

## References

- [1] A. Aguzzi. Prions and antiprions. *Biol. Chem.*, 378:1393–1395, 1997.
- [2] A. Aguzzi, F. Montrasio, and P. S. Kaeser. Prions: Health scare and biological challenge. *Nature Rev. Mol. Cell Biol.*, 2:118–126, 2001.
- [3] B. Al-Lazikani, J. Jung, Z. Xiang, and B. Honig. Protein structure prediction. *Curr. Opin. Struct. Biol.*, 5:51–56, 2001.
- [4] B. J. Alder and T. E. Wainwright. Studies in molecular dynamics. I. General method. *J. Chem. Phys.*, 31:459–466, 1959.
- [5] M. P. Allen and D. J. Tildesley. *Computer Simulation of Liquids*. Oxford University Press, New York, NY, 1990.
- [6] W. F. Anderson. The best of times, the worst of times. *Science*, 288:627–629, 2000.
- [7] K. Ashrafi, F. Y. Chang, J. L. Watts, A. G. Fraser, R. S. Kamath, J. Ahringer, and G. Ruvkun. Genome-wide RNAi analysis of *Caenorhabditis elegans* fat regulatory genes. *Nature*, 421:268–272, 2003.
- [8] D. Baker and A. Sali. Protein structure prediction and structural genomics. *Science*, 294:93–96, 2001.
- [9] N. Ban, P. Nissen, J. Hansen, P. B. Moore, and T. A. Steitz. The complete atomic structure of the large ribosomal subunit at 2.4 Å resolution. *Science*, 289:905–920, 2000.
- [10] M. M. Barnhart, J. S. Pinkner, G. E. Soto, F. G. Sauer, S. Langermann, G. Waksman, C. Frieden, and S. J. Hultgren. PapD-like chaperones provide the missing information for folding of pilin proteins. *Proc. Natl. Acad. Sci. USA*, 97:7709–7714, 2000.
- [11] J. C. Beauchamp and N. W. Isaacs. Methods for X-ray diffraction analysis of macromolecular structures. *Curr. Opin. Chem. Biol.*, 3:525–529, 1999.

- [12] H. J. C. Berendsen. A glimpse of the holy grail. *Science*, 282:642–643, 1998.
- [13] R. Bonneau and D. Baker. Ab initio protein structure prediction: Progress and prospects. *Ann. Rev. Biophys. Biomol. Struct.*, 30:173–189, 2001.
- [14] R. Bonneau, J. Tsai, I. Ruczinski, and D. Baker. Functional inferences from blind *ab initio* protein structure predictions. *J. Struct. Biol.*, 134:186–190, 2001.
- [15] J. U. Bowie, R. Lüthy, and D. Eisenberg. A method to identify protein sequences that fold into a known three-dimensional structure. *Science*, 253:164–170, 1991.
- [16] D. B. Boyd. Rational drug design: Controlling the size of the haystack. *Mod. Drug Dis.*, 1:41–47, 1998.
- [17] S. F. Brady, K. J. Stauffer, W. C. Lumma, G. M. Smith, H. G. Ramjit, S. D. Lewis, B. J. Lucas, S. J. Gardell, E. A. Lyle, S. D. Appleby, J. J. Cook, M. A. Holahan, M. T. Stranieri, J. J. Lynch, Jr., J. H. Lin, I.-W. Chen, K. Vastag, A. M. Naylor-Olsen, and J. P. Vacca. Discovery and development of the novel potent orally active thrombin inhibitor N-(9-Hydroxy-9-fluorenicarboxy)propyl *trans*-4-Aminocyclohexylmethyl amide (L-372,460): Coapplication of structure-based design and rapid multiple analogue synthesis on solid support. *J. Med. Chem.*, 41(3):401–406, 1998.
- [18] C. Branden and J. Tooze. *Introduction to Protein Structure*. Garland Publishing Inc., New York, NY, second edition, 1999. ([www.proteinstructure.com/](http://www.proteinstructure.com/)).
- [19] P. Bratley, B. L. Fox, and L. E. Schrage. *A Guide to Simulation*. Springer-Verlag, New York, NY, 1987.
