**, T.L. Blundell. "Phylogenetic relationships from three-dimensional protein structures." *Methods Enzymol* **183**, 670-690, 1990.
17. M.S. Johnson, J.P. Overington, **A. Sali**. "Knowledge-based protein modelling: Human plasma kallikrein and human neutrophil defensin." In: Chemistry: Techniques Structure and Function. Ed: J.J. Vilafranca, pp. 567-574, Academic Press, Inc., 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.
19. T.L. Blundell, M.S. Johnson, J.P. Overington, **A. Sali**. "Knowledge-based protein modeling and the design of novel molecules." In: Protein design and the development of new therapeutics and vaccines. Ed: J.B. Hook, G. Poste, pp. 209-227, Plenum Press, New York, NY, 1990.
20. T.L. Blundell, J.B. Cooper, **A. Sali**, Z.Y. Zhu. "Comparisons of the sequences, 3-D structures and mechanisms of pepsin-like and retroviral aspartic proteinases." *Adv Exp Med Biol* **306**, 443-453, 1991.
21. T.L. Blundell, J.B. Cooper, D. Donnelly, H. Driessen, Y. Edwards, F. Eisenmenger, C. Frazao, M. Johnson, K. Niefind, M. Newman, J. Overington, **A. Sali**, C. Slingsby, V. Nalini, Z.Y. Zhu. "Patterns of

sequence variation in families of homologous proteins." In: *Methods in Protein Sequence Analysis*. Ed: H. Jornval, J.O. Hoog, A.M. Gustavsson, pp. 373-385, Birkhauser Verlag, Basel, Switzerland, 1991.

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

23. **A. Sali**, B. Veerapandian, J.B. Cooper, D.S. Moss, T. Hofmann, T.L. Blundell. "Domain flexibility in aspartic proteinases." *Proteins* **12**, 158-170, 1992.

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

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

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

27. M.S. Johnson, J.P. Overington, **A. Sali**, T.L. Blundell. "From the comparative analysis of proteins to similarity-based modelling." In: *Computer Modelling of Biomolecular Processes*. Ed: V.A. Ratner, N.A. Kolchanov, pp. 191-196, Nova Science Publishers, 1992.

28. J.P. Overington, Z.Y. Zhu, **A. Sali**, M.S. Johnson, R. Sowdhamini, G.V. Louie, T.L. Blundell. "Molecular recognition in protein families: a database of aligned three-dimensional structures of related proteins." *Biochem Soc Trans* **21 (Pt 3)**, 597-604, 1993.

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

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

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

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

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

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

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

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

37. M. Karplus, A. Caflich, **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. Pullman et al,

pp. 69-84, Kluwer Academic Publishers, 1995.

38. **A. Sali**. "MODELLER: Implementing 3D protein modeling." In: *mc²*, **2**, pp. 5, Molecular Simulations Inc., 1995.
39. X.D. Wu, B. Knudsen, S.M. Feller, J. Zheng, **A. Sali**, D. Cowburn, H. Hanafusa, J. Kuriyan. "Structural basis for the specific interaction of lysine-containing proline-rich peptides with the amino-terminal SH3 domain of c-Crk." *Structure* **3**, 215-226, 1995.
40. R. Matsumoto, **A. Sali**, N. Ghildyal, M. Karplus, R.L. Stevens. "Packaging of proteases and proteoglycans in the granules of mast cells and other hematopoietic cells. A cluster of histidines on mouse mast cell protease 7 regulates its binding to heparin serglycin proteoglycans." *J Biol Chem* **270**, 19524-19531, 1995.
41. **A. Sali**. "Comparative protein modeling by satisfaction of spatial restraints." *Mol Med Today* **1**, 270-277, 1995.
42. **A. Sali**, E. Shakhnovich, M. Karplus. "Protein Folding Studied by Monte Carlo Simulations." In: *Protein Folds: A Distance Based Approach*. Ed: H. Bohr, S. Brunak, pp. 202-216, CRC Press Inc., 1995.
43. **A. Sali**, E. Shakhnovich, M. Karplus. "Thermodynamics and kinetics of protein folding from lattice Monte Carlo simulations." In: *DIMACS Series in Discrete Mathematics and Theoretical Computer Science*. Ed: D. Shalloway, G. Xue, P. Pardalos, **23**, pp. 199-213, American Mathematical Society, 1995.
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." *Curr Opin Biotechnol* **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." *J Immunol* **157**, 3744-3751, 1996.
48. N. Ghildyal, D.S. Friend, R.L. Stevens, K.F. Austen, C. Huang, J.F. Penrose, **A. Sali**, M.F. Gurish. "Fate of two mast cell tryptases in V3 mastocytosis and normal BALB/c mice undergoing passive systemic anaphylaxis: prolonged retention of exocytosed mMCP-6 in connective tissues, and rapid accumulation of enzymatically active mMCP-7 in the blood." *The Journal of Experimental Medicine* **184**, 1061-1073, 1996.
49. L.Z. Xu, R. Sanchez, **A. Sali**, N. Heintz. "Ligand specificity of brain lipid-binding protein." *J Biol Chem* **271**, 24711-24719, 1996.
50. A.R. Dinner, **A. Sali**, M. Karplus. "The folding mechanism of larger model proteins: role of native structure." *Proc Natl Acad Sci U S A* **93**, 8356-8361, 1996.
51. S. Wu, H. de Lencastre, **A. Sali**, A. Tomasz. "A phosphoglucomutase-like gene essential for the optimal expression of methicillin resistance in *Staphylococcus aureus*: molecular cloning and DNA sequencing." *Microbial Drug Resistance* **2**, 277-286, 1996.
52. M. Russel, N.A. Linderoth, **A. Sali**. "Filamentous phage assembly: variation on a protein export theme." *Gene* **192**, 23-32, 1997.
53. C. Huang, G.W. Wong, N. Ghildyal, M.F. Gurish, **A. Sali**, R. Matsumoto, W.T. Qiu, R.L. Stevens.

- "The trypsin, mouse mast cell protease 7, exhibits anticoagulant activity in vivo and in vitro due to its ability to degrade fibrinogen in the presence of the diverse array of protease inhibitors in plasma." *J Biol Chem* **272**, 31885-31893, 1997.
54. R. Sanchez, **A. Sali**. "Comparative protein modeling as an optimization problem." *Journal of Molecular Structure (Theochem)* **398**, 489-496, 1997.
55. R. Sanchez, **A. Sali**. "Advances in comparative protein-structure modelling." *Curr Opin Struct Biol* **7**, 206-214, 1997.
56. D. Koulich, M. Orlova, A. Malhotra, **A. Sali**, S.A. Darst, S. Borukhov. "Domain organization of *Escherichia coli* transcript cleavage factors GreA and GreB." *J Biol Chem* **272**, 7201-7210, 1997.
57. J.E. Hunt, D.S. Friend, M.F. Gurish, E. Feyfant, **A. Sali**, C. Huang, N. Ghildyal, S. Stechschulte, K.F. Austen, R.L. Stevens. "Mouse mast cell protease 9, a novel member of the chromosome 14 family of serine proteases that is selectively expressed in uterine mast cells." *J Biol Chem* **272**, 29158-29166, 1997.
58. R. Sanchez, **A. Sali**. "Evaluation of comparative protein structure modeling by MODELLER-3." *Proteins Suppl* **1**, 50-58, 1997.
59. B. Guenther, R. Onrust, **A. Sali**, M. O'Donnell, J. Kuriyan. "Crystal structure of the delta' subunit of the clamp-loader complex of *E. coli* DNA polymerase III." *Cell* **91**, 335-345, 1997.
60. R. Sanchez, A.Ya. Badretdinov, E. Feyfant, **A. Sali**. "Homology protein structure modeling." *Transactions of the American Crystallographic Association* **32**, 81-91, 1997.
61. Y. Sheng, S.A. Krilis, **A. Sali**. "Site-directed mutagenesis of recombinant human beta 2-glycoprotein I. Effect of phospholipid binding and anticardiolipin antibody activity." *Ann N Y Acad Sci* **815**, 331-333, 1997.
62. C.M. Dobson, **A. Sali**, M. Karplus. "Protein folding: A perspective from theory and experiment." *Angewandte Chemie Int Ed* **37**, 868-893, 1998.
63. C. Huang, **A. Sali**, R.L. Stevens. "Regulation and function of mast cell proteases in inflammation." *J Clin Immunol* **18**, 169-183, 1998.
64. D.A. Kandiah, **A. Sali**, Y. Sheng, E.J. Victoria, D.M. Marquis, S.M. Coutts, S.A. Krilis. "Current insights into the "antiphospholipid" syndrome: clinical, immunological, and molecular aspects." *Advanced Immunology Journal* **70**, 507-563, 1998.
65. A. Gutin, **A. Sali**, V. Abkevich, M. Karplus, E. Shakhnovich. "Temperature dependence of the folding rate in a simple protein model: Search for a glass transition." *J Chem Phys* **108**, 6466-6483, 1998.
66. E. Wolf, A. Vassilev, Y. Makino, **A. Sali**, Y. Nakatani, S.K. Burley. "Crystal structure of a GCN5-related N-acetyltransferase: *Serratia marcescens* aminoglycoside 3-N-acetyltransferase." *Cell* **94**, 439-449, 1998.
67. R. Sanchez, **A. Sali**. "Large-scale protein structure modeling of the *Saccharomyces cerevisiae* genome." *Proc Natl Acad Sci U S A* **95**, 13597-13602, 1998.
68. **A. Sali**. "100,000 protein structures for the biologist." *Nat Struct Biol* **5**, 1029-1032, 1998.
69. R. Sanchez, **A. Sali**. "MODBASE: A database of comparative protein structure models." *Bioinformatics* **15**, 1060-1061, 1999.

70. R. Sanchez, **A. Sali**. "Comparative protein structure modeling in genomics." *Journal of Computational Physics* **151**, 388-401, 1999.
71. G. Wu, A. Fiser, B. ter Kuile, **A. Sali**, M. Muller. "Convergent evolution of *Trichomonas vaginalis* lactate dehydrogenase from malate dehydrogenase." *Proc Natl Acad Sci U S A* **96**, 6285-6290, 1999.
72. T. Nagata, V. Gupta, D. Sorce, W.Y. Kim, **A. Sali**, B.T. Chait, K. Shigesada, Y. Ito, M.H. Werner. "Immunoglobulin motif DNA recognition and heterodimerization of the PEBP2/CBF Runt domain." *Nat Struct Biol* **6**, 615-619, 1999.
73. J.M. Miwa, I. Ibanez-Tallon, G.W. Crabtree, R. Sanchez, **A. Sali**, L.W. Role, N. Heintz. "lynx1, an endogenous toxin-like modulator of nicotinic acetylcholine receptors in the mammalian CNS." *Neuron* **23**, 105-114, 1999.
74. G.W. Wong, Y. Tang, E. Feyfant, **A. Sali**, L. Li, Y. Li, C. Huang, D.S. Friend, S.A. Krilis, R.L. Stevens. "Identification of a new member of the tryptase family of mouse and human mast cell proteases which possesses a novel COOH-terminal hydrophobic extension." *J Biol Chem* **274**, 30784-30793, 1999.
75. S.K. Burley, S.C. Almo, J.B. Bonanno, M. Capel, M.R. Chance, T. Gaasterland, D. Lin, **A. Sali**, F.W. Studier, S. Swaminathan. "Structural genomics: beyond the human genome project." *Nat Genet* **23**, 151-157, 1999.
76. **A. Sali**, J. Kuriyan. "Challenges at the frontiers of structural biology (Reprinted from Trends in Biochemical Science, vol 12, Dec., 1999)." *Trends Cell Biol* **9**, M20-M24, 1999.
77. **A. Sali**. "Functional links between proteins." *Nature* **402**, 23, 25-26, 1999.
78. P. Baldi, M. Borodovsky, S. Brunak, C. Burge, J. Fickett, S. Henikoff, E. Koonin, **A. Sali**, C. Sander, G. Stormo. "The Second Georgia Tech International Conference on Bioinformatics: Sequence, Structure and Function." *Bioinformatics* **15**, 865-866, 1999.
79. C. Huang, G. Morales, A. Vagi, K. Chanasyk, M. Ferrazzi, C. Burklow, W.T. Qiu, E. Feyfant, **A. Sali**, R.L. Stevens. "Formation of enzymatically active, homotypic, and heterotypic tetramers of mouse mast cell tryptases. Dependence on a conserved Trp-rich domain on the surface." *J Biol Chem* **275**, 351-358, 2000.
80. M.A. Marti-Renom, A.C. Stuart, A. Fiser, R. Sanchez, F. Melo, **A. Sali**. "Comparative protein structure modeling of genes and genomes." *Annu Rev Biophys Biomol Struct* **29**, 291-325, 2000.
81. R. Sanchez, U. Pieper, N. Mirkovic, P.I.W. de Bakker, E. Wittenstein, **A. Sali**. "ModBase, a database of annotated comparative protein structure models." *Nucleic Acids Res* **28**, 250-253, 2000.
82. A.R. Dinner, **A. Sali**, L.J. Smith, C.M. Dobson, M. Karplus. "Understanding protein folding via free-energy surfaces from theory and experiment." *Trends Biochem Sci* **25**, 331-339, 2000.
83. R. Sanchez, **A. Sali**. "Comparative protein structure modeling. Introduction and practical examples with modeller." *Methods Mol Biol* **143**, 97-129, 2000.
84. G. Wu, A.G. McArthur, A. Fiser, **A. Sali**, M.L. Sogin, M. Muller. "Core histones of the amitochondriate protist, *Giardia lamblia*." *Mol Biol Evol* **17**, 1156-1163, 2000.
85. A. Fiser, R.K.G. Do, **A. Sali**. "Modeling of loops in protein structures." *Protein Sci* **9**, 1753-1773, 2000.

