

# Michael Levitt: Curriculum Vitae and Bibliography

## **PERSONAL:**

1947 Born in Pretoria, South Africa.  
1968 Married (Rina) with three children (Daniel, Reuven, and Adam).

## **EDUCATION:**

1964-1967 B.Sc. Special Degree in Physics, King's College, London, UK.  
1968-1971 Ph.D. in Biophysics, MRC Laboratory of Molecular Biology and Cambridge University, Cambridge, UK..

## **PROFESSIONAL EXPERIENCE:**

1972-1974 EMBO Postdoctoral Fellow with Shneior Lifson, Weizmann Institute, Rehovot, Israel.  
1974-1979 Staff Scientist, Structural Studies, MRC Laboratory Molecular Biology, Cambridge, UK (Tenured from 1977).  
1977-1979 Visiting Scientist with Francis Crick, Salk Institute, La Jolla, California.  
1979-1987 Associate & Full Professor of Chemical Physics, Department of Chemical Physics, Weizmann Institute, Israel. Chair from 1980-1983, Full Professor from 1983.  
1986-1987 Visiting Scientist, MRC Laboratory of Molecular Biology, Cambridge.  
1987- Professor of Structural Biology, Department of Structural Biology, Stanford University School of Medicine, Stanford. Chair from July 1993 to June 2004.  
1995-1996 Sabbatical Professor, Department of Structural Biology, Weizmann Institute, Rehovot.  
2003-2004 Sabbatical in Paris at Université de Paris, Paris, France.

## **HONORS AND AWARDS:**

1967-1968 Royal Society Exchange Fellowship with S. Lifson, Weizmann Institute, Israel.  
1970-1974 Research Fellowship. Gonville and Caius College, Cambridge.  
1972-1976 European Molecular Biology Organization Fellowship. Weizmann Institute, Israel.  
1981 Member of the European Molecular Biology Organization.  
1986 Federation of European Biochemical Societies Anniversary Prize (for protein folding).  
1997-1999 Co-director of Program in Mathematics and Molecular Biology (PMMB).  
2001- Fellow of the Royal Society.  
2002- Member of the US National Academy of Science.  
2002-2004 Blaise Pascal Professor of Research, Fondation de l'Ecole Normale Supérieure, Paris  
2010- Member of the American Academy of Arts & Sciences.

## **FEDERAL GOVERNMENT AND INTERNATIONAL REVIEW SERVICE:**

1983-1988 Scientific Advisory Committee, European Molecular Biology Laboratory, Heidelberg, Germany.  
1984-1988 Member of Course Committee, European Molecular Biology Organization, Heidelberg.  
1989- Ad Hoc reviewer for NIH, NSF and DOE.  
1992- Reviewer for British Medical Research Council and Swedish National Research Foundation.  
1992- Editorial Boards of *Structure* and *Current Opinion in Structural Biology*.  
1995-1999 Charter Member of NIH BBKA Study Section.  
1998- Reviewer of Sloan-DOE fellowships in Computation Biology.  
1999 Member of ad hoc committee advising Dr. Varmus, NIH Director, on computing.  
2002- Editor of *Journal of Molecular Biology*.  
2002- Editorial Board Member of *Proceedings of National Academy of Science*.  
2004-2006 Member and then Chair of NIH ZRG1 BCMB-Q(90) Study Section.  
2007- Editor of *PloS Computational Biology*.

2010- Reviewer of NIH Pioneer Awards  
2010- Reviewer for NIH College of Reviewers

#### SHORT WORKING VISITS:

1975 Visiting Faculty Member, Dept. Biological Sciences, Columbia, New York.  
1981 Research Consultant, Laboratory of Chemical Physics, NIH, Bethesda.  
1982 Visiting Scientist, Laboratory of Chemical Physics, NIH, Bethesda.  
1983 Visiting Professor, Department of Structural Biology, Stanford.  
1983 Visiting Professor, School of Pharmacology, UCSF, San Francisco.  
1984 Visiting Scholar, Dept. Inorganic Chemistry, University of Sydney, Sydney, Australia.  
1985 Research Consultant, Whitehead Institute, Cambridge, Massachusetts.  
1986 Visiting Scientist, DCRT, National Institutes of Health, Bethesda, Maryland.  
1986 Visiting Professor, School of Pharmacology, UCSF, San Francisco.  
2008 Visiting Scientist, D.E.Shaw Research, New York.

#### INDUSTRIAL ASSOCIATIONS:

1985-1997 Consultant, DuPont and DuPont-Merck Pharmaceuticals, Wilmington, Delaware.  
1987- Consultant, Protein Design Laboratory, Palo Alto, California.  
1987-1994 Consultant, Amgen, Thousand Oaks, California.  
1989-1993 Consultant, Affymax, Palo Alto, California.  
1990-2001 Consultant & Founder, Molecular Applications Group, Palo Alto, California.  
1991-1994 Consultant, Sterling Drug Inc., Malvern, Pennsylvania.  
1993-2003 Consultant, 3-D Pharmaceuticals, Philadelphia.  
1999-2002 Consultant, Signature Biosciences.  
2000-2003 Consultant, Structural Bioinformatics, San Diego.  
2001-2005 Consultant, Affinium, Toronto.  
2001-2004 Consultant, Protein Mechanics, Mountain View, California.  
2002-2005 Consultant, Predix Pharmaceuticals, Tel Aviv.  
2002-2009 Consultant, Algodign, Cupertino, California.  
2003-2004 Consultant, Receptron, Mountain View, California.  
2005-2007 Consultant, Keddem Bioscience, Israel.  
2008- Consultant, CoCrystal Discovery, California.

#### BIBLIOGRAPHY (total of 164):

1. Levitt, M., and S. Lifson. Refinement of Protein Conformations Using a Macromolecular Energy Minimization Procedure. *J. Mol. Biol.* **46**, 269-279 (1969).
2. Levitt, M. Detailed Molecular Model for Transfer Ribonucleic Acid. *Nature* **224**, 759-763 (1969).
3. Warshel, A., M. Levitt and S. Lifson. Consistent Force Field for Calculation of Vibrational Spectra and Conformations of Some Amides and Lactam Rings. *J. Mol. Spect.* **33**, 84-98 (1970).
4. Levitt, M. Folding of Nucleic Acids. In *Polymerization in Biological Systems*, Ciba Foundation Symposium **7**, Elsevier, Amsterdam, pp. 146-171 (1972).
5. Levitt, M. Orientation of Double-Helical Segments in Crystals of Yeast Phenylalanine Transfer RNA. *J.Mol.Biol.* **80**, 255-263 (1973).
6. Levitt, M. Energy Refinement of Hen Egg-White Lysozyme. *J.Mol.Biol.* **82**, 393-420 (1974).
7. Levitt, M. On the Nature of the Binding of Hexa-N-Acetyl Glucosamine Substrate to Lysozyme. In *Peptides, Polypeptides and Proteins*, Wiley, New York, pp. 99-113 (1974).