- [20] S. E. Brenner. A tour of structural genomics. *Nat. Genet.*, 2:801–809, 2001.
- [21] R. Brimacombe. The bacterial ribosome at atomic resolution. *Structure*, 8:R195–R200, 2000.
- [22] C. L. Brooks, III. Viewing protein folding from many perspectives. *Proc. Natl. Acad. Sci. USA*, 99:1099–1100, 2002.
- [23] C. L. Brooks, III. With a little help ... *Nature*, 420:33–34, 2002.
- [24] C. L. Brooks, III, M. Karplus, and B. M. Pettitt. *Proteins: A Theoretical Perspective of Dynamics, Structure, and Thermodynamics*, volume LXXI of *Advances in Chemical Physics*. John Wiley & Sons, New York, NY, 1988.
- [25] C. L. Brooks, III, J. N. Onuchic, and D. J. Wales. Statistical thermodynamics: Taking a walk on a landscape. *Science*, 293:612–613, 2001.
- [26] A. T. Brünger, P. D. Adams, and L. M. Rice. New applications of simulated annealing in X-ray crystallography and solution NMR. *Structure*, 5:325–336, 1997.
- [27] M. Bucciantini, E. Giannoni, F. Chiti, F. Baroni, L. Formigli, J. Zurdo, N. Taddei, G. Ramponi, C. M. Dobson, and M. Stefani. Inherent toxicity of aggregates implies a common mechanism for protein misfolding diseases. *Nature*, 416:507–511, 2002.
- [28] C. Bustamante, Z. Bryant, and S. B. Smith. Ten years of tension: Single-molecule DNA mechanics. *Nature*, 421:423–427, 2003.
- [29] A. A. Camargo, S. J. de Souza, R. R. Brentani, and A. J. G. Simpson. Human gene discovery through experimental definition of transcribed regions of the human genome. *Curr. Opin. Chem. Biol.*, 6:13–16, 2001.
- [30] C. R. Cantor and P. R. Schimmel. *Biophysical Chemistry*, volume 1–3. W. H. Freeman and Company, San Francisco, 1980.

- [31] A. P. Carter, W. M. Clemons, D. E. Brodersen, R. J. Morgan-Warren, B. T. Wimberly, and V. Ramakrishnan. Functional insights from the structure of the 30S ribosomal subunit and its interactions with antibiotics. *Nature*, 407:340–348, 2000.
- [32] D. A. Case. NMR refinement. In P. von Ragué Schleyer (Editor-in Chief), N. L. Allinger, T. Clark, J. Gasteiger, P. A. Kollman, and H. F. Schaefer, III, editors, *Encyclopedia of Computational Chemistry*, volume 3, pages 1866–1876. John Wiley & Sons, West Sussex, England, 1998.
- [33] L. Castagnoli, M. Scarpa, M. Kokkinidis, D.W. Banner, D. Tsernoglou, and G. Cesareni. Genetic and structural analysis of the CoIE1 Rop (Rom) protein. *Embo. J.*, 8:621–629, 1989.
- [34] J. H. Cate, M. M. Yusupov, C. Zh. Yusupova, T. N. Earnest, and H. F. Noller. X-ray crystal structure of 70S ribosome functional complexes. *Science*, 285:2095–2104, 1999.
- [35] M. Cavazzana-Calvo, S. Hacein-Bey, G. de Saint Basile, F. Gross, E. Yvon, P. Nusbaum, F. Selz, C. Hue, S. Certain, J.-L. Casanova, P. Bousso, F. Le Deist, and A. Fischer. Gene therapy of human severe combined immunodeficiency (SCID)-X1 disease. *Science*, 288:669–672, 2000.
- [36] T. R. Cech. The ribosome is a ribozyme. *Science*, 289:878–879, 2000.
- [37] 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. He, R. Huang, V. Ilyin, L. McMahan, U. Pieper, S. Ray, M. Vidal, and L. K. Wang. Structural genomics: A pipeline for providing structures for the biologist. *Prot. Sci.*, 11:723–738, 2002.
- [38] T. E. Cheatham, III, J. L. Miller, T. Fox, T. A. Darden, and P. A. Kollman. Molecular dynamics simulations of solvated biomolecular systems: The particle mesh Ewald method leads to stable trajectories of DNA, RNA, and proteins. *J. Amer. Chem. Soc.*, 117:4193–4194, 1995.