86. W. Liedtke, Y. Choe, M.A. Marti-Renom, A.M. Bell, C.S. Denis, **A. Sali**, A.J. Hudspeth, J.M. Friedman, S. Heller. "Vanilloid receptor-related osmotically activated channel (VR-OAC), a candidate vertebrate osmoreceptor." *Cell* **103**, 525-535, 2000.
87. S.K. Jin, S. Martinek, W.S. Joo, J.R. Wortman, N. Mirkovic, **A. Sali**, M.D. Yandell, N.P. Pavletich, M.W. Young, A.J. Levine. "Identification and characterization of a p53 homologue in *Drosophila melanogaster*." *Proc Natl Acad Sci U S A* **97**, 7301-7306, 2000.
88. R. Sanchez, U. Pieper, F. Melo, N. Eswar, M.A. Marti-Renom, M.S. Madhusudhan, N. Mirkovic, **A. Sali**. "Protein structure modeling for structural genomics." *Nat Struct Biol* **7**, 986-990, 2000.
89. A. Fiser, R. Sanchez, F. Melo, **A. Sali**. "Comparative protein structure modeling." In: Computational Biochemistry and Biophysics. Ed: M. Watanabe, B. Roux, A. Mackerell, O. Becker, pp. 275-312, Marcel Dekker, 2000.
90. C.M. Groft, R. Beckmann, **A. Sali**, S.K. Burley. "Crystal structures of ribosome anti-association factor IF6." *Nat Struct Biol* **7**, 1156-1164, 2000.
91. S. Gopal, M. Schroeder, U. Pieper, A. Sczyrba, G. Aytakin-Kurban, S. Bekiranov, J.E. Fajardo, N. Eswar, R. Sanchez, **A. Sali**, T. Gaasterland. "Homology-based annotation yields 1,042 new candidate genes in the *Drosophila melanogaster* genome." *Nat Genet* **27**, 337-340, 2001.
92. V.A. Eyrich, M.A. Marti-Renom, D. Przybylski, M.S. Madhusudhan, A. Fiser, F. Pazos, A. Valencia, **A. Sali**, B. Rost. "EVA: continuous automatic evaluation of protein structure prediction servers." *Bioinformatics* **17**, 1242-1243, 2001.
93. M.A. Marti-Renom, V.A. Ilyin, **A. Sali**. "DBAli: a database of protein structure alignments." *Bioinformatics* **17**, 746-747, 2001.
94. G.W. Wong, L. Li, M.S. Madhusudhan, S.A. Krilis, M.F. Gurish, M.E. Rothenberg, **A. Sali**, R.L. Stevens. "Trypsin 4, a new member of the chromosome 17 family of mouse serine proteases." *J Biol Chem* **276**, 20648-20658, 2001.
95. L.G. Barrientos, R. Campos-Olivas, J.M. Louis, A. Fiser, **A. Sali**, A.M. Gronenborn. "¹H, ¹³C, ¹⁵N resonance assignments and fold verification of a circularly permuted variant of the potent HIV-inactivating protein cyanovirin-N." *J Biomol NMR* **19**, 289-290, 2001.
96. **A. Sali**. "Target practice." *Nat Struct Biol* **8**, 482-484, 2001.
97. J.B. Bonanno, C. Edo, N. Eswar, U. Pieper, M.J. Romanowski, V. Ilyin, S.E. Gerchman, H. Kycia, F.W. Studier, **A. Sali**, S.K. Burley. "Structural genomics of enzymes involved in sterol/isoprenoid biosynthesis." *Proc Natl Acad Sci U S A* **98**, 12896-12901, 2001.
98. C.M. Spahn, R. Beckmann, N. Eswar, P.A. Penczek, **A. Sali**, G. Blobel, J. Frank. "Structure of the 80S ribosome from *Saccharomyces cerevisiae*--tRNA-ribosome and subunit-subunit interactions." *Cell* **107**, 373-386, 2001.
99. R. Beckmann, C.M.T. Spahn, N. Eswar, J. Helmers, P.A. Penczek, **A. Sali**, J. Frank, G. Blobel. "Architecture of the protein-conducting channel associated with the translating 80S ribosome." *Cell* **107**, 361-372, 2001.
100. G.W. Wong, S. Yasuda, M.S. Madhusudhan, L. Li, Y. Yang, S.A. Krilis, **A. Sali**, R.L. Stevens. "Human trypsin epsilon (PRSS22), a new member of the chromosome 16p13.3 family of human serine proteases expressed in airway epithelial cells." *J Biol Chem* **276**, 49169-49182, 2001.

101. M. Borodovsky, E. Koonin, C. Burge, J. Fickett, J. Logsdon, **A. Sali**, G. Stormo, I. Zhulin. "The third Georgia Tech - Emory international conference on bioinformatics: in silico biology; bioinformatics after human genome November 15-18, 2001, Atlanta, Georgia, USA." *Bioinformatics* **17**, 859-861, 2001.
102. C.M. Groft, R. Beckmann, **A. Sali**, S.K. Burley. "Response to Paoli." *Nat Struct Biol* **8**, 745, 2001.
103. D. Baker, **A. Sali**. "Protein structure prediction and structural genomics." *Science* **294**, 93-96, 2001.
104. J. Vernal, A. Fiser, **A. Sali**, M. Muller, J.J. Cazzulo, C. Nowicki. "Probing the specificity of a trypanosomal aromatic alpha-hydroxy acid dehydrogenase by site-directed mutagenesis." *Biochem Biophys Res Commun* **293**, 633-639, 2002.
105. F. Melo, R. Sanchez, **A. Sali**. "Statistical potentials for fold assessment." *Protein Sci* **11**, 430-448, 2002.
106. A.C. Stuart, V.A. Ilyin, **A. Sali**. "LigBase: a database of families of aligned ligand binding sites in known protein sequences and structures." *Bioinformatics* **18**, 200-201, 2002.
107. M.A. Marti-Renom, M.S. Madhusudhan, A. Fiser, B. Rost, **A. Sali**. "Reliability of assessment of protein structure prediction methods." *Structure* **10**, 435-440, 2002.
108. **A. Sali**, M.A. Marti-Renom, M.S. Madhusudhan, A. Fiser, B. Rost. "Reply to Moult et al." *Structure* **10**, 292-293, 2002.
109. A. Fiser, M. Feig, C.L. Brooks, **A. Sali**. "Evolution and physics in comparative protein structure modeling." *Accounts of Chemical Research* **35**, 413-421, 2002.
110. U. Pieper, N. Eswar, A.C. Stuart, V.A. Ilyin, **A. Sali**. "MODBASE, a database of annotated comparative protein structure models." *Nucleic Acids Res* **30**, 255-259, 2002.
111. M.R. Chance, A.R. Bresnick, S.K. Burley, J.S. Jiang, C.D. Lima, **A. Sali**, S.C. Almo, J.B. Bonanno, J.A. Buglino, S. Boulton, H. Chen, N. Eswar, G.S. He, R. Huang, V. Ilyin, L. McMahan, U. Pieper, S. Ray, M. Vidal, L.K. Wang. "Structural genomics: A pipeline for providing structures for the biologist." *Protein Sci* **11**, 723-738, 2002.
112. K.R. Rajashankar, M.R. Chance, S.K. Burley, J. Jiang, S.C. Almo, A.R. Bresnick, T. Dodatko, R. Huang, G. He, H. Chen, M. Sullivan, J. Toomey, R.A. Thirumuruhan, W.A. Franklin, **A. Sali**, U. Pieper, N. Eswar, V. Ilyin, L. McMahan. "Structural Genomics at the National Synchrotron Light Source." *NSLS Activity Report 2001* **2**, 28-32, 2002.
113. Y. Yang, L.X. Li, G.W. Wong, S.A. Krilis, M.S. Madhusudhan, **A. Sali**, R.L. Stevens. "RasGRP4, a new mast cell-restricted Ras guanine nucleotide-releasing protein with calcium- and diacylglycerol-binding motifs - Identification of defective variants of this signaling protein in asthma, mastocytosis, and mast cell leukemia patients and demonstration of the importance of RasGRP4 in mast cell development and function." *J Biol Chem* **277**, 25756-25774, 2002.
114. M.A. Marti-Renom, B. Yerkovich, **A. Sali**. "Comparative protein structure prediction." In: *Current Protocols in Protein Science*, pp. 2.9.1-2.9.22, John Wiley & Sons, 2002.
115. G.M. Iverson, S. Reddel, E.J. Victoria, K.A. Cockerill, Y.X. Wang, M.A. Marti-Renom, **A. Sali**, D.M. Marquis, S.A. Krilis, M.D. Linnik. "Use of single point mutations in domain I of beta(2)-glycoprotein I to determine fine antigenic specificity of antiphospholipid autoantibodies." *J Immunol* **169**, 7097-7103, 2002.
116. A. Fiser, **A. Sali**. "Modeller: generation and refinement of homology-based protein structure

models." *Methods Enzymol* **374**, 461-491, 2003.

117. V.A. Ilyin, U. Pieper, A.C. Stuart, M.A. Marti-Renom, L. McMahan, **A. Sali**. "ModView, visualization of multiple protein sequences and structures." *Bioinformatics* **19**, 165-166, 2003.

118. M.A. Marti-Renom, B. Yerkovich, **A. Sali**. "Modeling protein structure from its sequence." In: Current Protocols in Bioinformatics, **V. 5 January Issue**, pp. 5.1.1-5.1.32, John Wiley & Sons, Inc., Hoboken, NJ, 2003.

119. A. Fiser, **A. Sali**. "Comparative Protein Structure Modeling." In: Protein Structure. Ed: D. Chasman, pp. 167-206, Marcel Dekker, Inc., 2003.

120. **A. Sali**, R. Glaeser, T. Earnest, W. Baumeister. "From words to literature in structural proteomics." *Nature* **422**, 216-225, 2003.

121. C. Klammt, I. Maslennikov, M. Bayrhuber, C. Eichmann, N. Vajpai, E. Chiu, K. Blain, L. Esquivies, J. Kwon, B. Balana, U. Pieper, **A. Sali**, P. Slesinger, W. Kwiatkowi, R. Riek, S. Choe, I.Y.Y. Koh, V.A. Eylich, M.A. Marti-Renom, D. Przybylski, M.S. Madhusudhan, N. Eswar, O. Grana, F. Pazos, A. Valencia, **A. Sali**, B. Rost. "EVA: evaluation of protein structure prediction servers." *Nucleic Acids Res* **31**, 3311-3315, 2003.