8. Schulz, G.E., C.D. Barry, J. Friedman, P.Y. Chou, G.D. Fasman, A.V. Finkelstein, V.I. Lim, O.B. Ptitsyn, E.A. Kabat, T.T. Wu, M. Levitt, B. Robson and K. Nagano. Comparison of Predicted and Experimentally Determined Secondary Structure of Adenylate Kinase. *Nature* **250**, 140-142 (1974).
9. Levitt, M., and A. Warshel. Computer Simulation of Protein Folding. *Nature* **253**, 694-698 (1975).
10. Warshel, A., and M. Levitt. Theoretical Studies of Enzymic Reactions: Dielectric, Electrostatic, and Steric Stabilization of the Carbonium Ion in the Reaction of Lysozyme. *J.Mol.Biol.* **103**, 227-249 (1976).
11. Levitt, M. A Simplified Representation of Protein Conformations for Rapid Simulation of Protein Folding. *J.Mol.Biol.* **104**, 59-107 (1976).
12. Levitt, M., and C. Chothia. Structural Patterns in Globular Proteins. *Nature* **261**, 552-558 (1976).
13. Warshel, A., and M. Levitt. Folding and Stability of Helical Proteins: Carp Myogen. *J.Mol.Biol.* **106**, 421-437 (1976).
14. Levitt, M., and J. Greer. Automatic Identification of Secondary Structure in Globular Proteins. *J.Mol.Biol.* **114**, 181-239 (1977).
15. Chothia, C., M. Levitt and D. Richardson. Structure of Proteins: Packing of  $\alpha$ -Helices and Pleated Sheets. *Proc. Nat. Acad. Sci. USA* **74**, 4130-4134 (1977).
16. Finch, J.T., L.C. Lutter, D. Rhodes, R.S. Brown, B. Rushton, M. Levitt, and A. Klug. Structure of the Nucleosome Core Particles of Chromatin. *Nature* **269**, 29-35 (1977).
17. Levitt, M. Protein Folding as a Random Walk. Proceedings of 7-th Taniguichi Symposium, 1977.
18. Levitt, M., and A. Warshel. Extreme Conformational Flexibility of the Furanose Ring in DNA and RNA. *J. Am. Chem. Soc.* **100**, 2607-2613 (1978).
19. Jack, A., and M. Levitt. Refinement of Large Structures by Simultaneous Minimization of Energy and R Factor. *Acta Crystallogr.* **A34**, 931-935 (1978).
20. Levitt, M. How Many Base-Pairs per Turn Does DNA have in Solution and in Chromatin? Some Theoretical Calculations. *Proc. Nat. Acad. Sci. USA* **75**, 640-644 (1978).
21. Levitt, M. Conformational Preferences of Amino Acids in Globular Proteins. *Biochemistry* **17**, 4277-4285 (1978).
22. Janin, J., S. Wodak, M. Levitt and B. Maigret. The Conformation of Amino Acid Side Chains in Proteins. *J.Mol.Biol.* **125**, 357-386 (1978).
23. Prunell, A., R.D. Kornberg, L. Lutter, A. Klug, M. Levitt and F.H.C. Crick. Periodicity of Deoxyribonuclease I Digestion of Chromatin. *Science* **204**, 855-858 (1979).
24. Lifson, S., and M. Levitt. On Obtaining Energy Parameters from Crystal Structure Data. *Computers and Chemistry* **3**, 49-51 (1979).
25. Levitt, M. Computer Studies of Protein Molecules. In *Protein Folding*, Elsevier/North Holland, pp. 17-40 (1980).
26. Levitt, M. Effect of Proline Residues on Protein Folding. *J.Mol.Biol.* **145**, 251-263 (1981).
27. Chothia, C., M. Levitt and D. Richardson. Helix to Helix Packing in Proteins. *J.Mol.Biol.* **145**, 215-250 (1981).
28. Levitt, M. The Molecular Dynamics of Hydrogen Bonds in Bovine Pancreatic Trypsin Inhibitor Protein. *Nature* **294**, 379-380 (1981).
29. Levitt, M. Hydrogen Bond and Internal Solvent Dynamics of BPTI Protein. *Ann. N.Y. Acad. Sci.* **367**, 162-181 (1981).
30. Levitt, M., and R.J. Feldmann. Conformational Dynamics of Pancreatic Trypsin Inhibitor: A Movie. In *Structural Aspects of Recognition and Assembly in Biological Macromolecules*, Elsevier/North Holland (1981).

31. Levitt, M. Protein Conformation, Dynamics and Folding by Computer Simulation. *Ann. Rev. Biophys. Bioeng.* **11**, 251-271 (1982).
32. Levitt, M. Computer Simulation of DNA Double Helix Dynamics. *Cold Spring Harbor Symp. Quant. Biol.* **47**, 251-261 (1983).
33. Levitt, M. Molecular Dynamics of Native Protein: I. Computer Simulation of Trajectories. *J.Mol.Biol.* **168**, 595-620 (1983).
34. Levitt, M. Molecular Dynamics of Native Protein: II. Analysis and Nature of Motion. *J.Mol.Biol.* **168**, 595-620 (1983).
35. Levitt, M. Protein Folding by Restrained Energy Minimization and Molecular Dynamics. *J.Mol.Biol.* **170**, 723-764 (1983).
36. Levitt, M., C. Sander and P.S. Stern. Normal-Mode Dynamics of a Protein: Bovine Pancreatic Trypsin Inhibitor. *Int. J. Quant. Chem: Quant. Biol. Symp.*, **10**, 181-199 (1983).
37. Henry, E.R., M. Levitt and W.A. Eaton. Molecular Dynamics Simulation of Photodissociation of Carbon Monoxide from Hemoglobin. *Proc. Natl. Acad. Sci. USA*, **82**, 2034-2038 (1985).
38. Levitt, M., C. Sander and P.S. Stern. Protein Normal-Mode Dynamics: Trypsin Inhibitor, Crambin, Ribonuclease and Lysozyme. *J.Mol.Biol.* **181**, 423-447 (1985).
39. Pattabiraman, N., M. Levitt, T. E. Ferrin and R. Langridge. Computer Graphics in Real Time Docking with Energy Calculations and Minimization. *J. Comput. Chem.* **6**, 432-436 (1985).
40. Chothia, C., A.M. Lesk, M. Levitt, A.G. Amit, R.A. Mariuzza, S.E.V. Phillips, and R.J. Poljak. The Predicted Structure of Immunoglobulin D1.3 and its Comparison with the Crystal Structure. *Science*, **233**, 755-758 (1986).
41. Lesk, A.M., M. Levitt and C. Chothia. Alignment of the Amino Acid Sequences of Distantly Related Proteins Using Variable Gap Penalties. *Protein Engineering*, **1**, 77-78 (1986).
42. Levitt, M., and R. Sharon. Simulating Protein Dynamics in Solution. In *Crystallography in Molecular Biology*, ed. Moras D. et al. NATO ASI Series A: Life Sciences, Vol. **126**, pp. 197-207 (1987).
43. Anglister, J., M. Bond, T. Frey, D. Leahy, M. Levitt, H.M. McConnell, and M. Whittaker. Contribution of Tryptophan Residues to the Combining Site of a Monoclonal Anti-Dinitrophenyl Spin-Label Antibody. *Biochemistry*, **26**, 6058-6064 (1987).
44. Levitt, M. and M.F. Perutz. Aromatic Rings Act as Hydrogen Bond Acceptors. *J. Mol. Biol.* **201**, 751-754 (1988).
45. Levitt, M. and R. Sharon. Accurate Simulation of Protein Dynamics in Solution. *Proc. Natl. Acad. Sci. USA*. **85**, 7557-7561 (1988).
46. Levitt, M. A Calculated Conformation for the Folding Transition State of Bovine Pancreatic Trypsin Inhibitor. In *Protein Structure and Protein Engineering*, ed. Winnacker E.L. and Huber, R. Springer-Verlag, Berlin, Heidelberg, pp. 45-50 (1988).
47. Levitt, M. Molecular Dynamics of Macromolecules in Water. *Chemica Scripta*, **29A**, 197-203 (1989).
48. Levy, R., O. Assulin, T. Scherf, M. Levitt, and J. Anglister. Probing Antibody Diversity by 2D NMR: Comparison of Amino Acid Sequences, Predicted Structures, and Observed Antibody-Antigen Interactions in Complexes of Two Antipeptide Antibodies. *Biochemistry*, **28**, 7168-7175 (1989).
49. Matsumura, M., W.J. Becktel, M. Levitt and B.W. Matthews. Stabilization of Phage T4 Lysozyme by Engineered Disulfide Bonds. *Proc. Natl. Acad. Sci. USA*. **86**, 6562-6566 (1989).
50. Chothia, C., A.M. Lesk, M. Levitt, A. Tramontano, S.J. Smith-Gill, G. Air, S. Sheriff, E.A. Padlan, D. Davies, W.R. Tulip and P.M. Colman. The Conformations of Immunoglobulin Hypervariable Regions. *Nature*, **342**, 877-883 (1989).