- [39] Z. Chen, Y. Li, E. Chen, D. L. Hall, P. L. Darke, C. Culberson, J. A. Shafer, and L. C. Kuo. Crystal structure at 1.9-Å resolution of human immunodeficiency (HIV) II protease complexed with L-735,524, an orally bioavailable inhibitor of the HIV proteases. *J. Biol. Chem.*, 269:26344–26348, 1994.
- [40] G. M. Clore and A. M. Gronenborn. New methods of structure refinement for macromolecular structure determination by NMR. *Proc. Natl. Acad. Sci. USA*, 95:5891–5898, 1998.
- [41] G. M. Clore and C. D. Schwieters. Theoretical and computational advances in biomolecular NMR spectroscopy. *Curr. Opin. Struct. Biol.*, 12:146–153, 2002.
- [42] F. E. Cohen. Protein misfolding and prion diseases. *J. Mol. Biol.*, 293:313–320, 1999.
- [43] F. S. Collins and K. G. Jegalian. Deciphering the code of life. *Sci. Amer.*, 281:86–91, 1999.
- [44] D. Crothers and D. Eisenberg. *Physical Chemistry with Applications to the Life Sciences*. Benjamin/Cummings, Menlo Park, CA, 1979.
- [45] V. Daggett. Long timescale simulations. *Curr. Opin. Struct. Biol.*, 10:160–164, 2000.
- [46] S. Dalal, S. Balasubramanian, and L. Regan. Protein alchemy: Changing  $\beta$ -sheet into  $\alpha$ -helix. *Nature Struct. Biol.*, 4:548–552, 1997.

- [47] X. Daura, B. Jaun, D. Seebach, W. F. Van Gunsteren, and A. Mark. Reversible peptide folding in solution by molecular dynamics simulation. *J. Mol. Biol.*, 280:925–932, 1998.
- [48] K. Davies. *Cracking the Genome: Inside the Race to Unlock Human DNA*. The Free Press (A Simon & Schuster Division), New York, NY, 2001.
- [49] K. A. Dill, S. Bromberg, K. Yue, K. M. Fiebig, D. P. Yee, P. D. Thomas, and H. S. Chan. Principles of protein folding — A perspective from simple exact models. *Protein Science*, 4:561–602, 1995.
- [50] K. A. Dill and H. S. Chan. From Levinthal to pathways to funnels. *Nature Struct. Biol.*, 4:10–19, 1997.
- [51] A. R. Dinner and M. Karplus. Comment on the communication “The key to solving the protein-folding problem lies in an accurate description of the denatured state” by van Gunsteren et al. *Angew. Chem. Int. Ed.*, 40:4615–4616, 2001.
- [52] C. M. Dobson. Getting out of shape. *Nature*, 418:729–730, 2002.
- [53] J. A. Doudna. A molecular contortionist. *Nature*, 388:830–831, 1997.
- [54] D. A. Doyle, J. Morais Cabral, R. A. Pfuetzner, A. Kuo, J. M. Gulbis, S. L. Cohen, B. T. Chait, and R. MacKinnon. The structure of the potassium channel: Molecular basis of K<sup>+</sup> conduction and selectivity. *Science*, 280:69–77, 1998.
- [55] Y. Duan and P. A. Kollman. Pathways to a protein folding intermediate observed in a 1-microsecond simulation in aqueous solution. *Science*, 282:740–744, 23 October 1998.
- [56] Y. Duan, P. A. Kollman, and S. C. Harvey. Protein folding and beyond. In E. Keinan and I. Schechter, editors, *Chemistry for the 21st Century*. Wiley-VCH, Weinheim, Germany, 2000.
- [57] Y. Duan, L. Wang, and P. A. Kollman. The early stage of folding of villin head-piece subdomain observed in a 200-nanosecond fully solvate molecular dynamics simulation. *Proc. Natl. Acad. Sci. USA*, 95:9897–9902, 1998.