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

123. N. Eswar, B. John, N. Mirkovic, A. Fiser, V.A. Ilyin, U. Pieper, A.C. Stuart, M.A. Marti-Renom, M.S. Madhusudhan, B. Yerkovich, **A. Sali**. "Tools for comparative protein structure modeling and analysis." *Nucleic Acids Res* **31**, 3375-3380, 2003.

124. H.X. Gao, J. Sengupta, M. Valle, A. Korostelev, N. Eswar, S.M. Stagg, P. Van Roey, R.K. Agrawal, S.C. Harvey, **A. Sali**, M.S. Chapman, J. Frank. "Study of the structural dynamics of the *E-coli* 70S ribosome using real-space refinement." *Cell* **113**, 789-801, 2003.

125. S.A. Lee, E.L. Shen, A. Fiser, **A. Sali**, S. Guo. "The zebrafish forkhead transcription factor Foxi1 specifies epibranchial placode-derived sensory neurons." *Development* **130**, 2669-2679, 2003.

126. M.A. Marti-Renom, A. Fiser, M.S. Madhusudhan, B. John, A.C. Stuart, N. Eswar, U. Pieper, M.-Y. Shen, **A. Sali**. "Modeling protein structure from its sequence." In: Current Protocols in Bioinformatics, **V. 5**, pp. 5.1.1-5.1.32, John Wiley & Sons, Inc., 2003.

127. **A. Sali**. "NIH workshop on structural proteomics of biological complexes." *Structure* **11**, 1043-1047, 2003.

128. A. Fiser, **A. Sali**. "ModLoop: automated modeling of loops in protein structures." *Bioinformatics* **19**, 2500-2501, 2003.

129. N. Mirkovic, M.A. Marti-Renom, B.L. Weber, **A. Sali**, A.N. Monteiro. "Structure-based assessment of missense mutations in human BRCA1: implications for breast and ovarian cancer predisposition." *Cancer Res* **64**, 3790-3797, 2004.

130. A. Rossi, Q. Deveraux, B. Turk, **A. Sali**. "Comprehensive search for cysteine cathepsins in the human genome." *Biol Chem* **385**, 363-372, 2004.

131. M.A. Marti-Renom, M.S. Madhusudhan, **A. Sali**. "Alignment of protein sequences by their profiles." *Protein Sci* **13**, 1071-1087, 2004.

132. F. Alber, N. Eswar, **A. Sali**. "Structure determination of macromolecular complexes by experiment and computation." *Practical Bioinformatics*, Ed: J.Bujnicki **15**, 73-96, 2004.
133. B. John, **A. Sali**. "Detection of homologous proteins by an intermediate sequence search." *Protein Sci* **13**, 54-62, 2004.
134. S.M. Maurer, A. Rai, **A. Sali**. "Finding Cures for Tropical Diseases: Is Open Source An Answer?" *Minnesota Journal of Law, Science & Technology* **6**, 169-175, 2004.
135. U. Pieper, N. Eswar, H. Braberg, M.S. Madhusudhan, F.P. Davis, A.C. Stuart, N. Mirkovic, A. Rossi, M.A. Marti-Renom, A. Fiser, B. Webb, D. Greenblatt, C.C. Huang, T.E. Ferrin, **A. Sali**. "MODBASE, a database of annotated comparative protein structure models, and associated resources." *Nucleic Acids Res* **32**, D217-D222, 2004.
136. S.M. Maurer, A. Rai, **A. Sali**. "Finding Cures for Tropical Diseases: Is Open Source An Answer?" In: *Biotechnology: Essays From Its Heartland*. Ed: L.y.n.n. Laboratory Yarris, **June 2004**, pp. 33-37, 2004.
137. M.R. Chance, A. Fiser, **A. Sali**, U. Pieper, N. Eswar, G. Xu, J.E. Fajardo, T. Radhakannan, N. Marinkovic. "High-throughput computational and experimental techniques in structural genomics." *Genome Res* **14**, 2145-2154, 2004.
138. M. Jacobson, **A. Sali**. "Comparative Protein Structure Modeling and Its Applications to Drug Discovery." In: *Annual Reports in Medicinal Chemistry*. Ed: J. Overington, **39**, pp. 259-276, Inpharmatica Ltd., London, 2004.
139. R.B. Russell, F. Alber, P. Aloy, F.P. Davis, D. Korkin, M. Pichaud, M. Topf, **A. Sali**. "A structural perspective on protein-protein interactions." *Curr Opin Struct Biol* **14**, 313-324, 2004.
140. D. Devos, S. Dokudovskaya, F. Alber, R. Williams, B.T. Chait, **A. Sali**, M.P. Rout. "Components of coated vesicles and nuclear pore complexes share a common molecular architecture." *PLoS Biology* **2**, e380, 2004.
141. S.M. Maurer, A. Rai, **A. Sali**. "Finding Cures for Tropical Diseases: Is Open Source an Answer?" *PLoS Medicine* **1**, e56, 2004.
142. J. Espadaler, R. Aragues, N. Eswar, M.A. Marti-Renom, E. Querol, F.X. Aviles, **A. Sali**, B. Oliva. "Detecting remotely related proteins by their interactions and sequence similarity." *Proc Natl Acad Sci U S A* **102**, 7151-7156, 2005.
143. M. Topf, M.L. Baker, B. John, W. Chiu, **A. Sali**. "Structural characterization of components of protein assemblies by comparative modeling and electron cryo-microscopy." *J Struct Biol* **149**, 191-203, 2005.
144. R. Karchin, L. Kelly, **A. Sali**. "Improving functional annotation of non-synonymous SNPs with information theory." *Pac Symp Biocomput*, 397-408, 2005.
145. M.S. Madhusudhan, M.A. Marti-Renom, N. Eswar, B. John, U. Pieper, R. Karchin, M.i.n.-y.i. Shen, **A. Sali**. "Comparative Protein Structure Modeling." In: *Proteomics Protocols Handbook*. Ed: J.M. Walker, pp. 831-860, Humana Press Inc., Totowa, NJ, 2005.
146. F. Alber, M.F. Kim, **A. Sali**. "Structural characterization of assemblies from overall shape and subcomplex compositions." *Structure* **13**, 435-445, 2005.
147. F.P. Davis, **A. Sali**. "PIBASE: a comprehensive database of structurally defined protein interfaces." *Bioinformatics* **21**, 1901-1907, 2005.

148. R. Karchin, M. Diekhans, L. Kelly, D.J. Thomas, U. Pieper, N. Eswar, D. Haussler, **A. Sali**. "LS-SNP: large-scale annotation of coding non-synonymous SNPs based on multiple information sources." *Bioinformatics* **21**, 2814-2820, 2005.
149. S. Yasuda, N. Morokawa, G.W. Wong, A. Rossi, M.S. Madhusudhan, **A. Sali**, Y.S. Askew, R. Adachi, G.A. Silverman, S.A. Krilis, R.L. Stevens. "Urokinase-type plasminogen activator is a preferred substrate of the human epithelium serine protease tryptase epsilon/PRSS22." *Blood* **105**, 3893-3901, 2005.
150. J. Dvorak, M. Delcroix, A. Rossi, V. Vopalensky, M. Pospisek, M. Sedinova, L. Mikes, M. Sajid, **A. Sali**, J.H. Mckerrow, P. Horak, C.R. Caffrey. "Multiple cathepsin B isoforms in schistosomula of *Trichobilharzia regenti*: Identification, characterization and putative role in migration and nutrition." *International Journal of Parasitology* **35**, 895-910, 2005.
151. **A. Sali**, W. Chiu. "Macromolecular assemblies highlighted." *Structure* **13**, 339-341, 2005.
152. D. Korkein, F.P. Davis, **A. Sali**. "Localization of protein-binding sites within families of proteins." *Protein Sci* **14**, 2350-2360, 2005.
153. M.Y. Shen, F.P. Davis, **A. Sali**. "The optimal size of a globular protein domain: A simple sphere-packing model." *Chem Phys Lett* **405**, 224-228, 2005.
154. J.B. Bonanno, S.C. Almo, A. Bresnick, M.R. Chance, A. Fiser, S. Swaminathan, J. Jiang, F.W. Studier, L. Shapiro, C.D. Lima, T.M. Gaasterland, **A. Sali**, K. Bain, I. Feil, X. Gao, D. Lorimer, A. Ramos, J.M. Sauder, S.R. Wasserman, S. Emtage, K.L. D'Amico, S.K. Burley. "New York-Structural GenomiX Research Consortium (NYSGXRC): a large scale center for the protein structure initiative." *J Struct Funct Genom* **6**, 225-232, 2005.
155. M. Topf, **A. Sali**. "Combining electron microscopy and comparative protein structure modeling." *Curr Opin Struct Biol* **15**, 578-585, 2005.
156. S.A. McMahon, J.L. Miller, J.A. Lawton, D.E. Kerkow, A. Hodes, M.A. Marti-Renom, S. Doulatov, E. Narayanan, **A. Sali**, J.F. Miller, P. Ghosh. "The C-type lectin fold as an evolutionary solution for massive sequence variation." *Nature Structural Molecular Biology* **12**, 886-892, 2005.
157. D. Devos, S. Dokudovskaya, R. Williams, F. Alber, N. Eswar, B.T. Chait, M.P. Rout, **A. Sali**. "Simple fold composition and modular architecture of the nuclear pore complex." *Proc Natl Acad Sci U S A* **103**, 2172-2177, 2006.
158. M.S. Madhusudhan, M.A. Marti-Renom, R. Sanchez, **A. Sali**. "Variable gap penalty for protein sequence-structure alignment." *Protein Engineering, Design & Selection* **19**, 129-133, 2006.
159. C. Lima, J. Puglisi, **A. Sali**, L. Szewczak. "Editorial." *Structure* **14**, 801, 2006.
160. U. Pieper, N. Eswar, F.P. Davis, H. Braberg, M.S. Madhusudhan, A. Rossi, M. Marti-Renom, R. Karchin, B.M. Webb, D. Eramian, M.Y. Shen, L. Kelly, F. Melo, **A. Sali**. "MODBASE: a database of annotated comparative protein structure models and associated resources." *Nucleic Acids Res* **34**, D291-295, 2006.
161. M. Topf, M.L. Baker, M.A. Marti-Renom, W. Chiu, **A. Sali**. "Refinement of protein structures by iterative comparative modeling and CryoEM density fitting." *J Mol Biol* **357**, 1655-1668, 2006.
162. D. Korkein, F.P. Davis, F. Alber, T. Luong, M.Y. Shen, V. Lucic, M.B. Kennedy, **A. Sali**. "Structural modeling of protein interactions by analogy: application to PSD-95." *PLoS Computational Biology* **2**,