51. Queen, C., W.P. Schneider, H.E. Selick, P.W. Payne, N.F. Landolfi, J.F. Duncan, N.M. Avdalovic, M. Levitt, R.P. Junghans and T.A. Waldmann. A Humanized Antibody that Binds to the IL-2 Receptor. *Proc. Natl. Acad. Sci. USA*. **86**, 10029-10033 (1989).
52. Zilber, B., T. Scherf, M. Levitt and J. Anglister. NMR Derived Model for a Peptide-Antibody Complex. *Biochemistry*, **29**, 10032-10041 (1990).
53. Levitt, M. Protein Folding. *Curr. Opinions Struct. Biol.* **1**, 224-229 (1991).
54. Lee, C. and M. Levitt. Accurate Prediction of the Stability and Activity Effects of Site-directed Mutagenesis of a Protein Core. *Nature*, **352**, 448-451 (1991).
55. Levitt, M. Real-Time Interactive Frequency Filtering of Molecular Dynamics Trajectories. *J. Mol. Biol.* **220**, 1-4 (1991).
56. Theriault, T.P, G. S. Rule, D.J. Leahy, M. Levitt and H. M. McConnell. Structural and Kinetic Studies of the Fab Fragment of a Monoclonal Anti-Spin Label Antibody by NMR. *J. Mol. Biol.* **221**, 257-270 (1991).
57. Daggett, V. and M. Levitt. A Molecular Dynamics Simulation of the C-Terminal Fragment of the L7/L12 Ribosomal Protein in Solution. *Chemical Phys.* **158**, 501-512 (1991).
58. Narhi, L.O., Y. Stabinsky, M. Levitt, L. Miller, R. Sachdev, S. Finley, S. Park, C. Kolvenbach, T. Arakawa and M. Zukowski. Enhanced Stability of Subtilisin by Three Point Mutations. *Biotechnology and Applied Biochemistry* **1**, 12-24 (1991).
59. Daggett, V. and M. Levitt. Molecular Dynamics Simulation of Helix Denaturation. *J. Mol. Biol.* **223**, 1121-1138 (1992).
60. Hinds, D.A. and M. Levitt. A Lattice Model for Protein Structure Prediction at Low Resolution. *Proc. Natl. Acad. Sci. USA*. **89**, 2536-2540 (1992).
61. Levitt, M. Accurate Modeling of Protein Conformation by Automatic Segment Matching. *J. Mol. Biol.* **226**, 507-533(1992).
62. Daggett, V. and M. Levitt. A Model of The Molten Globule State From Molecular Dynamics Simulations. *Proc. Natl. Acad. Sci. USA*. **89**, 5142-5146 (1992).
63. Scherf, T., R. Hiller, F. Naider, M. Levitt and Y. Anglister. Induced Peptide Conformations in Different Antibody Complexes: Molecular Modeling of the Three-Dimensional Structure of Peptide-Antibody Complexes Using NMR Distance Restraints. *Biochemistry* **31**, 6884-6897 (1992).
64. Subbiah, S., Laurents, D. V. and M. Levitt. Structural Similarity of DNA-binding Domains of Bacteriophage Repressors and the Globin Core. *Current Biol.* **3**, 141-148 (1993).
65. Daggett, V. and M. Levitt. Realistic Simulation of Native Protein Dynamics in Solution and Beyond. *Ann. Rev. Biophys & Biomol. Struct.* **22**, 353-380 (1993).
66. Daggett, V. and M. Levitt. Protein Unfolding Pathways Explored Through Molecular Dynamics Simulations. *J. Mol. Biol.* **232** 600-618 (1993).
67. Levitt, M. and B. Park. Water: Now You See It, Now You Don't. *Structure.* **1** 223-226 (1993).
68. Daggett, V. and M. Levitt. Protein Folding <-> Unfolding Dynamics. *Current Opinions in Structural Biology* **4** 291-295 (1994).
69. Laurents, D.V., S. Subbiah and M. Levitt. Different Protein Sequences Can Give Rise to Highly Similar Folds Through Different Stabilizing Interactions. *Protein Science* **3** 1938-1944 (1994).
70. Hinds, D.A. and M. Levitt. Exploring Conformational Space with a Simple Lattice Model for Protein Structure. *J. Mol. Biol.* **243** 668-682 (1994).
71. Hinds, D.A. and M. Levitt. Simulation of Protein-Folding Pathways: Lost in (Conformational) Space?. *Trends in Biotechnology.* **13** 23-27(1995).