- [58] R. L. Dunbrack, Jr., D. L. Gerloff, M. Bower, X. Chen, O. Lichtarge, and F. E. Cohen. Meeting review: the second meeting on the critical assessment of techniques for protein structure prediction (CASP2), Asilomar, California, December 13–16, 1996. *Fold. Design*, 2:R27–R42, 1997.
- [59] R. Dutzler, E. B. Campbell, M. Cadene, B. T. Chait, and R. MacKinnon. X-ray structure of a CIC chloride channel at 3.0 Å reveals the molecular basis of anion selectivity. *Nature*, 415:287–294, 2002.
- [60] H. J. Dyson and P. E. Wright. Insights into protein folding from NMR. *Annu. Rev. Phys. Chem.*, 47:369–395, 1996.
- [61] H. J. Dyson and P. E. Wright. Coupling of folding and binding for unstructured proteins. *Curr. Opin. Struct. Biol.*, 12:54–60, 2002.
- [62] L. O. Elkin. Rosalind Franklin and the double helix. *Physics Today*, 56:42–48, 2003.
- [63] R. J. Ellis. Molecular chaperones: Avoiding the crowd. *Curr. Biol.*, 7:R531–R533, 1999.
- [64] R. J. Ellis. Molecular chaperones: Pathways and networks. *Curr. Biol.*, 9:R137–R139, 1999.

- [65] R. R. Ernst, G. Bodenhausen, and A. Wokaum. *Principles of Nuclear Magnetic Resonance in One and Two Dimensions*, volume 14 of *International Series of Monographs on Chemistry*. Clarendon Press, Oxford, New York, NY, 1987.
- [66] W. E. Evans and M. V. Relling. Pharmacogenomics: Translating functional genomics into rational therapeutics. *Science*, 286:487–491, 1999.
- [67] C. Ezzell. Proteins rule. *Sci. Amer.*, 286:40–47, 2002.
- [68] W. A. Fenton and A. L. Horwich. GroEL-mediated protein folding. *Protein Sci.*, 6:743–760, 1997.
- [69] M. Ferrer, T. A. Kapoor, T. Strassmaier, W. Weissenhorn, J. J. Skehel, D. Oprian, S. L. Schreiber, D. C. Wiley, and S. C. Harrison. Selection of gp41-mediated HIV-1 cell entry inhibitors from biased combinatorial libraries of non-natural binding elements. *Nature Struct. Biol.*, 6:953–960, 1999.
- [70] A. Fersht. *Structure and Mechanism in Protein Science: A Guide to Enzyme Catalysis and Protein Folding*. W. H. Freeman and Company, New York, NY, 1999.
- [71] A. R. Fersht and V. Daggett. Protein folding and unfolding at atomic resolution. *Cell*, 108:573–582, 2002.
- [72] J. Fiaux, E. B. Bertelsen, A. L. Horwich, and K. Wüthrich. NMR analysis of a 900K GroEL–GroES complex. *Nature*, 418:207–211, 2002.
- [73] D. Filmore. Taming the beast. *Mod. Drug Dis.*, 4:40–46, 2001.
- [74] J. Frank. *Three-Dimensional Electron Microscopy of Macromolecular Assemblies*. Academic Press, San Diego, CA, 1996.
- [75] J. Frank. How the ribosome works. *Sci. Amer.*, 86:428–439, 1998.
- [76] D. Frenkel and B. Smit. *Understanding Molecular Simulations. From Algorithms to Applications*. Academic Press, San Diego, CA, 1996.
- [77] R. A. Friesner and J. R. Gunn. Computational studies of protein folding. *Annu. Rev. Biophys. Biomol. Struct.*, 25:315–342, 1996.
- [78] E. A. Galburt and B. L. Stoddard. Time-resolved macromolecular crystallography. *Phys. Today*, 54:33–39, 1989.
- [79] H. H. Gan, R. A. Perlow, S. Roy, J. Ko, M. Wu, J. Huang, S. Yan, A. Nicoletta, J. Vafai, D. Sun, L. Wang, J. E. Noah, S. Pasquali, and T. Schlick. Analysis of protein sequence/structure similarity relationships. *Biophys. J.*, 83:2781–2791, 2002.