163. D. Eramian, M.Y. Shen, D. Devos, F. Melo, **A. Sali**, M.A. Marti-Renom. "A composite score for predicting errors in protein structure models." *Protein Sci* **15**, 1653-1666, 2006.
164. S. Dokudovskaya, R. Williams, D. Devos, **A. Sali**, B.T. Chait, M.P. Rout. "Protease accessibility laddering: a proteomic tool for probing protein structure." *Structure* **14**, 653-660, 2006.
165. N. Eswar, B. Webb, M.A. Marti-Renom, M.S. Madhusudhan, D. Eramian, M.Y. Shen, U. Pieper, **A. Sali**. "Comparative protein structure modeling using Modeller." *Current Protocols in Bioinformatics* **Chapter 5**, Unit 5.6, 2006.
166. A. Rossi, M.A. Marti-Renom, **A. Sali**. "Localization of binding sites in protein structures by optimization of a composite scoring function." *Protein Sci* **15**, 2366-2380, 2006.
167. F.P. Davis, H. Braberg, M.Y. Shen, U. Pieper, **A. Sali**, M.S. Madhusudhan. "Protein complex compositions predicted by structural similarity." *Nucleic Acids Res* **34**, 2943-2952, 2006.
168. T.D. Nguyen, J.M. Gow, L.W. Chinn, L. Kelly, H. Jeong, C.C. Huang, D. Stryke, M. Kawamoto, S.J. Johns, E. Carlson, T. Taylor, T.E. Ferrin, **A. Sali**, K.M. Giacomini, D.L. Kroetz. "PharmGKB submission update: IV. PMT submissions of genetic variations in ATP-Binding cassette transporters to the PharmGKB network." *Pharmacol Rev* **58**, 1-2, 2006.
169. H.M. Berman, S.K. Burley, W. Chiu, **A. Sali**, A. Adzhubei, P.E. Bourne, S.H. Bryant, R.L. Dunbrack Jr., K. Fidelis, J. Frank, A. Godzik, K. Henrick, A. Joachimiak, B. Heymann, D. Jones, J.L. Markley, J. Moult, G.T. Montelione, C. Orengo, M.G. Rossmann, B. Rost, H. Saibil, T. Schwede, D.M. Standley, J.D. Westbrook. "Outcome of a workshop on archiving structural models of biological macromolecules." *Structure* **14**, 1211-1217, 2006.
170. A. Colubri, A.K. Jha, M.Y. Shen, **A. Sali**, R.S. Berry, T.R. Sosnick, K.F. Freed. "Minimalist representations and the importance of nearest neighbor effects in protein folding simulations." *J Mol Biol* **363**, 835-857, 2006.
171. M.Y. Shen, **A. Sali**. "Statistical potential for assessment and prediction of protein structures." *Protein Sci* **15**, 2507-2524, 2006.
172. N. Eswar, B. Webb, M.A. Marti-Renom, M.S. Madhusudhan, D. Eramian, M.Y. Shen, U. Pieper, **A. Sali**. "Comparative protein structure modeling using MODELLER." *Curr Protoc Bioinformatics* **Chapter 5**, Unit 5.6.1-5.6.30, 2006.
173. R. Karchin, A.N. Monteiro, S.V. Tavtigian, M.A. Carvalho, **A. Sali**. "Functional Impact of Missense Variants in BRCA1 Predicted by Supervised Learning." *PLoS Computational Biology* **3**, e26, 2007.
174. L. Kelly, R. Karchin, **A. Sali**. "Protein interactions and disease phenotypes in the ABC transporter superfamily." *Pac Symp Biocomput*, 51-63, 2007.
175. N. Eswar, **A. Sali**. "Comparative Modeling of Drug Target Proteins." In: Volume 4 Computer-Assisted Drug Design, Comprehensive Medicinal Chemistry II. Ed: J. Taylor, D. Triggler, J.S. Mason, pp. 215-236, Elsevier Ltd, Oxford, UK, 2007.
176. M.A. Carvalho, S.M. Marsillac, R. Karchin, S. Manoukian, S. Grist, R.F. Swaby, T.P. Urmenyi, E. Rondinelli, R. Silva, L. Gayol, L. Baumbach, R. Sutphen, J.L. Pickard-Brzosowicz, K.L. Nathanson, **A. Sali**, D. Goldgar, F.J. Couch, P. Radice, A.N. Monteiro. "Determination of cancer risk associated with germ line BRCA1 missense variants by functional analysis." *Cancer Res* **67**, 1494-1501, 2007.

177. S.X. Wang, K.C. Pandey, J. Scharfstein, J. Whisstock, R.K. Huang, J. Jacobelli, R.J. Fletterick, P.J. Rosenthal, M. Abrahamson, L.S. Brinen, A. Rossi, **A. Sali**, J.H. McKerrow. "The structure of chagasin in complex with a cysteine protease clarifies the binding mode and evolution of an inhibitor family." *Structure* **15**, 535-543, 2007.

178. E. Feyfant, **A. Sali**, A. Fiser. "Modeling mutations in protein structures." *Protein Sci* **16**, 2030-2041, 2007.

179. N. Soranzo, L. Kelly, L. Martinian, M.W. Burley, M. Thom, **A. Sali**, D.L. Kroetz, D.B. Goldstein, S.M. Sisodiya. "Lack of support for a role for RLIP76 (RALBP1) in response to treatment or predisposition to epilepsy." *Epilepsia* **48**, 674-683, 2007.

180. K. Bajaj, M.S. Madhusudhan, B.V. Adkar, P. Chakrabarti, C. Ramakrishnan, **A. Sali**, R. Varadarajan. "Stereochemical criteria for prediction of the effects of proline mutations on protein stability." *PLoS Comput Biol* **3**, e241, 2007.

181. R. Aragues, **A. Sali**, J. Bonet, M.A. Marti-Renom, B. Oliva. "Characterization of protein hubs by inferring interacting motifs from protein interactions." *PLoS Comput Biol* **3**, 1761-1771, 2007.

182. M.A. Marti-Renom, A. Rossi, F. Al-Shahrour, F.P. Davis, U. Pieper, J. Dopazo, **A. Sali**. "The AnnoLite and AnnoLyze programs for comparative annotation of protein structures." *BMC Bioinformatics* **8 Suppl 4**, S4, 2007.

183. M.A. Marti-Renom, U. Pieper, M.S. Madhusudhan, A. Rossi, N. Eswar, F.P. Davis, F. Al-Shahrour, J. Dopazo, **A. Sali**. "DBAli tools: mining the protein structure space." *Nucleic Acids Res* **35**, W393-397, 2007.

184. F.P. Davis, D.T. Barkan, N. Eswar, J.H. McKerrow, **A. Sali**. "Host pathogen protein interactions predicted by comparative modeling." *Protein Sci* **16**, 2585-2596, 2007.

185. S.C. Almo, J.B. Bonanno, J.M. Sauder, S. Emtage, T.P. DiIorenzo, V. Malashkevich, S.R. Wasserman, S. Swaminathan, S. Eswaramoorthy, R. Agarwal, D. Kumaran, M. Madegowda, S. Ragumani, Y. Patskovsky, J. Alvarado, U.A. Ramagopal, J. Faber-Barata, M.R. Chance, **A. Sali**, A. Fiser, Z.Y. Zhang, D.S. Lawrence, S.K. Burley. "Structural genomics of protein phosphatases." *J Struct Funct Genom* **8**, 121-140, 2007.

186. F. Melo, **A. Sali**. "Fold assessment for comparative protein structure modeling." *Protein Sci* **16**, 2412-2426, 2007.

187. **A. Sali**, C.D. Lima, M. Kostic. "Structural genomics." *Structure* **15**, 1341, 2007.

188. V.D. Winn, R. Haimov-Kochman, A.C. Paquet, Y.J. Yang, M.S. Madhusudhan, M. Gormley, K.T. Feng, D.A. Bernlohr, S. McDonagh, L. Pereira, **A. Sali**, S.J. Fisher. "Gene expression profiling of the human maternal-fetal interface reveals dramatic changes between midgestation and term." *Endocrinology* **148**, 1059-1079, 2007.

189. C.V. Robinson, **A. Sali**, W. Baumeister. "The molecular sociology of the cell." *Nature* **450**, 973-982, 2007.

190. F. Alber, S. Dokudovskaya, L.M. Veenhoff, W. Zhang, J. Kipper, D. Devos, A. Suprpto, O. Karni-Schmidt, R. Williams, B.T. Chait, **A. Sali**, M.P. Rout. "The molecular architecture of the nuclear pore complex." *Nature* **450**, 695-701, 2007.

191. F. Alber, S. Dokudovskaya, L.M. Veenhoff, W. Zhang, J. Kipper, D. Devos, A. Suprpto, O. Karni-Schmidt, R. Williams, B.T. Chait, M.P. Rout, **A. Sali**. "Determining the architectures of macromolecular

assemblies." *Nature* **450**, 683-694, 2007.

192. N. Eswar, D. Eramian, B. Webb, M.Y. Shen, **A. Sali**. "Protein structure modeling with MODELLER." *Methods Mol Biol* **426**, 145-159, 2008.

193. T. Schwede, **A. Sali**, N. Eswar, M.C. Peitsch. "Protein Structure Modeling." In: Computational Structural Biology. Ed: T. Schwede, M.C. Peitsch, pp. 3-35, World Scientific Publishing Ltd., Singapore, 2008.

194. Y. Cong, M. Topf, **A. Sali**, P. Matsudaira, M. Dougherty, W. Chiu, M.F. Schmid. "Crystallographic conformers of actin in a biologically active bundle of filaments." *J Mol Biol* **375**, 331-336, 2008.

195. C.R. Booth, A.S. Meyer, Y. Cong, M. Topf, **A. Sali**, S.J. Ludtke, W. Chiu, J. Frydman. "Mechanism of lid closure in the eukaryotic chaperonin TRiC/CCT." *Nat Struct Mol Biol* **15**, 746-753, 2008.

196. S.K. Burley, S.C. Almo, J.B. Bonanno, M.R. Chance, S. Emtage, A. Fiser, **A. Sali**, J.M. Sauder, S. Swaminathan. "Structure Genomics of Protein Superfamilies." In: Structural Bioinformatics, 2nd Edition. Ed: J. Gu, P.E. Bourne, Wiley-Blackwell, New York, NY, 2008.

197. F. Alber, B.T. Chait, M.P. Rout, **A. Sali**. "Integrative Structure Determination of Protein Assemblies by Satisfaction of Spatial Restraints." In: Protein-protein interactions and networks: identification, characterization and prediction. Ed: A. Panchenko, T. Przytycka, pp. 99-114, Springer-Verlag, London, UK, 2008.

198. P. Chandramouli, M. Topf, J.F. Menetret, N. Eswar, J.J. Cannone, R.R. Gutell, **A. Sali**, C.W. Akey. "Structure of the mammalian 80S ribosome at 8.7 Å resolution." *Structure* **16**, 535-548, 2008.

199. F. Alber, F. Forster, D. Korkin, M. Topf, **A. Sali**. "Integrating diverse data for structure determination of macromolecular assemblies." *Annu Rev Biochem* **77**, 443-477, 2008.

200. M. Topf, K. Lasker, B. Webb, H. Wolfson, W. Chiu, **A. Sali**. "Protein structure fitting and refinement guided by cryo-EM density." *Structure* **16**, 295-307, 2008.

201. J. Espadaler, N. Eswar, E. Querol, F.X. Aviles, **A. Sali**, M.A. Marti-Renom, B. Oliva. "Prediction of enzyme function by combining sequence similarity and protein interactions." *BMC Bioinformatics* **9**, 249, 2008.

202. F. Agüero, B. Al-Lazikani, M. Aslett, M. Berriman, F.S. Buckner, R.K. Campbell, S. Carmona, I.M. Carruthers, A.W. Chan, F. Chen, G.J. Crowther, M.A. Doyle, C. Hertz-Fowler, A.L. Hopkins, G. McAllister, S. Nwaka, J.P. Overington, A. Pain, G.V. Paolini, U. Pieper, S.A. Ralph, A. Riechers, D.S. Roos, **A. Sali**, D. Shanmugam, T. Suzuki, W.C. Van Voorhis, C.L. Verlinde. "Genomic-scale prioritization of drug targets: the TDR Targets database." *Nat Rev Drug Discov* **7**, 900-907, 2008.

203. R. Karchin, M. Agarwal, **A. Sali**, F. Couch, M.S. Beattie. "Classifying Variants of Undetermined Significance in BRCA2 with Protein Likelihood Ratios." *Cancer Inform* **6**, 203-216, 2008.

204. K.A. Krukenberg, F. Forster, L.M. Rice, **A. Sali**, D.A. Agard. "Multiple conformations of *E. coli* Hsp90 in solution: insights into the conformational dynamics of Hsp90." *Structure* **16**, 755-765, 2008.

205. D. Eramian, N. Eswar, M.Y. Shen, **A. Sali**. "How well can the accuracy of comparative protein structure models be predicted?" *Protein Sci* **17**, 1881-1893, 2008.