72. Levitt, M., M. Hirshberg, R. Sharon and V. Daggett. Potential Energy Function and Parameters for Simulations of the Molecular Dynamics of Proteins and Nucleic Acids in Solution. *Computer Physics Communications*, **91**, 215-231 (1995).
73. Park, B. and M. Levitt. The Complexity and Accuracy of Discrete State Models of Protein Structure. *J. Mol. Biol.*, **249**, 493-507 (1995).
74. Gerstein, M., J. Tsai and M. Levitt. The Volume of Atoms on the Protein Surface: Calculated from Simulation using Voronoi Polyhedra. *J. Mol. Biol.*, **249**, 955-966 (1995).
75. Huang, E.S., S. Subbiah and M. Levitt. Recognizing Native Folds by the Arrangement of Hydrophobic and Polar Residues. *J. Mol. Biol.*, **252**, 709-720 (1995).
76. Shoham, S., T. Scherf, J. Anglister, M. Levitt, E. A. Merritt and W. G. J. Hol. Structural Diversity in a Conserved Cholera Toxin Epitope Involved in Ganglioside Binding. *Protein Science*, **4**, 841-848 (1995).
77. Tsai, J., M. Gerstein and M. Levitt. Keeping the Shape but Changing the Charge: A Simulation Study of Urea and its Iso-Steric Analogues. *J. Chem. Phys.*, **104**, 9417-9430 (1996).
78. Huang, E.S., J. Tsai, S. Subbiah and M. Levitt. Using a Hydrophobic Contact Potential to Evaluate Native and Near-Native Folds Generated by Molecular Dynamics Simulations. *J. Mol. Biol.*, **257**, 716-725(1996).
79. Hinds, D.A. and M. Levitt. From Structure to Sequence and Back Again. *J. Mol. Biol.*, **258**, 201-209 (1996).
80. Gerstein, M. and Levitt, M. Using Iterative Dynamic Programming to Obtain Accurate Pairwise and Multiple Alignments of Protein Structures. *Proc Int Conf Intell Syst Mol Biol.* **4**, 59-67(1996).
81. Levitt, M. Through the Breach. *Curr Opin Struct Biol.* **6(2)**, 193-194 (1996).
82. Park, B. and M. Levitt. Energy Functions that Discriminate X-ray and Near-Native Folds from Well-Constructed Decoys. *J. Mol. Biol.*, **258**, 367-392 (1996).
83. Zhou, Z., Payne, P., Vasquez, M., Kuhn, N. and M. Levitt. Finite-Difference Solution of the Poisson-Boltzmann Equation: Complete Elimination of Self-Energy. *J. Comp. Chem.* **11**, 1344-1351 (1996).
84. Park, B., Huang, E. S. and M. Levitt. Factors Affecting the Ability of Energy Functions to Discriminate Correct from Incorrect Folds. *J. Mol. Biol.*, **266**, 831-846 (1997).
85. Levitt, M., Hirshberg, M., Sharon, R., Laidig, K.E., and Daggett, V. Calibration and Testing of a Water Model for Simulation of the Molecular Dynamics of Proteins and Nucleic Acids in Solution. *J. Phys. Chem. B* **25**, 5051-5061 (1997).
86. Hirshberg, M. and M. Levitt. Simulating the Dynamics of the DNA Double Helix in Solution. In *Dynamics and the Problem of Recognition in Biological Macromolecules*, ed. Jardetzky, O. and Lefevre, J. Plenum Press, New York, pp. 173-191 (1997).
87. Levitt, M., M. Gerstein, E.S. Huang, S. Subbiah and J. Tsai. Protein Folding: The End-Game. *Ann. Rev. Biochemistry*, **66**, 549-579 (1997).
88. Gerstein, M. and M. Levitt. A Structural Census of the Current Population of Protein Sequences. *Proc. Natl. Acad. Sci.*, **99**, 11911-11916 (1997).
89. Tsai, J., M. Gerstein, and M. Levitt. Simulating the Minimum Core for Hydrophobic Collapse in Globular Proteins. *Protein Science*, **6**, 1-11 (1997).
90. Levitt, M. Competitive Assessment of Protein Fold Recognition and Alignment Accuracy. *Proteins, Struct., Funct. and Gen. Suppl.* **1**, 92-104 (1997).
91. Marchler-Bauer, A., Levitt, M and S. Bryant. A Retrospective Analysis of the CASP2 Threading Predictions. *Proteins, Struct., Funct. and Gen. Suppl.* **1**, 83-91 (1997).
92. Gerstein, M. and M. Levitt. Comprehensive Assessment of Automatic Structural Alignment against a Manual Standard, the SCOP Classification of Proteins. *Protein Science*, **7**, 445-456 (1998).
93. Levitt, M and M. Gerstein. A Unified Statistical Framework for Sequence Comparison and Structure Comparison. *Proc. Natl. Acad. Sci.*, **95**, 5913-5920 (1998).

94. Gerstein, M. and M. Levitt. Simulating Water and the Molecules of Life. *Scientific American*, Nov. 100-105, (1998).
95. Lee C. and M. Levitt. Packing as a Structural Basis of Protein Stability: Understanding Mutant Properties from Wildtype Structure. *Pac. Symp. Biocomput.* 245-255 (1998).
96. Huang E.S., P. Koehl, M. Levitt, R.V. Pappu and J.W. Ponder. Accuracy of side-chain prediction upon near-native protein backbones generated by *Ab initio* folding methods. *Proteins*, **33**, 204-217 (1998).
97. Samudrala, R., Xia, Y., Levitt, M. and E.S. Huang. A Combined Approach for *Ab Initio* Construction of Low Resolution Protein Tertiary Structures from Sequence. *Pac Symp Biocomput.* 505-516 (1999).
98. Brenner S.E., D. Barken, and M. Levitt M. The PRESAGE Database for Structural Genomics. *Nucleic Acids Res.* **27**, 251-3 (1999).
99. Koehl P. and M. Levitt. A Brighter Future for Protein Structure Prediction. *Nat Struct Biol.* **6**, 108-111 (1999).
100. Samudrala, R., Y. Xia, E.S. Huang, and M. Levitt. *Ab Initio* Protein Structure Prediction Using a Combined Hierarchical Approach. *Proteins, Struct., Funct. and Gen. Suppl.* **3S**, 194-198 (1999).
101. Tsai, J., M. Levitt and D. Baker. Hierarchy of Structure Loss in MD Simulations of SRC SH3 Domain Unfolding. *J. Mol. Biol.* **291**, 215-225 (1999).
102. Koehl P. and M. Levitt. De Novo Protein Design. I. In Search of Stability and Specificity. *J. Mol. Biol.* **293**, 1161-1181 (1999).
103. Koehl P. and M. Levitt. De Novo Protein Design. II. Plasticity in Sequence Space. *J. Mol. Biol.* **293**, 1183-1193 (1999).
104. Koehl P. and M. Levitt. Structure-Based Conformational Preferences of Amino Acids. *Proc. Natl. Acad. Sci. USA*, **96**, 12524-12529 (1999).
105. Brenner S.E, Koehl, P. and M. Levitt. The Astral Compendium for Protein Structure and Sequence Analysis *Nucleic Acids Res.*,**28**, 254-256 (2000).
106. Brenner, S. E. and M. Levitt. Expectations from Structural Genomics. *Protein Science*, **9**, 197-200 (2000).
107. Samudrala R, Xia Y, Levitt M, Cotton NJ, Huang ES, and R. Davis. Probing Structure-Function Relationships of the DNA Polymerase Alpha-Associated Zinc-Finger Protein Using Computational Approaches. *Pac. Symp. Biocomput.*, **12**, 179-190 (2000).
108. Yona, G. and M. Levitt. A Unified Sequence-Structure Classification of Protein Sequences: Combining Sequence and Structure in a Map of the Protein Space. *RECOMB 2000*, pp. 308-317, ACM (2000).
109. Samudrala, R. Huang, E.S., Koehl, P. and M. Levitt. Constructing side chains on near-native main chains for *ab initio* protein structure prediction. *Protein Eng.* **3**, 453-457 (2000).
110. Xia, Y., Huang, E.S., Levitt, M. and Samudrala, R. *Ab initio* construction of protein tertiary structures using a hierarchical approach. *J. Mol. Biol.*, **300**, 171-185 (2000).
111. Samudrala R, Levitt M. Decoys 'R' Us: A database of incorrect protein conformations for evaluating scoring functions. *Protein Science*, **9**, 1399-1401 (2000).
112. Yona, G. and M. Levitt. Towards A Complete Map of the Protein Space Based on a Unified Sequence And Structure Analysis of All Known Proteins. *Proceedings of ISMB.* **8**, 395-406 (2000).
113. Xia. Y. and M. Levitt. Extracting Knowledge-Based Energy Functions from Protein Structures by Error Rate Minimization: Comparison of Methods Using Lattice Model. *J. Chem. Phys.* **113**, 9318-9330 (2000).
114. Fain, B. and M. Levitt. A Novel Method for Sampling Alpha-helical Protein Backbones, *J. Mol. Biol.*, **305**, 191-201 (2001).
115. Levitt, M. The Birth of Computational Structural Biology, *Nature Struct. Biol.*, **8**, 392-393 (2001).
114. Raschke, T.M., Tsai, J. and M. Levitt. Quantification of the Hydrophobic Interaction by Simulations of the Aggregation of Small Hydrophobic Solutes in Water. *Proc. Natl. Acad. Sci.*, **98**, 5965-5660 (2001).