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

207. C.M. Anderson, D. Korkein, D.L. Smith, S. Makovets, J.J. Seidel, **A. Sali**, E.H. Blackburn. "Tel2 mediates activation and localization of ATM/Tel1 kinase to a double-strand break." *Genes Dev* **22**, 854-859, 2008.
208. R.A. Chiang, **A. Sali**, P.C. Babbitt. "Evolutionarily conserved substrate substructures for automated annotation of enzyme superfamilies." *PLoS Comput Biol* **4**, e1000142, 2008.
209. S. Mahrus, J.C. Trinidad, D.T. Barkan, **A. Sali**, A.L. Burlingame, J.A. Wells. "Global Sequencing of Proteolytic Cleavage Sites in Apoptosis by Specific Labeling of Protein N Termini." *Cell* **134**, 866-876, 2008.
210. I.I. Serysheva, S.J. Ludtke, M.L. Baker, Y. Cong, M. Topf, D. Eramian, **A. Sali**, S.L. Hamilton, W. Chiu. "Subnanometer-resolution electron cryomicroscopy-based domain models for the cytoplasmic region of skeletal muscle RyR channel." *Proc Natl Acad Sci U S A* **105**, 9610-9615, 2008.
211. S. Graslund, P. Nordlund, J. Weigelt, B.M. Hallberg, J. Bray, O. Gileadi, S. Knapp, U. Oppermann, C. Arrowsmith, R. Hui, J. Ming, S. dhe-Paganon, H. Park, A. Savchenko, A. Yee, A. Edwards, R. Vincentelli, C. Cambillau, R. Kim, S. Kim, Z. Rao, Y. Shi, T.C. Terwilliger, C. Kim, L. Hung, G.S. Waldo, Y. Peleg, S. Albeck, T. Unger, O. Dym, J. Prilusky, J.L. Sussman, R.C. Stevens, S.A. Lesley, I.A. Wilson, A. Joachimiak, F. Collart, I. Dementieva, M.I. Donnelly, W.H. Eschenfeldt, Y. Kim, L. Stols, R. Wu, M. Zhou, S.K. Burley, J.S. Emtage, J.M. Sauder, D. Thompson, K. Bain, J. Luz, T. Gheyi, F. Zhang, S. Atwell, S.C. Almo, J.B. Bonanno, A. Fiser, S. Swaminathan, F.W. Studier, M.R. Chance, **A. Sali**, T.B. Acton, R. Xiao, L. Zhao, L.C. Ma, J.F. Hunt, L. Tong, K. Cunningham, M. Inouye, S. Anderson, H. Janjua, R. Shastry, C.K. Ho, D. Wang, H. Wang, M. Jiang, G.T. Montelione, D.I. Stuart, R.J. Owens, S. Daenke, A. Schutz, U. Heinemann, S. Yokoyama, K. Bussow, K.C. Gunsalus. "Protein production and purification (vol 5, pg 135, 2008)." *Nat Methods* **5**, 369-369, 2008.
212. N. Eswar, **A. Sali**. "Protein Structure Modeling." In: *From Molecules to Medicine, Structure of Biological Macromolecules and Its Relevance in Combating New Diseases and Bioterrorism*. Ed: J.L. Sussman, P. Spadon, pp. 139-151, Springer-Verlag, Dordrecht, The Netherlands, 2009.
213. U. Pieper, R. Chiang, J.J. Seffernick, S.D. Brown, M.E. Glasner, L. Kelly, N. Eswar, J.M. Sauder, J.B. Bonanno, S. Swaminathan, S.K. Burley, X. Zheng, M.R. Chance, S.C. Almo, J.A. Gerlt, F.M. Raushel, M.P. Jacobson, P.C. Babbitt, **A. Sali**. "Target selection and annotation for the structural genomics of the amidohydrolase and enolase superfamilies." *J Struct Funct Genom* **10**, 107-125, 2009.
214. U. Pieper, N. Eswar, B.M. Webb, D. Eramian, L. Kelly, D.T. Barkan, H. Carter, P. Mankoo, R. Karchin, M.A. Marti-Renom, F.P. Davis, **A. Sali**. "MODBASE, a database of annotated comparative protein structure models and associated resources." *Nucleic Acids Res* **37**, D347-354, 2009.
215. F.A. Hays, Z. Roe-Zurz, M. Li, L. Kelly, F. Gruswitz, **A. Sali**, R.M. Stroud. "Ratiocinative screen of eukaryotic integral membrane protein expression and solubilization for structure determination." *J Struct Funct Genom* **10**, 9-16, 2009.
216. M. Li, F.A. Hays, Z. Roe-Zurz, L. Vuong, L. Kelly, C.M. Ho, R.M. Robbins, U. Pieper, J.D. O'Connell 3rd, L.J. Miercke, K.M. Giacomini, **A. Sali**, R.M. Stroud. "Selecting optimum eukaryotic integral membrane proteins for structure determination by rapid expression and solubilization screening." *J Mol Biol* **385**, 820-830, 2009.
217. M.E. Peterson, F. Chen, J.G. Saven, D.S. Roos, P.C. Babbitt, **A. Sali**. "Evolutionary constraints on structural similarity in orthologs and paralogs." *Protein Sci* **18**, 1306-1315, 2009.
218. D. Russel, K. Lasker, J. Phillips, D. Schneidman-Duhovny, J.A. Velazquez-Muriel, **A. Sali**. "The structural dynamics of macromolecular processes." *Curr Opin Cell Biol* **21**, 97-108, 2009.

219. T. Schwede, **A. Sali**, B. Honig, M. Levitt, H.M. Berman, D. Jones, S.E. Brenner, S.K. Burley, R. Das, N.V. Dokholyan, R.L. Dunbrack Jr, K. Fidelis, A. Fiser, A. Godzik, Y.J. Huang, C. Humblet, M.P. Jacobson, A. Joachimiak, S.R. Krystek Jr, T. Kortemme, A. Kryshtafovych, G.T. Montelione, J. Moulton, D. Murray, R. Sanchez, T.R. Sosnick, D.M. Standley, T. Stouch, S. Vajda, M. Vasquez, J.D. Westbrook, I.A. Wilson. "Outcome of a workshop on applications of protein models in biomedical research." *Structure* **17**, 151-159, 2009.
220. L. Orti, R.J. Carbajo, U. Pieper, N. Eswar, S.M. Maurer, A.K. Rai, G. Taylor, M.H. Todd, A. Pineda-Lucena, **A. Sali**, M.A. Marti-Renom. "A kernel for open source drug discovery in tropical diseases." *PLoS Negl Trop Dis* **3**, e418, 2009.
221. K.C. Pandey, D.T. Barkan, **A. Sali**, P.J. Rosenthal. "Regulatory elements within the prodomain of falcipain-2, a cysteine protease of the malaria parasite *Plasmodium falciparum*." *PLoS One* **4(5):e5694**, 2009.
222. R.M. Stroud, S. Choe, J. Holton, H.R. Kaback, W. Kwiatkowski, D.L. Minor, R. Riek, **A. Sali**, H. Stahlberg, W. Harries. "2007 Annual progress report synopsis of the Center for Structures of Membrane Proteins." *J Struct Funct Genom* **10**, 193-208, 2009.
223. L. Orti, R.J. Carbajo, U. Pieper, N. Eswar, S.M. Maurer, A.K. Rai, G. Taylor, M.H. Todd, A. Pineda-Lucena, **A. Sali**, M.A. Marti-Renom. "A kernel for the Tropical Disease Initiative." *Nat Biotechnol* **27**, 320-321, 2009.
224. O. Fornes, R. Aragues, J. Espadaler, M.A. Marti-Renom, **A. Sali**, B. Oliva. "ModLink+: Improving fold recognition by using protein-protein interactions." *Bioinformatics* **25**, 1506-1512, 2009.
225. S. Nickell, F. Beck, S.H.W. Scheres, A. Korinek, F. Forster, K. Lasker, O. Mihalache, N. Sun, I. Nagy, **A. Sali**, J. Plitzko, J.-M. Carazo, M. Mann, W. Baumeister. "Insights into the Molecular Architecture of the 26S Proteasome." *Proc Natl Acad Sci U S A* **29**, 11943-11947, 2009.
226. K. Lasker, M. Topf, **A. Sali**, H.J. Wolfson. "Inferential optimization for simultaneous fitting of multiple components into a cryoEM map of their assembly." *J Mol Biol* **388**, 180-194, 2009.
227. M.S. Madhusudhan, B.M. Webb, M.A. Marti-Renom, N. Eswar, **A. Sali**. "Alignment of multiple protein structures based on sequence and structure features." *Protein Eng Des Sel* **22**, 569-574, 2009.
228. J.A. DeGrasse, K.N. DuBois, D. Devos, T.N. Siegel, **A. Sali**, M.C. Field, M.P. Rout, B.T. Chait. "The Establishment of Nuclear Pore Complex Architecture Occurred Early in Evolution." *Mol Cell Proteomics* **8**, 2119-2130, 2009.
229. L. Kelly, U. Pieper, N. Eswar, F.A. Hays, M. Li, Z. Roe-Zurz, D. Kroetz, K.M. Giacomini, R.M. Stroud, **A. Sali**. "A survey of integral alpha-helical membrane proteins." *J Struct Funct Genomics* **10**, 269-280, 2009.
230. T. Lezon, **A. Sali**, I. Bahar. "Global motions of the nuclear pore complex: Insights from Elastic Network Models." *PLoS Comp Biol* **5**, e1000496, 2009.
231. D.J. Taylor, B. Devkota, A.D. Huang, M. Topf, N. Eswar, **A. Sali**, S.C. Harvey, J. Frank. "Comprehensive Molecular Structure of the Eukaryotic Ribosome." *Structure* **17**, 1591-1604, 2009.
232. H. Fan, J.J. Irwin, B.M. Webb, G. Klebe, B. Shoichet, **A. Sali**. "Molecular Docking Screens Using Comparative Models of Proteins." *J Chem Inf Model* **49**, 2512-2527, 2009.
233. F. Forster, K. Lasker, F. Beck, S. Nickell, **A. Sali**, W. Baumeister. "An Atomic Model AAA-

- ATPase/20S core particle sub-complex of the 26S proteasome." *Biochem Biophys Res Commun* **388**, 228-233, 2009.
234. D. Kroetz, N. Ahituv, E. Burchard, S. Guo, **A. Sali**, K. Giacomini. "The Pharmacogenomics Center of the University of California, San Francisco: At the interface of genomics, biological mechanism and drug therapy." *Pharmacogenomics* **10**, 1569-1576, 2009.
235. F.P. Davis, **A. Sali**. "The overlap of small molecule and protein binding sites within families of protein structures." *PLoS Comp Biol* **6**, e1000668, 2010.
236. D. Barkan, D. Hostetter, S. Mahrus, U. Pieper, J. Wells, C. Craik, **A. Sali**. "Prediction of Protease Substrates using Sequence and Structure Features." *Bioinformatics* **26**, 1714-1722, 2010.
237. F. Gruswitz, S. Chaudhary, J. Ho, A. Schlessinger, P. Bobak, C. Ho, **A. Sali**, C. Westhoff, R. Stroud. "Function of Human Rh based on Structure of RhCG at 2.1 Å." *Proc Natl Acad Sci U S A* **107**, 9638-9643, 2010.
238. L. Chen, B. Pawlikowski, A. Schlessinger, S. More, D. Stryke, S.J. Johns, M. Portman, T.E. Ferrin, **A. Sali**, K. Giacomini. "Role of organic cation transporter 3 (SLC22A3) and Its missense variants in the pharmacologic action of metformin." *Pharmacogenet Genomics* **20**, 687-699, 2010.
239. A. Schlessinger, P. Matsson, J.E. Shima, U. Pieper, S.W. Yee, L. Kelly, L. Apeltsin, R.M. Stroud, T.E. Ferrin, K.M. Giacomini, **A. Sali**. "Comparison of Human Solute Carriers." *Protein Sci* **19**, 412-428, 2010.
240. D. Schneidman-Duhovny, M. Hammel, **A. Sali**. "FoXS: A Web Server for Rapid Computation and Fitting of SAXS Profiles." *Nucleic Acids Res* **38**, 541-544, 2010.
241. K. Lasker, J.L. Phillips, D. Russel, J. Velazquez-Muriel, D. Schneidman-Duhovny, B. Webb, A. Schlessinger, **A. Sali**. "Integrative Structure Modeling of Macromolecular Assemblies from Proteomics Data." *Mol Cell Proteomics* **9**, 1689-1702, 2010.
242. P. Sampathkumar, S.A. Ozyurt, J. Do, K.T. Bain, M. Dickey, L.A. Rodgers, T. Gheyi, **A. Sali**, S.J. Kim, J. Phillips, U. Pieper, J. Fernandez-Martinez, J.D. Franke, A. Martel, H. Tsuruta, S. Atwell, D.A. Thompson, J.S. Emtage, S.R. Wasserman, M.P. Rout, J.M. Sauder, S.K. Burley. "Structures of the autoproteolytic domain from the *Saccharomyces cerevisiae* nuclear pore complex component, Nup 145." *Proteins: Struct Funct Bioinform* **78**, 1992-1998, 2010.
243. P. Sampathkumar, F. Lu, X. Zhao, Z. Li, J. Gilmore, K. Bain, M.E. Rutter, T. Gheyi, K. Schwinn, J. Bonanno, U. Pieper, J.E. Fajardo, A. Fiser, S. Almo, A. Swaminathan, M. Chance, D. Baker, S. Atwell, D. Thompson, J.S. Emtage, S. Wasserman, **A. Sali**, J.M. Sauder, S. Burley. "Structure of a putative BenF-like porin from *Pseudomonas fluorescens* Pf-5 at 2.6 Å resolution." *Proteins: Struct Funct Bioinform* **78**, 3056-3062, 2010.
244. K. Lasker, **A. Sali**, H.J. Wolfson. "Determining macromolecular assembly structures by molecular docking and fitting into an electron density map." *Proteins: Struct Funct Bioinform* **78**, 3205-3211, 2010.
245. L. Chen, M. Takizawa, E. Chen, A. Schlessinger, J.H. Choi, J. Segenthaler, **A. Sali**, M. Kubo, S. Nakamura, Y. Iwamoto, N. Iwasaki, K.M. Giacomini. "Genetic polymorphisms in the organic cation transporter 1, OCT1, in Chinese and Japanese populations, exhibit altered function." *J Pharmacol Exp Ther* **1**, 42-50, 2010.
246. L. Kelly, H. Fukushima, R. Karchin, J.M. Gow, L.W. Chinn, U. Pieper, M.R. Segal, D.L. Kroetz, **A. Sali**. "Functional Hot Spots in Human ATP-binding Cassette Transporter Nucleotide Binding Domains." *Protein Sci* **19**, 2110-2121, 2010.

247. F. Forster, K. Lasker, S. Nickell, **A. Sali**, W. Baumeister. "Toward an integrated structural model of the 26S proteasome." *Mol Cell Proteomics* **9**, 1666-1677, 2010.
248. D. Schneidman-Duhovny, M. Hammel, **A. Sali**. "Macromolecular docking restrained by a small angle X-ray scattering profile." *J Struct Biol* **3**, 461-471, 2011.
249. L. Kelly, H. Fukushima, R. Karchin, J.M. Gow, L.W. Chinn, U. Pieper, M.R. Segal, D.L. Kroetz, **A. Sali**. "Response to "Predictable difficulty or difficulty to predict" by Tamas Aranyi, Krisztina Fulop, Orsolya Symmons, Viola Pomozi, and Andras Varadi." *Protein Sci* **20**, 4-5, 2011.
250. U. Pieper, B.M. Webb, D.T. Barkan, D. Schneidman-Duhovny, A. Schlessinger, H. Braberg, Z. Yang, E.C. Meng, E.F. Pettersen, C.C. Huang, R.S. Datta, P. Sampathkumar, M.S. Madhusudhan, K. Sjolander, T.E. Ferrin, S.K. Burley, **A. Sali**. "ModBase, a database of annotated comparative protein structure models, and associated resources." *Nucleic Acids Res* **39**, 465-474, 2011.
251. S.S. Kamat, A. Bagaria, D. Kumaran, G.P. Holmes-Hampton, H. Fan, **A. Sali**, J.M. Sauder, S.K. Burley, P.A. Lindahl, S. Swaminathan, F.M. Raushel. "Catalytic Mechanism and Three-Dimensional Structure of Adenine Deaminase." *Biochemistry* **50**, 1917-1927, 2011.
252. B. Webb, K. Lasker, D. Schneidman-Duhovny, E. Tjioe, J. Phillips, S.J. Kim, J. Velazquez-Muriel, D. Russel, **A. Sali**. "Modeling of Proteins and their Assemblies with the Integrative Modeling Platform." In: *Methods in Molecular Biology*, pp. 377-397, Humana Press, 2011.
253. P. Sampathkumar, T. Gheyi, S.A. Miller, K.T. Bain, M. Dickey, J.B. Bonanno, Kim. S.J., J. Phillips, U. Pieper, J. Fernandez-Martinez, J. Franke, A. Martel, H. Tsuruta, S. Atwell, D.A. Thompson, J.S. Emtage, S.R. Wasserman, M.P. Rout, **A. Sali**, J.M. Sauder, S.K. Burley. "Structure of the C-terminal domain of *Saccharomyces cerevisiae* Nup133, a component of the Nuclear Pore Complex." *Proteins: Struct Funct Bioinform* **79**, 1672-1677, 2011.
254. S.S. Kamat, H. Fan, J.M. Sauder, S.K. Burley, B.K. Shoichet, **A. Sali**, F.M. Raushel. "Enzymatic deamination of the epigenetic base N-6-methyladenine." *J Am Chem Soc* **133**, 2080-2083, 2011.
255. S. Dokudovskaya, F. Waharte, A. Schlessinger, U. Pieper, D.P. Devos, I.M. Cristea, R. Williams, J. Salamero, B.T. Chait, **A. Sali**, M.C. Field, M.C. Rout, C. Dargemont. "A conserved coatomer-related complex containing Sec13 and Seh1 dynamically associates with the vacuole in *Saccharomyces cerevisiae*." *Mol Cell Proteomics* **10**, M110.006478, 2011.
256. M. Field, **A. Sali**, M. Rout. "On a bender: Bars, ESCRTs, COPs, and finally getting your coat." *J Cell Biol* **193**, 963-972, 2011.
257. H. Fan, D. Schneidman, J.J. Irwin, G. Dong, B. Shoichet, **A. Sali**. "Statistical Potential for Modeling and Ranking Protein-Ligand Interactions." *J Chem Inf Model* **51**, 3078-3092, 2011.
258. S. Jager, P. Cimermancic, N. Gulbahce, J. Johnson, K. McGovern, S. Clarke, M. Shales, G. Mercenne, K. Li, H. Barry, G. Jang, E. Akiva, L. Pache, J. Marlett, S. Roth, M. Stephens, I. D'Orso, J. Fernandes, M. Fahey, C. Mahon, A. O'Donoghue, A. Todorovic, J. Morris, D. Maltby, T. Alber, G. Cagney, F. Bushman, J. Young, S. Chanda, W. Sundquist, T. Kortemme, R. Hernandez, C. Craik, A. Burlingame, **A. Sali**, A. Frankel, N. Krogan. "Global Landscape of HIV-Human Protein Complexes." *Nature* **481**, 365-370, 2011.
259. S. Jager, D.Y. Kim, K. Shindo, E. Kwon, R. LaRue, C. Mahon, P. Cimermancic, L. Yen, D. Stanley, M. Li, A. Burlingame, **A. Sali**, C. Craik, R. Harris, J. Gross, N. Krogan. "Vif Hijacks CBF β to Degrade APOBEC3G and Promote HIV-1 Infection." *Nature* **481**, 371-375, 2011.

260. E. Tjioe, K. Lasker, B. Webb, H. Wolfson, **A. Sali**. "MultiFit: A web server for fitting multiple protein structures into their electron microscopy density map." *Nucleic Acids Res* **39**, 167-170, 2011.
261. J. Carlsson, R. Coleman, V. Setola, J. Irwin, H. Fan, A. Schlessinger, **A. Sali**, B. Roth, B. Shoichet. "Structure-based Ligand Discovery Against a Homology Model and X-ray Structure of the Dopamine D3 Receptor." *Nat Chem Biol* **7**, 769-778, 2011.
262. A. Schlessinger, E. Geier, H. Fan, J. Irwin, B. Shoichet, K. Giacomini, **A. Sali**. "Structure-based Discovery of Prescription Drugs that Interact with the Norepinephrine Transporter, NET." *Proc Natl Acad Sci USA* **108**, 15810-15815, 2011.
263. J. Choi, S. Yee, A. Ramirez, K. Morrissey, G. Jang, P. Joski, J. Mefford, S. Hesselon, A. Schlessinger, G. Jenkins, R. Castro, S. Johns, D. Stryke, **A. Sali**, T. Ferrin, J. Witte, P. Kwok, D. Roden, R. Wilke, C. McCarty, R. Davis, K. Giacomini. "A Common Promoter Variant in MATE2-K Is Associated with Poor Response to Metformin." *Clin Pharmacol Ther* **90**, 674-684, 2011.
264. A.M. Goble, H. Fan, **A. Sali**, F.M. Raushel. "Discovery of a Cytokinin Deaminase." *ACS Chem Biol* **6**, 1036-1040, 2011.
265. J. Gerlt, K. Allen, S. Almo, R. Armstrong, P. Babbitt, J. Cronan, D. Dunaway-Mariano, H. Imker, M. Jacobson, W. Minor, C. Poulter, F. Raushel, **A. Sali**, B. Shoichet, J. Sweedler. "The Enzyme Function Initiative." *Biochemistry* **50**, 9950-9962, 2011.
266. Z. Yang, K. Lasker, D. Schneidman-Duhovny, B. Webb, C. Huang, E. Pettersen, T. Goddard, E. Meng, **A. Sali**, T. Ferrin. "UCSF Chimera, MODELLER, and IMP: an integrated Modeling System." *J Struct Biol* **179**, 269-278, 2012.
267. K. Lasker, J. Velazquez-Muriel, B. Webb, Z. Yang, T.E. Ferrin, **A. Sali**. "Macromolecular assembly structures by comparative modeling and electron microscopy." In: *Methods in Molecular Biology*. Ed: J. Walker, pp. 331-350, Humana Press, New York, NY, 2012.
268. H. Fan, J. Irwin, **A. Sali**. "Virtual Ligand Screening Against Comparative Protein Structure Models." *Methods Mol Biol* **819**, 105-126, 2012.
269. J. Fernandez-Martinez, J. Phillips, M. Sekedat, R. Diaz-Avalos, J. Velazquez-Muriel, J. Franke, R. Williams, D. Stokes, B. Chait, **A. Sali**, M. Rout. "Structure-function Map for a Heptameric Component of the Nuclear Pore Complex." *J Cell Biol* **196**, 419-434, 2012.
270. R. Henderson, **A. Sali**, M. Baker, B. Carragher, B. Devkota, K. Downing, E. Egelman, Z. Feng, J. Frank, N. Grigorieff, W. Jiang, S. Ludtke, O. Medalia, P. Penczek, P. Rosenthal, M. Rossmann, M. Schmid, G. Schroder, A. Steven, D. Stokes, J. Westbrook, W. Wriggers, H. Yang, J. Young, H. Berman, W. Chiu, G. Kleywegt, C. Lawson. "Outcome of the First Electron Microscopy Validation Task Force Meeting." *Structure* **20**, 205-214, 2012.
271. P. Weinkam, J. Pons, **A. Sali**. "Structure-based Model of Allostery Predicts Coupling Between Distant Sites." *Proc Natl Acad Sci USA* **109**, 4875-4880, 2012.
272. D. Russel, K. Lasker, B. Webb, J. Velazquez-Muriel, E. Tjioe, D. Schneidman-Duhovny, B. Peterson, **A. Sali**. "Putting the pieces together: integrative structure determination of macromolecular assemblies." *PLoS Biol* **10**, e1001244, 2012.
273. G. Pathare, I. Nagy, S. Bohn, P. Unverdorben, A. Hubert, R. Korner, S. Nickell, K. Lasker, **A. Sali**, T. Tamura, T. Nishioka, F. Forster, W. Baumeister, A. Bracher. "The proteasomal subunit Rpn6 is a molecular clamp holding the core and regulatory subcomplexes together." *Proc Natl Acad Sci USA* **109**, 149-154, 2012.