117. Fain, B., Y. Xia, and M. Levitt. Determination of Optimal Chebyshev-Expanded Hydrophobic Discrimination Function for Globular Proteins. *IBM J. Res. Dev.* **45**, 525-532 (2001).
118. Chandonia J.M., Walker N.S., Lo Conte L., Koehl P., Levitt M., and Brenner S.E. ASTRAL compendium enhancements. *Nucleic Acids Res.* **30**, 260-263 (2002).
119. Koehl P. and M. Levitt. Improved Recognition of Native-Like Protein Structures Using a Family of Designed Sequences. *Proc Natl. Acad. Sci U S A.* **99**, 691-696 (2002).
120. Koehl P. and M. Levitt. Protein Topology and Stability Define the Space of Allowed Sequences. *Proc Natl. Acad. Sci U S A.* **99**, 1280-1285 (2002).
121. Yona G. and M. Levitt. Within the Twilight Zone: A Sensitive Profile-Profile Comparison Tool Based on Information Theory. *J Mol Biol.* **315**: 1257-1275 (2002).
122. Xia, Y and M. Levitt. Roles of Mutation and Recombination in the Evolution of Protein Thermodynamics. *Proc Natl. Acad. Sci U S A.* **99**: 10382-10387 (2002).
123. Fain, B., Xia, Y. and M. Levitt. Design of an Optimal Chebyshev-Expanded Discrimination Function for Globular Proteins. *Protein Sci.* **11**: 2010-2021 (2002).
124. Samudrala R. and M. Levitt. A Comprehensive Analysis of 40 Blind Protein Structure Predictions. *BMC Struct. Biol.* **2**: 3-10 (2002).
125. Kolodny, R., Koehl, P., Guibas, L., and M. Levitt. Small Libraries of Protein Fragments Model Native Protein Structures Accurately. *J Mol Biol.* **323**: 297-307 (2002).
126. Koehl, P. and M. Levitt. Sequence Variations within Protein Families are Linearly Related to Structural Variations. *J. Mol. Biol.* **323**: 551-562 (2002).
127. Tsai, J. and M. Levitt. Evidence of Turn and Salt Bridge Contributions to  $\beta$ -Hairpin Stability: MD Simulations of C-terminal Fragment from the B1 Domain of Protein G. *Biophys. Chem.***102**: 187-201 (2002).
128. Kolodny, R. and M. Levitt. Protein Decoy Assembly Using Short Fragments under Geometric Constraints. *Biopolymers*, **68**: 278-285 (2003).
129. Keasar, C. and M. Levitt. A Novel Approach to Decoy Set Generation: Designing a Physical Energy Function Having Local Minima with Native Structure Characteristics. *J. Mol. Biol.* **329**: 159-174 (2003).
130. Fain B, and M. Levitt M. Funnel Sculpting for *in Silico* Assembly of Secondary Structure Elements of Proteins. *Proc Natl. Acad. Sci. U S A.* **100**: 10700-10705 (2003).
131. Chandonia, J. M., Hon, G., Walker, N.S., Lo Conte, L., Koehl, P., Levitt, M. and S.E. Brenner. The ASTRAL Compendium in 2004. *Nucleic Acids Res.* **32**: 189-192 (2004).
132. Xia, Y. and M. Levitt. Funnel-Like Organization in Sequence Space Determines the Distributions of Protein Stability and Folding Rate Preferred by Evolution. *Proteins*, **55**: 107-114 (2004).
133. Xia, Y. and M. Levitt. Simulating Protein Evolution in Sequence and Structure Space. *Curr. Opin. Struct. Biol.* **14**: 202-207 (2004).
134. Wang, K, Fain, B, Levitt, M, and R. Samudrala. Improved Protein Structure Selection Using Decoy-Dependent Discriminatory Functions. *BMC Struct. Biol.* **4**: 1-18 (2004).
135. Bryant, R., Edelsbrunner, H., Koehl, P. and M. Levitt. The Area Derivative of a Space-Filling Diagram. *Discrete & Computational Geometry*, **32**: 293-308 (2004).
136. Batada N.N., Westover K.D., Bushnell D.A., Levitt M, Kornberg R.D. Diffusion of nucleoside triphosphates and role of the entry site to the RNA polymerase II active center. *Proc Natl. Acad. Sci U S A.* **101**: 17361-17364. (2004).
137. Raschke, T. M. and M. Levitt. Detailed Hydration Maps of Benzene and Cyclohexane Reveal Distinct Water Structures. *J. Phys. Chem.* **108**, 13492-13500 (2004).



138. Kolodny R., Koehl P. and M. Levitt. Comprehensive evaluation of protein structure alignment methods: scoring by geometric measures. *J. Mol. Biol.* **346**: 1173-1188 (2005).
139. Kolodny, R., Guibas, L., Levitt, M. and Koehl, P. Inverse Kinematics in Biology: The Protein Loop Closure Problem. *International Journal of Robotics Research*, **24**, 2–3: 151-163 (2005).
140. Raschke, T. M. and M. Levitt. Nonpolar Solutes Enhance Water Structure within Hydration Shells, While Reducing Interactions between Them. *Proc. Natl. Acad. Sci. USA.* **102**: 6777-6782. (2005).
141. Sykes M.T. and M. Levitt. Describing RNA structure by Libraries of Clustered Nucleotide Doublets. *J. Mol. Biol.* **352**: 26-38 (2005).
142. Summa, C.M., Levitt, M. and Degrado W.F. An Atomic Environment Potential for Use in Protein Structure Prediction. *J. Mol. Biol.* **352**: 986-1001 (2005).
143. Batada, N.N., Shepp, L.A., Siegmund, D.O. and M. Levitt. Spatial Regulation and the Rate of Signal Transduction Activation., *PLoS Comput Biol.* **2**(5): e44 (2006).
144. Janin J, and M. Levitt. Theory and simulation: Accuracy and Reliability in Modelling Proteins and Complexes. *Curr. Opin. Struct Biol.* 16(2):139-141 (2006).
145. Minary, P. and M. Levitt. Discussion of “Equi-energy sampler” by Kou, Zhou and Wong. *Annals Statistics* **34**: 1636–1641 (2006).
146. Summa C. M. and M. Levitt. Near-Native Structure Refinement Using in Vacuo Energy Minimization. *Proc. Natl. Acad. Sci. USA.* **104**: 3177-3182 (2007).
147. M. Levitt. Growth of Novel Protein Structural Data. *Proc. Natl. Acad. Sci. USA.* **104**: 3183-3188 (2007).
148. Sykes, M.T. and M. Levitt. Simulations of RNA base pairs in a nanodroplet reveal solvation-dependent stability. *Proc. Natl. Acad. Sci. USA.* **104**: 12336-12340 (2007).
149. Schröder, G., Brunger, A. and M. Levitt. Deformable Elastic Network Model to Combine Initial Structural Information with Low Resolution Data: Application to Real-Space Refinement. *Structure*, **15**:1630-1641 (2007).
150. Minary, P. and M. Levitt. Probing Protein Fold Space with a Simplified Model. *J. Mol. Biol.* **375**: 920-933 (2008).
151. Weiss, D., Rashcke, T. M. and M. Levitt. How Hydrophobic Buckminsterfullerene Affects Surrounding Water Structure. *J. Chem. Phys.* **112**: 2981-2990 (2008).
152. Samson, A. O. and M. Levitt. Inhibition Mechanism of the Acetylcholine Receptor by R-Neurotoxins as Revealed by Normal-Mode Dynamics. *Biochemistry*, **47**: 4065–4070 (2008).
153. Chopra, G., Summa, C. and M. Levitt. Solvent Dramatically Affects Protein Structure Refinement. *Proc. Natl. Acad. Sci. USA.* **105**: 20239-20244 (2008).
154. Weiss, D. and M. Levitt. “Can Morphing Methods Predict Intermediate Structures? *J. Mol. Biol.* **385**: 665-674 (2009).
155. Samson, A. O. and M. Levitt. Protein segment finder: an online search engine for segment motifs in the PDB, *Nucleic Acid Research*, **37**: D224-D228 (2009).
156. Shmygelska, A. and M. Levitt. Generalized Ensemble Methods for *De Novo* Structure Prediction. *Proc. Natl. Acad. Sci. USA.* **106**: 1415-1420 (2009).
157. Schwede, T., Sali, A., Honig, B., Levitt, M., Berman, H.M., Jones, D., Brenner, S.E., Burley, S.K., Das, R., Dokholyan, N.V., Dunbrack, R.L. Jr, Fidelis, K., Fiser, A., Godzik, A., Huang, Y.J., Humblet, C., Jacobson, M.P., Joachimiak, A., Krystek, S.R. Jr, Kortemme, T., Kryshtafovych, A., Montelione, G.T., Moulton, J., Murray, D., Sanchez, R., Sosnick, T.R., Standley, D.M., Stouch, T., Vajda, S., Vasquez, M., Westbrook, J.D., Wilson, I.A. Outcome of a Workshop on Applications of Protein Models in Biomedical Research. Outcome of a Workshop on Applications of Protein Models in Biomedical Research. *Structure*, **17**: 151-9 (2009).

158. Wang, D., Bushnell, D.A., Huang, X, Westover, K.D., Levitt, M. and R.D. Kornberg Structural Basis of Transcription: Backtracked RNA Polymerase II at 3.4 Å Resolution. *Science* **324**: 1203-1206 (2009).
159. Levitt, M.. Nature of the Protein Universe. *Proc. Natl. Acad. Sci USA*. **106**: 11078-11084 (2009).
160. Kalisman, N. and M. Levitt. Insights into the Intra-Ring Subunit Order Of TRiC/CCT: A Structural and Evolutionary Analysis. *Proc. Pacific Symp. Bioinf.* 2010.
161. Zhang, J., Baker, M. L., Schröder, G., Douglas, N. R., Reissmann, S., Jakana, J., Dougherty, M., Fu, C. J, Levitt, M., Ludtke, S. J., Frydman, J., and W. Chiu. Mechanism of Folding Chamber Closure in a Group II Chaperonin. *Nature* , **463**: 379-384 (2010).
162. Schröder, G., Brunger, A. and M. Levitt. Super-Resolution Biomolecular Crystallography with Low-Resolution Data. *Nature*, **464**: 1218-1222 (2010).
163. Saha M, Levitt M, Chiu W "MOTIF-EM: an automated computational tool for identifying conserved regions in CryoEM structures." *Bioinformatics*, **26(12)**: I301-309 (2010).
164. Chopra G., Kalisman N. and M. Levitt M. Consistent refinement of submitted models at CASP using a knowledge-based potential. *Proteins*, June 2010 (online).

#### **COMPUTER PROGRAMS RELEASED FOR CIRCULATION:**

- 1974 Warshel, A., and M. Levitt. QCPE/PI: A Program for the Consistent Force Field Evaluation of Equilibrium Geometries and Vibrational Frequencies of Molecules. QCPE 247, Quantum Chemistry Program Exchange, Indiana University (1974).
- 1989 Levitt, M., and N. Kuhn. MacImdad: A Program for Interactive Molecular Display and Design on the Macintosh computer.

#### **INVITED LECTURES (total of 2054):**

1. Ciba Foundation Symposium on Polymerization in Biological Systems, London, March 1972.
2. Penn Lecture, University of Pennsylvania, Philadelphia, July 1975.
3. Chemical Society (Theoretical Group), London, England, February 1976.
4. Gordon Research Conference on Biopolymers, Holderness, New Hampshire, June 1976.
5. Tenth International Congress of Biochemistry, Hamburg, Germany, July 1976.
6. Table Ronde Roussel UCLAF on Biomolecular Evolution, Paris, France, November 1976.
7. Twelfth Winter Seminar, Klosters, Switzerland, January 1977.
8. Taniguichi International Symposium on Biophysics, Hakone, Japan, September 1977.
9. Gordon Research Conference on Theoretical Biology, Tilton, New Hampshire, June 1978.
10. Gordon Research Conference on Diffraction in Molecular Biology, Andover, NH, June 1978.
11. Gordon Research Conference on Biopolymers, Plymouth, New Hampshire, June 1978.
12. Stanford Conference on Molecular Structural Methods in Biological Research, Stanford, Nov. 1978.
13. Gordon Research Conference on Proteins, New Hampton, New Hampshire, June 1979.
14. Eleventh International Congress of Biochemistry, Toronto, Canada, July 1979.
15. Konferenz der Gesellschaft für Biologische Chemie "Protein Folding", Regensburg, Germany, September 1979.
16. Seventh Katzir Conference, "Structural Aspects of Recognition and Assembly in Biological Macromolecules", Nof-Ginossar, Israel, February 1980.
17. EMBO-SKMB Workshop, "Dynamic Aspects of Globular Protein Molecules", Kandersteg, Switzerland, September 1980.
18. Swedish Biophysical and Biochemical Society Meeting, Uppsala, Sweden, November 1980.
19. Gordon Research Conference on Proteins, New Hampton, New Hampshire, June 1981.
20. Gordon Research Conference on Biopolymers, Holderness, New Hampshire, June 1982.
21. Fourth Lita Annenberg Hazen Biomedical Workshop, Aspen Institute for Humanistic Studies, Aspen, Colorado, August 1983.
22. Pontifical Academy of Sciences Study Group, Vatican City, Italy, November, 1983.