274. K. Lasker, F. Forster, S. Bohn, T. Walzthoeni, E. Villa, P. Unverdorben, F. Beck, R. Aebersold, **A. Sali**, W. Baumeister. "Molecular architecture of the 26S proteasome holocomplex determined by an integrative approach." *Proc Natl Acad Sci USA* **109**, 1380-1387, 2012.
275. P. Sampathkumar, S.J. Kim, D. Manglicmot, K.T. Bain, J. Gilmore, T. Gheyi, J. Phillips, U. Pieper, J. Fernandez-Martinez, J. Franke, T. Matsui, H. Tsuruta, S. Atwell, D. Thompson, J.S. Emtage, S. Wasserman, M. Rout, **A. Sali**, J.M. Sauder, S.C. Almo, S.K. Burley. "Atomic structure of the Nuclear Pore Complex targeting domain of Nup116 homologue from the yeast, *Candida glabrata*." *Proteins: Struct Funct Bioinform* **8**, 2110-2116, 2012.
276. C. Klammt, I. Maslennikov, M. Bayrhuber, C. Eichmann, N. Vajpai, E. Chiu, K. Blain, L. Esquivies, H. Kwon, B. Balana, U. Pieper, **A. Sali**, P. Slesinger, W. Kwiatkowski, R. Rick, S. Choe. "Facile Backbone structure determination of human membrane proteins by NMR spectroscopy." *Nat Methods* **8**, 834-839, 2012.
277. D. Schneidman-Duhovny, A. Rossi, A. Avila-Sakar, S.J. Kim, J. Velazquez-Muriel, P. Strop, H. Liang, K.A. Krukenberg, M. Liao, H.M. Kim, S. Sobhanifar, V. Dotsch, A. Raipal, J. Pons, D.A. Agard, Y. Cheng, **A. Sali**. "A Method for Integrative Structure Determination of Protein-Protein Complexes." *Bioinformatics* **28**, 3282-3289, 2012.
278. V. Puizdar, T. Zajc, E. Zerovnik, M. Renko, U. Pieper, N. Eswar, **A. Sali**, I. Dolenc, V. Turk. "Biochemical Characterization and Structural Modeling of Human Cathepsin E Variant 2 in Comparison to the Wild-type Protein." *Biol Chem* **393**, 177-186, 2012.
279. A. Morin, J. Urban, P.D. Adams, I. Foster, **A. Sali**, D. Baker, P. Sliz. "Shining Light into Black Boxes." *Science* **336**, 159-160, 2012.
280. H. Braberg, B. Webb, E. Tjioe, U. Pieper, **A. Sali**, M.S. Madhusudhan. "SALIGN: A webserver for alignment of multiple protein sequences and structures." *Bioinformatics* **15**, 2072-2073, 2012.
281. J.A. Horst, U. Pieper, **A. Sali**, L. Zhan, G. Chopra, R. Samudrala, J.D.B. Featherstone. "Strategic protein target analysis for developing drugs to stop dental caries." *Adv Dent Res* **22**, 86-93, 2012.
282. J. Trinidad, D. Barkan, B. Gulledge, A. Thalhammer, **A. Sali**, R. Schoepfer, A. Burlingame. "Global Identification and Characterization of Both O-GlcNAcylation and Phosphorylation at the Murine Synapse." *Mol Cell Proteomics* **11**, 215-229, 2012.
283. O. Martinez-Avila, S. Wu, S.J. Kim, Y. Cheng, F. Khan, R. Samudrala, **A. Sali**, J. Horst, S. Habelitz. "Self-assembly of Filamentous Amelogenin Requires Calcium and Phosphate: From Dimers via Nanoribbons to Fibrils." *Biomacromolecules* **13**, 3494-3502, 2012.
284. J.A. Velazquez-Muriel, K. Lasker, D. Russel, J. Phillips, B. Webb, D. Schneidman-Duhovny, **A. Sali**. "Assembly of macromolecular complexes by satisfaction of spatial restraints from electron microscopy images." *Proc Natl Acad Sci USA* **109**, 18821-18826, 2012.
285. P. Kolb, K. Phan, Z. Gao, A. Marko, **A. Sali**, K.A. Jacobson. "Limits of ligand selectivity from docking to models: In silico screening for A1 adenosine receptor antagonists." *PLoS One* **7**, e49910, 2012.
286. A. Schlessinger, M.B. Wittwer, A. Dahlin, N. Khuri, M. Bonomi, H. Fan, K. Giacomini, **A. Sali**. "High Selectivity of the γ -Aminobutyric Acid Transporter 2 (GAT-2, SLC6A13) Revealed by Structure-based Approach." *J Biol Chem* **287**, 37745-37756, 2012.
287. D. Schneidman-Duhovny, S.J. Kim, **A. Sali**. "Integrative structural modeling with small angle X-ray

scattering profiles." *BMC Struct Biol* **12**, 17, 2012.

288. J.L. Markley, H. Akutsu, T. Asakura, M. Baldus, R. Boelens, A. Bonvin, R. Kaptein, A. Bax, I. Bezsonova, M.R. Gryk, J.C. Hoch, D.M. Korzhnev, M. Maciejewski, D. Case, W. Chazin, T. Cross, S. Dames, H. Kessler, O. Lange, T. Madl, B. Reif, M. Sattler, D. Eliezer, A. Fersht, J. Forman-Kay, L. Kay, J. Fraser, J. Gross, T. Kortemme, **A. Sali**, T. Fujiwara, K. Gardner, X. Luo, J. Rizo-Rey, M. Rosen, R. Gil, C. HO, G. Rule, A. Gronenborn, R. Ishima, J. Klein-Seetharaman, P. Tang, P. van der Wel, Y. Xu, S. Grzesiek, S. Hiller, J. Seelig, E. Laue, H. Mott, D. Nietlispach, I. Barsukiv, L. Lian, D. Middleton, T. Blumenschein, G. Moore, I. Campbell, J. Schnell, I. Vakonakis, A. Watts, M. Conte, J. Mason, M. Pfuhl, M. Sanderson, J. Craven, M. Williamson, C. Dominguez, G. Roberts, U. Gunther, M. Overduin, J. Werner, P. Williamson, C. Blindauer, M. Crump, P. Driscoll, T. Frenkiel, A. Golovanov, S. Matthews, J. Parkinson, D. Uhrin, M. Williams, D. Neuhaus, H. Oschkinat, A. Ramos, D. Shaw, C. Steinbeck, M. Vendruscolo, G. Vuister, K. Walters, H. Weinstein, K. Wuthrich, S. Yodoyama. "In support of the BMRB." *Nat Struct Mol Biol* **19**, 854-860, 2012.

289. H. Fan, D. Hitchcock, R. Seidel, B. Hillerich, H. Lin, S. Almo, **A. Sali**, B. Shoichet, F. Raushel. "The Assignment of Pterin Deaminase Activity to an Enzyme of Unknown Function Guided by Homology Modeling and Docking." *J Am Chem Soc* **135**, 795-803, 2013.

290. M.B. Wittwer, A.A. Zur, N. Khuri, Y. Kido, A. Kosaka, X. Zhang, K.M. Morrissey, **A. Sali**, Y. Huang, K.M. Giacomini. "Discovery of potent, selective multidrug and toxin extrusion Transporter 1 (MATE1, SLC47A1) inhibitors through prescription drug profiling and computational modeling." *J Med Chem* **56**, 781-795, 2013.

291. U. Pieper, A. Schlessinger, E. Kloppmann, G.A. Chang, J.J. Chou, M. Dumont, B. Fox, P. Fromme, W. Hendrickson, M. Malkowski, D. Rees, D. Stokes, M.H.B. Stowell, M. Wiener, B. Rost, R. Stroud, R. Stevens, **A. Sali**. "Coordinating the impact of structural genomics on the human α -helical transmembrane proteome." *Nat Struct Mol Biol* **20**, 135-138, 2013.

292. P. Sampathkumar, S.J. Kim, P. Upla, W. Rice, J. Phillips, B. Timney, U. Pieper, J. Bonanno, J. Fernandez-Martinez, Z. Hakhverdyan, N. Ketaren, T. Matsui, R. Weiss, D. Stokes, J.M. Sauder, S. Burley, **A. Sali**, M. Rout, S. Almo. "Structure, dynamics, evolution and function of a major scaffold component in the Nuclear Pore Complex." *Structure* **21**, 560-571, 2013.

293. H. Gradisar, S. Bozic, T. Doles, D. Vengust, I. Hafner-Bratkovic, A. Mertelj, B. Webb, **A. Sali**, S. Klavzar, R. Jerala. "Design of a single-chain polypeptide tetrahedron assembled from coiled-coil segments." *Nat Chem Biol* **9**, 362-366, 2013.

294. B. Pedersen, H. Kumar, A. Waight, A. Risenmay, Z. Roe-Zurz, B. Chau, A. Schlessinger, M. Bonomi, W. Harries, **A. Sali**, A. Johri, R. Stroud. "Crystal structure of a eukaryotic phosphate transporter." *Nature* **496**, 533-536, 2013.

295. A. Schlessinger, N. Khuri, K. Giacomini, **A. Sali**. "Molecular modeling and ligand docking for Solute Carrier (SLC) transporters." *Curr Top Med Chem* **13**, 843-856, 2013.

296. T. van Dam, M. Townsend, M. Turk, A. Schlessinger, **A. Sali**, M. Field, M. Huynen. "Evolution of modular intraflagellar transport from a coatomer-like progenitor." *Proc Natl Acad Sci USA* **110**, 6943-6948, 2013.

297. A. Waight, B. Pedersen, A. Schlessinger, M. Bonomi, B. Chau, Z. Roe-Zurz, A. Risenmay, **A. Sali**, R. Stroud. "Structural basis for alternating access of a Eukaryotic Calcium/Proton exchanger." *Nature* **499**, 107-110, 2013.

298. M. Guttman, P. Weinkam, **A. Sali**, K. Lee. "All-atom ensemble modeling to analyze small angle X-ray scattering of glycosylated proteins." *Structure* **21**, 321-331, 2013.