23. Protein Structure and Dynamics, Daresbury, England, November 1983.
24. Site-Directed Mutagenesis and Protein Structure and Function, Banbury Center, Cold Spring Harbor Laboratory, New York, March 1984.
25. Molecular Dynamics and Protein Structure, University of North Carolina, Chapel Hill, May 1984.
26. EMBO Workshop on Protein Folding, Cambridge, England, August 1984.
27. NSF Workshop on Applications of Supercomputers for Life Sciences, Airlie, Virginia, Dec. 1984.
28. Twentieth Winter Seminar, Klosters, Switzerland, January 1985.
29. Tenth Edmond de Rothschild School on the Structure of DNA and of Chromatin, Neve Ilan, Israel, April 1985.
30. Gordon Research Conference on Proteins, New Hampton, New Hampshire, June 1985.
31. EUCHEM Conference on Computer Modeling in Macromolecular Chemistry, Stockholm, July 1985.
32. EMBO/NATO 4-th European Meeting on Protein Crystallography, Bischenberg, France, Sept. 1985.
33. Dynamics of Proteins and Nucleic Acids, Bielefeld, Germany, November 1985.
34. ACS Meeting on Computer-Aided Drug Design, New York, April 1986.
35. DNAX Research Meeting, Stanford, May 1986.
36. FEBS Seventeenth Annual Meeting, Berlin, Germany, August 1986.
37. EMBO Course on Modern Analysis of Biological Structures, Pavia, Italy, September 1986.
38. CECAM/EC Workshop on Force Fields for Computer Simulations on Macromolecules, Paris, France, September 1986.
39. Third European Seminar on Computer-Aided Molecular Design, London, England, October 1986.
40. British Biophysical Society meeting on Protein Structure and Function, Cambridge, April 1987.
41. Cold Spring Harbor Symposium on Quantitative Biology: Evolution of Catalytic Function in Proteins and Nucleic Acids, Cold Spring Harbor, New York, May 1987.
42. Gordon Research Conference on Nucleic Acids, Holderness, New Hampshire, June 1987.
43. International Union of Pure and Applied Biophysics meeting on Protein and Nucleic Acid, Jerusalem, Israel, August 1987.
44. Thirteenth Taniguichi International Symposium of Biophysics, Kyoto, Japan, November 1987.
45. Thirty-ninth Mosbacher Kolloquium on Protein Structure and Protein Engineering, Mosbach, Germany, April 1988.
46. Oholo Conference on Computer Assisted Modeling, Eilat, Israel, April 1988.
47. Sweden-Israeli Workshop on Molecular Basis for Molecular Recognition, Stockholm, Aug. 1988.
48. FMC Lecturer, Chemistry Department, Princeton University, October 1988.
49. Nobel Symposium on Structure and Dynamics in Biological Systems, Snogeholms Slott, Lund, Sweden, December 1988.
50. Twenty-fourth Winter Seminar, Klosters, Switzerland, January 1989.
51. American Society for Cell Biology Joint Annual Meeting, San Francisco, California, January 1989.
52. UCLA Symposium on Biotechnology and Human Genetic Pre-disposition to Disease, Steamboat Springs, Colorado, March 1989.
53. Fourth International Conference on Supercomputing, Santa Clara, California, May 1989.
53. Spetsai Summer School on Molecular and Cellular Biology: Protein and Genetic Engineering, Spetsai, September 1989.
54. 3rd Structural Biology Symposium, Berkeley, California, January 1990.
55. Mathematical Approaches to DNA, Santa Fe, New Mexico, January 1990.
56. The Pauling Lecture in Chemistry, Stanford, California, February 1990.
57. Protein Folding Seminar at the AAAS Annual Meeting, New Orleans, February 1990.
58. Protein and Drug Design and Delivery, San Francisco, California, February 1990.
59. National Research Council Computer Board meeting on Computing and Molecular Biology: Mapping and Interpreting Biological Information, Washington, April 1990.
60. Gordon Research Conference on Computational Chemistry, Plymouth, NH, June 1990.
61. United Nations UNIDO ICGEB workshop on Computer Applications in Molecular Biology, Trieste, July 1990.
62. Frontiers in Human Retrovirology and Related Topics, Bethesda, August 1990.
63. Keck Symposium on Computational Biology, Houston, November 1990.

64. First USSR-Israel Workshop on Peptides and Proteins, Rehovot, Israel, December 1990.
65. Grand Challenges in Chemistry, Tallahassee, Florida, January 1992.
66. NSF Discussion Meeting on Protein Folding, Puerto Rico, March 1992.
67. Keystone Symposium of Transcription, Copper Mountain, April 1992.
68. Apple European Consortium Meeting, EUC 92, Bruges, Belgium, April 1992.
69. Gordon Research Conference on Biopolymers, Newport, Rhode Island, June 1992.
70. AAAS Science Innovation '92, San Francisco, July 1992.
71. Protein Society Meeting, San Diego, July 1992.
72. Understanding Protein Folding, Stockholm, Sweden, August 1992.
73. Nucleic Acid Structure, Santa Fe, New Mexico, November 1992.
74. International School on NMR, Erice, Sicily, March 1993.
75. Protein Dynamics and Thermodynamics, Jerusalem, Israel, March 1993.
76. ACS Protein Folding Symposium, Chicago, August 1993.
77. Twenty-Ninth Winter Seminar, Klosters, Switzerland, January 1994.
78. New York Academy of Science, New York, February 1994.
79. Beckmann Symposium, Urbana, June 1994.
80. Gordon Research Conference on Biopolymers, Newport, Rhode Island, June 1994.
81. KITS Symposium on Biomolecular Computation, Lawrence, Kansas, September 1994.
82. Juan Gris Symposium on Protein Folding, Madrid, Spain, November 1994.
83. Fourteenth Marr Memorial Lecture, Cambridge, England, November 1994.
84. American Physical Society Symposium on Protein Folding, San Jose, California, March 1995.
85. ESF Workshop on Protein Folding, St. Feliu de Guixols, Spain, April 1995.
86. International School on NMR and Dynamics in Biology, Erice, Sicily, May 1995.
87. Symposium on Protein Folding, Cornell, Ithaca, October 1995.
88. Protein Folding and Bioinformatics, Santa Fe, New Mexico, November 1995.
89. Israeli-German Symposium on Bioinformatics, Tel Aviv, Israel, November 1995.
90. European Bioinformatics Institute, Genomics, Cambridge, England, May 1996.
91. Cambridge Healthtech Institute, Bioinformatics & Genome Research, Baltimore, June 1996.
92. Symposium in Honor of Aaron Klug's 70-th Birthday, Cambridge, England, September 1996.
93. Symposium in Honor of Harold Scheraga's 75-th Birthday, Cornell, New York, October 1996.
94. Bioinformatics and Structure, Jerusalem, Israel, November 1996.
95. Critical Assessment of Structure Prediction II, Asilomar, California, December 1996.
96. Statistics and Inference in Molecular Biology, Santa Fe, New Mexico, January 1997.
97. 2nd Johns Hopkins Protein Folding Meeting, Coolfont, West Virginia, March 1997.
98. 9th Minisymposium in Molecular Biophysics, Rutgers, New Jersey, April 1997.
99. Cambridge Healthtech Institute, Bioinformatics & Genome Research, San Francisco, May 1997.
100. Howard Hughes Institute, Protein Function from Primary Sequence, Chevy Chase, Sept. 1997.
101. National Academy of Science, Colloquium on Computational Biomolecular Science, Irvine, California, September 1997.
102. The Institute for Genomic Research, Symposium on Bioinformatics, Washington, DC, Oct. 1997.
103. NIH Intramural STEP Program, Training in Bioinformatics, Washington, DC, November 1997.
104. La Jolla Interfaces in Science 98, San Diego, February 1998.
105. Recomb 98, Symposium on Bioinformatics, New York City, March 1998.
106. Purdue Research Symposium, Purdue, Indiana, November 1998.
107. Mathematics and Molecular Biology, Santa Fe, New Mexico, January 1999.
108. Stanford Computer Science Forum, Stanford, California, March 1999.
109. Bioinformatics 99, Symposium on Bioinformatics, Lund, Sweden, April 1999.
110. UCSF 99, Symposium on Bioinformatics, San Francisco, April 1999.
111. International School on NMR and Dynamics in Biology, Erice, Sicily, June 1999.
112. Gordon Conference on computational NMR in Biology, Il Cioccio, Italy, June 1999.
113. Belgium Biophysical Society meeting on Protein Folding, Gembloux, Belgium, June 1999.
114. Glaxo-Wellcome/UNC Meeting on Bioinformatics, Chapel Hill, October 1999.
115. First International Structural Genomics Meeting, Cambridge, UK, April 2000.