299. P. Weinkam, Y.C. Chen, J. Pons, **A. Sali**. "Impact of mutations on the allosteric conformational equilibrium." *J Mol Biol* **425**, 647-661, 2013.
300. A. Ward, **A. Sali**, I. Wilson. "Integrative structural biology." *Science* **339**, 913-915, 2013.
301. E. Geier, A. Schlessinger, H. Fan, J. Gable, J. Irwin, **A. Sali**, K. Giacomini. "Structure-based ligand discovery for the Large-neutral Amino Acid Transporter 1, LAT-1." *Proc Natl Acad Sci USA* **110**, 5480-5485, 2013.
302. A. Schlessinger, S.W. Yee, **A. Sali**, K. Giacomini. "SLC classification: an update." *Clin Pharmacol Ther* **94**, 19-23, 2013.
303. J. Trewhella, W. Hendrickson, G. Kleywegt, **A. Sali**, M. Sato, T. Schwede, D. Svergun, J. Tainer, J. Westbrook, H. Berman. "Report of the wwPDB Small-Angle Scattering Task Force: Data Requirements for Biomolecular Modeling and the PDB." *Structure* **21**, 875-881, 2013.
304. D. Schneidman-Duhovny, M. Hammel, J. Tainer, **A. Sali**. "Accurate SAXS profile computation and its assessment by contrast variation experiments." *Biophys J* **105**, 962-974, 2013.
305. D. Hitchcock, H. Fan, J. Kim, M. Vetting, B. Hillerich, R. Seidel, S. Almo, B. Shoichet, **A. Sali**, F. Raushel. "Structure-guided Discovery of New Deaminase Enzymes." *J Am Chem Soc* **135**, 13927-13933, 2013.
306. C. Pandya, S. Brown, U. Pieper, **A. Sali**, D. Dunaway-Mariano, P. Babbitt, Y. Xia, K. Allen. "The consequences of domain insertion on sequence-structure divergence in a superfold." *Proc Natl Acad Sci USA* **110**, 3381-3387, 2013.
307. P. Weinkam, **A. Sali**. "Mapping Polymerization and Allostery of Hemoglobin S Using Point Mutations." *J Phys Chem B* **117**, 13058-13068, 2013.
308. G.Q. Dong, H. Fan, D. Schneidman-Duhovny, B. Webb, **A. Sali**. "Optimized atomic statistical potentials: Assessment of protein interfaces and loops." *Bioinformatics* **29**, 3158-3166, 2013.
309. F. Martinez-Jimenez, G. Papadatos, L. Yang, I.M. Wallace, V. Kumar, U. Pieper, **A. Sali**, J.R. Brown, J.P. Overington, M.A. Marti-Renom. "Target prediction for an open access set of compounds active against Mycobacterium tuberculosis." *PLoS Comp Biol*, *epub ahead of print*, 2013.
310. M. Kostic, C. Lima, **A. Sali**. "Celebrating 20 Years of Structural Biology." *Structure* **21**, 1477-1478, 2013.
311. A. Goble, R. Toro, X. Li, A. Ornelas, H. Fan, S. Eswaramoorthy, Y. Patskovsky, B. Hillerich, R. Seidel, **A. Sali**, B. Shoichet, S. Almo, S. Swaminathan, M. Tanner, F. Raushel. "Deamination of 6-Aminodeoxyfutasine in Menquinone Biosynthesis by Distantly Related Enzymes." *Biochemistry* **52**, 6525-6536, 2013.
312. C. Ryan, P. Cimermancic, Z. Szpiechy, **A. Sali**, R. Hernandez, N. Krogan. "High-resolution network biology: connecting sequence with function." *Nat Rev Genet* **14**, 865-879, 2013.
313. K. Berlin, C.A. Castaneda, D. Schneidman-Duhovny, **A. Sali**, A. Nava-Tudela, D. Fushman. "Recovering a representative conformational ensemble from underdetermined macromolecular structural data." *J Am Chem Soc* **135**, 16595-16609, 2013.
314. B. Webb, N. Eswar, H. Fan, N. Khuri, U. Pieper, G.Q. Dong, **A. Sali**. "Comparative Modeling of Drug Target Proteins." In: Chemistry, Molecular Sciences and Chemical Engineering. Ed: J. Reedijk,

Elsevier, Waltham, MA, 2014.

315. B. Webb, **A. Sali**. "Protein structure modeling with MODELLER." In: *Methods in Molecular Biology*. Ed: D. Kihara, **1137**, pp. 1-15, Springer, New York, 2014.

316. M. Bonomi, E.G. Muller, R. Pellarin, S.J. Kim, D. Russel, R. Ramsden, B.A. Sundin, T.A. Davis, **A. Sali**. "Determining protein complex structures based on a Bayesian model of in vivo FRET data." *Mol Cell Proteomics* **13**, 2812-2823, 2014.

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

318. K. Molnar, M. Bonomi, R. Pellarin, G. Clinthorne, G. Gonzalez, S. Goldberg, M. Goulian, **A. Sali**, W. DeGrado. "Cys-Scanning Disulfide Crosslinking and Bayesian Modeling Probe the Transmembrane Signaling Mechanism of the Histidine Kinase, PhoQ." *Structure* **22**, 1239-1251, 2014.

319. B. Webb, K. Lasker, J. Velazquez-Muriel, D. Schneidman-Duhovny, R. Pellarin, M. Bonomi, C. Greenberg, B. Raveh, E. Tjioe, D. Russel, **A. Sali**. "Modeling of proteins and their assemblies with the Integrative Modeling Platform." In: *Structural Genomics*. Ed: Y. Chen, pp. 277-295, Humana Press, London, UK, 2014.

320. Y. Spill, S.J. Kim, D. Schneidman-Duhovny, D. Russel, B. Webb, **A. Sali**, M. Nilges. "SAXS Merge: an automated statistical method to merge SAXS profiles using Gaussian processes." *J Synchrotron Radiat* **21**, 203-208, 2014.

321. G.Q. Dong, S. Calhoun, H. Fan, C. Kalyanaraman, N. London, M. Branch, S. Mashiyama, M. Jacobson, B. Shoichet, P. Babbitt, R. Armstrong, **A. Sali**. "Prediction of substrates for glutathione transferases by covalent docking." *J Chem Inf Model* **6**, 1687-1699, 2014.

322. R. Algret, J. Fernandez-Martinez, Y. Shi, S.J. Kim, R. Pellarin, P. Cimerancic, E. Cochet, **A. Sali**, B. Chait, M. Rout, S. Dokudovskaya. "Molecular Architecture and Function of the SEA Complex - a Modulator of the TORC1 Pathway." *Mol Cell Proteomics* **13**, 2855-2870, 2014.

323. T. Street, X. Zeng, R. Pellarin, M. Bonomi, **A. Sali**, M. Kelly, F. Chu, D. Agard. "Elucidating the mechanism of substrate recognition by the bacterial Hsp90 molecular chaperone." *J Mol Biol* **12**, 2393-2404, 2014.

324. X. Zeng-Elmore, X. Gao, R. Pellarin, D. Schneidman-Duhovny, X. Zhang, K. Kozacka, Y. Tang, **A. Sali**, R. Chalkley, R. Cote, F. Chu. "Molecular architecture of photoreceptor phosphodiesterase elucidated by chemical cross-linking and integrative modeling." *J Mol Biol* **426**, 3713-3728, 2014.

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

326. D. Schneidman-Duhovny, R. Pellarin, **A. Sali**. "Uncertainty in Integrative Structural Modeling." *Curr Opin Struct Biol* **28**, 96-104, 2014.

327. P. Cimerancic, M.H. Medema, J. Claesen, K. Kurita, L. Wieland Brown, K. Mavrommatis, A. Pati, P.A. Godfrey, M. Koehrsen, J. Clardy, B.W. Birren, E. Takano, **A. Sali**, R.G. Lington, M. Fischbach. "Insights into secondary metabolism from a global analysis of prokaryotic biosynthetic gene clusters." *Cell* **158**, 412-421, 2014.

328. M.H. Medema, P. Cimerancic, **A. Sali**, E. Takano, M. Fischbach. "A systematic computational

analysis of biosynthetic gene cluster evolution: Lessons for engineering biosynthesis." *PLoS Comput Biol* **10**, e1004016, 2014.

329. S.J. Kim, J. Fernandez-Martinez, P. Sampathkumar, A. Martel, T. Matsui, H. Tsuruta, T. Weiss, A. Markina-Inarrairaegui, J. Bonanno, M. Sauder, S. Burley, B.T. Chait, S. Almo, M. Rout, **A. Sali**.

"Integrative Structure-Function Mapping of the Nucleoporin Nup133 Suggests a Conserved Mechanism for Membrane Anchoring of the Nuclear Pore Complex." *Mol Cell Proteomics* **13**, 2911-2926, 2014.

330. Y. Shi, J. Fernandez-Martinez, E. Tjioe, R. Pellarin, S.J. Kim, R. Williams, D. Schneidman, **A. Sali**, M. Rout, B. Chait. "Structural characterization by cross-linking reveals the detailed architecture of a coatomer-related heptameric module from the nuclear pore complex." *Mol Cell Proteomics* **13**, 2927-2943, 2014.

331. B. Webb, **A. Sali**. "Comparative Protein Structure Modeling Using Modeller." In: Current Protocols in Bioinformatics, John Wiley and Sons, 2014.

332. E. Verschueren, J. VonDollen, P. Cimermancic, **A. Sali**, N. Gulbahce, N. Krogan. "Analyzing AP-MS data with Mass Spectrometry Interaction Statistics (MIST)." *Curr Protoc Bioinformatics* **49**, 8.19.1-8.19.16, 2015.

333. A. Politis, C. Schmidt, E. Tjioe, A. Sandercock, K. Lasker, Y. Gordiyenko, D. Russel, **A. Sali**, C. Robinson. "Topological models of heteromeric protein assemblies from mass spectrometry: Application to the yeast eIF3:eIF5 complex." *Chem Biol* **22**, 117-128, 2015.

334. J. Kollman, C. Greenberg, S. Li, M. Moritz, A. Zelter, K. Fong, J. Fernandez, **A. Sali**, J. Kilmartin, T. Davis, D. Agard. "Ring closure activates yeast γ TuRC for species-specific microtubule nucleation." *Nat Struct Mol Biol* **22**, 132-137, 2015.

335. J. Johnson, S. Santos, U. Pieper, **A. Sali**, N. Krogan, P. Beltrao. "Conservation and structural analysis of the *Xenopus laevis* phospho-proteome." *submitted*.

336. **A. Sali**, T. Schwede, J. Trehwella, H. Berman, G. Kleywegt, S. Burley, J. Markley, H. Nakamura, P. Adams, A. Bonvin, W. Chiu, M. Dal Peraro, F. Di Maio, T. Ferrin, K. Grunewald, A. Gutmanas, R. Henderson, G. Hummer, K. Iwasaki, G. Johnson, C. Lawson, J. Meiler, M. Marti-Renom, G. Montelione, M. Nilges, R. Nussinov, A. Patwardhan, J. Rappsilber, R. Read, H. Saibil, G. Schroder, C. Schwieters, C. Seidel, D. Svergun, M. Topf, E. Ulrich, S. Velanker, J. Westbrook. "Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop." *Structure*, *in press*.

337. L. Carter, S.J. Kim, D. Schneidman-Duhovny, S.t.o.e.h.r. J., G. Poncet-Montange, T. Weiss, H. Tsuruta, S. Prusiner, **A. Sali**. "Prion protein-antibody complexes characterized by chromatography-coupled small-angle X-ray scattering." *submitted*.

338. P. Cimermancic, P. Weinkam, J. Rettenmaier, D. Keedya, R. Woldeyes, J. Wells, J. Fraser, **A. Sali**. "Cryptic sites expand the druggable proteome." *submitted*.

339. Y. Shi, R. Pellarin, P./ Fridy, J. Fernandez-Martinez, M. Thompson, Y. Li, Q.J. Wang, **A. Sali**, M. Rout, B. Chait. "A strategy for dissecting the architectures of GFP-tagged endogenous macromolecular assemblies." *submitted*.

340. J. Luo, P. Cimermancic, S. Viswanath, C. Ebmeier, B. Kim, M. Dehecq, V. Raman, C. Greenberg, R. Pellarin, **A. Sali**, D. Taatjes, S. Hahn, J. Ranish. "Architecture of the human and yeast general transcription and DNA repair factor TFIIH." *submitted*.

341. P. Robinson, M. Trnka, R. Pellarin, C. Greenberg, D. Bushnell, R. Davis, A. Burlingame, **A. Sali**, R. Kornberg. "Molecular architecture of the mediator complex." *submitted*.

342. E. Lasater, E. Massi, A. Stecula, J. Politi, S. Tan, M. Gunthorpe, J. Holmes, F. Chehab, S.a.l.i. A., N. Shah. "Resistance profile of BCR-ABL T315 mutations." *submitted*.
343. D. Schneidman-Duhovny, N. Khuri, G.Q. Dong, M. Winter, E. Shifrut, N. Friedman, C. Craik, P. Paz, F. Aswad, **A. Sali**. "Predicting T-cell epitopes by integrated modeling of APC processing, MHCII presentation, and TCR recognition." *submitted*.
344. R. Reid, M. Sgobba, B. Raveh, G. Rastelli, **A. Sali**, D. Santi. "Analytical and simulation-based models for tetra-PEG hydrogel degradation and drug release." *submitted*.

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. Suprpto, 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. Suprpto, O. Karni, R. Williams, B.T. Chait, A. Sali, M.P. Rout. "The Molecular Architecture of the Nuclear Pore Complex." *Nature* 450, 695-701, 2007.

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.