116. IBM Workshop: Bioinformatics Comes of Age, Cambridge, Mass, June 2000.
117. Computational Chemistry Gordon Research Conference, Oxford, UK, July 2000.
118. CIME School on Mathematical Methods for Protein Structure Analysis and Design, Martina Franca, Italy, July 2000.
119. Swedish Biochemical Society Meeting, Linköping, Sweden, September 2000.
120. First SIAM Conference on Computation Science and Engineering, Washington, September 2000.
121. Anfinsen Memorial Lecture, Johns Hopkins Folding Meeting, Coolfont, March 2001.
122. Visiting lectures on Bioinformatics, University of Florence, Italy, May 2001.
123. Royal Society New Members meeting, London, UK, July 2001.
124. Laboratory of Molecular Biology, Cambridge, UK, July 2001.
125. SNBET visiting lectures in Sweden (Umeå, Stockholm, Lund, Göteborg, Uppsala), September 2001.
126. Fenner Conference on Bioinformation Science, Australian Academy of Sciences, Canberra, Australia, September, 2001.
127. Combio 2001 A New Dimension, Plenary talk, Canberra, Australia, September, 2001.
128. NIH Symposium on Structure Prediction, Cornell, Ithaca, New York, October 2001.
129. What is Information, Sde Boker, Israel, December 2001.
130. Mathematics and Molecular Biology, Santa Fe, New Mexico, January 2002.
131. Lifson Memorial Symposium, Rehovot, Israel, February 2002.
132. Kollman Memorial Symposium, UCSF, San Francisco, February 2002.
133. Protein Society, San Diego, August 2002.
134. Perutz Memorial Symposium, Cambridge, September 2002.
135. Bio-Informatics Institute, Singapore, October 2002.
136. The Scripps Institute, La Jolla, November 2002.
137. Triangle Research Symposium, Duke, November 2002.
138. Colloquium Andre Adoutte, Gif sur Yvette, France, February 2003.
139. Laboratoire d'Enzymologie et Biochimie Structurales, Gif sur Yvette, France, March 2003
140. Pasteur Institute, Paris, France, March 2003
141. Lauréats Chaires Blaise Pascal, Paris, France, May 2003.
142. Bio-Informatics Institute, Singapore, August 2003.
143. National Institute of Health Workshop on Structural Genomics, October 2003.
144. Seminar in Structural Biology, Weizmann Institute of Science, November 2003.
145. IBBMC, Paris Univ., Orsay, May 2004.
146. IBPC, Rue Curie, Paris 5, May 2004.
147. Ecole Polytechnique, Lozere, June 2004.
148. Paris Univ. Jussieu, Paris 5, July 2004.
149. IRNA, Jouy-en-Josas, Paris, September 2004.
150. Saclay, St. Aubin, Paris, September 2004.
151. University of Nancy, France. October 2004.
152. IHES, Poincare, Paris, November 2004.
153. Strasbourg, November 2004.
154. LEBS, Paris Univ., December 2004.
155. IBPC, Rue Curie, Paris 5, December 2004.
156. Genepole, Evry, Paris, December 2004.
157. IRNA, Jouy-en-Josas, Paris, December 2004.
158. "Protein Spaces and Evolution", ENS, Cachan, Paris, February 2005.
159. "Adventure in Computational Biology", Université de Paris Sud, February 2005.
160. "Adventure in Computational Biology", Weizmann Institute, March 2005.
161. "Fifty Years of Computational Structural Biology", Stanford, May 2005.
162. "Exploring Protein Spaces and Evolution", Hecht, Jerusalem, May 2005.
163. "Homology, Structure Templates and Refinement", Israeli Bioinformatics Society, Beer Sheva, May 2005.
164. "Exploring Protein Spaces and Evolution", Hadassah Medical School, Jerusalem, May 2005.
165. "Exploring the Protein Universe", Beijing, Protein Folding Meeting, July 2005.
166. "Classifying Protein Structures", Biogeometry, Greensboro, NC, August 2005.

167. "How Myosin (V) Walks", BioX-IIP, Stanford, August 2005.
168. "Exploring the Protein Universe", EU Conference, Haifa University, September 2005.
169. "Exploring Protein Spaces and Evolution", Stockholm University, September 2005.
170. "Mesoscale Modeling of Motion in Protein Complexes", M2CELL, Molecule to Cell, Abbey of Fontevraud, France, December 2005.
171. "Protein Models in Computational Structural Biology", Theoretical Computational Biology Symposium, Houston, December 2005.
172. "Mesoscale Modeling: Normal Modes of Myosin" Simbios, Stanford, February 2006.
173. "Mesoscale Modeling of Molecular Machines" Institute for Computational and Mathematical Engineering (ICME), Stanford, May 2006.
174. "Basic Interactions, Protein Architecture, Simulating Motion and Mesoscale Modeling", Bioinformatics Summer School, Lipari, July 2006.
175. "Mesoscale Modeling of Nanomachines", Theoretical Computational Biology Symposium, Houston, December 2006.
176. "Mesoscale Modeling of Nanomachines", Chemistry Colloquium, Weizmann Institute, March 2007.
177. "Interactions, Motion & Mesoscale Modeling", Computational Biology Summer School, Lipari, June 2007.
178. "Modeling Motion of Large Protein", Sino-American Symposium, Shanghai, July 2007.
179. "Mesoscale Modeling of Nanomachines", Georgia Tech. December 2007.
180. "Mesoscale Modeling of Nanomachines", D.E. Shaw Research. December 2007.
181. "Mesoscale Modeling of Nanomachines", INRIA March 2008.
182. "Mesoscale Modeling of Nanomachines", University of Pennsylvania, Philadelphia, April 2008.
183. "A Tale of Two Spaces: Sequence Meets Structure", NIH Structural Genomics Bottleneck's Keynote, Bethesda, April 2008.
184. "Mesoscale Modeling of Nanomachines", Parma Symposium. June 2008.
185. "Protein Structural Superposition", Computational Biology Summer School, Lipari, June 2008.
186. "A Tale of Two Spaces: Sequence Meets Structure", UCSF, San Francisco. July 2008.
187. "Mesoscale Modeling of Nanomachines", LASR 2008, Leeds, United Kingdom, July 2008.
188. "Mesoscale Modeling of Nanomachines", Columbia University, New York, May 2008.
189. "Mesoscale Modeling of Nanomachines", Welch Symposium, Houston, October 2008.
190. "A Tale of Two Spaces: Sequence Meets Structure", Burnham Institute, La Jolla, December 2008.
191. "Recent Work in Computational Biology", Bar Ilan University, Tel Aviv, December 2009.
192. "Refinement and Energy Functions", D.E. Shaw Research. March 2009.
193. "The Nature of the Protein Universe" Columbia C2B2 Meeting, Outside Speaker, New York, March 2009.
194. "Mesoscale Modeling of Nanomachines", Protein Flexibility Workshop, IRNIA, France, March 2009.
195. "Three lectures" International School on NMR and Dynamics in Biology, Erice, Sicily, June 2009.
196. "The Nature of the Protein Universe", EMBO Lecturer, 3DSeig, Stockholm, June 2009.
197. "Insights into Electrostatics: C60 and RNAP Simulations", Biomolecular Simulation, Stockholm, June 2009.
198. "A Tale of Two Potentials", Suddath Frontiers Symposium, GATECH, Atlanta, November 2009.
199. "Fun and Games in Computational Molecular Biology", New Opportunities Seminar, MIT November 2009.
200. "Reduced Models for Mesoscale Simulation", Pacific Symposium of Bioinformatics, Hawaii, January 2010.
201. "The Protein Universe: A Current Snapshot", Keystone Symposium, Breckenridge, January 2010
202. "Mesoscale Modeling of Nanomachines", Cryo-EM Workshop, Houston, January 2010.
203. "The Nature of the Protein Universe: A Tale of Two Spaces", Tri-Institutional Seminar. New York, January 2010.
204. "A Tale of Two Potentials", Frontiers in Computational Molecular Biophysics, Weizmann Institute, February 2010
205. "The Nature of the Protein Universe", Bioinformatics Institute, Singapore. March 2010.
206. "The Nature of the Protein Universe", ASBMB, Irving. April 2010.
207. "A Tale of Two Potentials", Protein Folding, Telluride. May 2010.
208. "Reduced Models for Mesoscale Simulation", International School on NMR and Dynamics in Biology, Erice, Sicily, June 2010.
209. "The Nature of the Protein Universe", International School on NMR and Dynamics in Biology, Erice, Sicily, June 2010.