- [80] F. Gao, E. Bailes, D. L. Robertson, Y. Chen, C. M. Rodenburg, S. F. Michael, L. B. Cummins, L. O. Arthur, M. Peeters, G. M. Shaw, P. M. Sharp, and B. H. Hahn. Origin of HIV-1 in the chimpanzee *pan troglodytes troglodytes*. *Nature*, 397:436–441, 1999.
- [81] H. Gould and J. Tobochnik. *An Introduction to Computer Simulation Methods: Applications to Physical Systems. Part 1*. Addison-Wesley, Reading, Massachusetts, 1988.
- [82] P. Green. Whole-genome disassembly. *Proc. Natl. Acad. Sci. USA*, 99:4143–4144, 2002.
- [83] P. Güntert. Structure calculation of biological macromolecules from NMR data. *Quart. Rev. Biophys.*, 31:145–237, 1998.
- [84] J. M. Haile. *Molecular Dynamics Simulations: Elementary Methods*. John Wiley & Sons, New York, NY, 1992.

- [85] P. Hammarström, F. Schneider, and J. W. Kelly. *Trans*-suppression of misfolding in an amyloid disease. *Science*, 293:2459–2462, 2001.
- [86] M. Hann and R. Green. Cheminformatics – A new name for an old problem? *Curr. Opin. Chem. Biol.*, 3:379–383, 1999.
- [87] U. H. E. Hansmann and Y. Okamoto. New Monte Carlo algorithms for protein folding. *Curr. Opin. Struct. Biol.*, 9:177–183, 1999.
- [88] T. Hansson, C. Oostenbrink, and W. F. van Gunsteren. Molecular dynamics simulations. *Curr. Opin. Struct. Biol.*, 12:190–196, 2002.
- [89] W. E. Harte, Jr., S. Swaminathan, and D. L. Beveridge. Molecular dynamics of HIV-1 protease. *Proteins: Struct. Func. Gen.*, 13:175–194, 1992.
- [90] F. U. Hartl and M. H.-Hartl. Molecular chaperones in the cytosol: Nascent chain to folded protein. *Science*, 295:1852–1858, 2002.
- [91] S. C. Harvey, M. Prabhakaran, B. Mao, and J. A. McCammon. Phenylalanine transfer RNA: Molecular dynamics simulation. *Science*, 223:1189–1191, 1984.
- [92] W. A. Hasteline. Beyond chicken soup. *Sci. Amer.*, 285:56–63, 2001.
- [93] H. A. Hauptman. The phase problem of X-ray crystallography. *Phys. Today*, 42:24–29, 1989.
- [94] D. J. Hazuda, P. Felock, M. Witmer, A. Wolfe, K. Stillmock, J. A. Grobler, A. Espe- seth, L. Gabryelski, W. Schleif, C. Blau, and Michael D. Miller. Inhibitors of strand transfer that prevent integration and inhibit HIV-1 replication in cells. *Science*, 287:646–650, 2000.
- [95] W. A. Hendrickson. Determination of macromolecular structures from anomalous diffraction of synchrotron radiation. *Science*, 254:51–58, 1991.
- [96] W. A. Hendrickson and C. Ogata. Phase determination from multiwavelength anomalous diffraction measurements. *Meth. Enzymol.*, 276:494–523, 1997.
- [97] B. Honig. Protein folding: From the Levinthal paradox to structure prediction. *J. Mol. Biol.*, 293:283–293, 1999.
- [98] W. A. Houry, D. Frishman, C. Eckerskorn, F. Lottspeich, and F. U. Hartl. Identification of *in vivo* substrates of the chaperonin GroEL. *Nature*, 402:147–154, 1999.
- [99] K. Howard. The bioinformatics gold rush. *Sci. Amer.*, 283:58–63, 2000.
- [100] H. Huang, R. Chopra, G. L. Verdine, and S. C. Harrison. Structure of a covalently trapped catalytic complex of HIV-1 reverse transcriptase: Implications for drug resistance. *Science*, 282:1669–1675, 1998.
- [101] T. Ideker, T. Galitski, and L. Hood. A new approach to decoding life: Systems biology. *Ann. Rev. Genom. Hum. Genet.*, 2:343–372, 2001.
- [102] S. Izrailev, A. R. Crofts, E. A. Berry, and K. Schulten. Steered molecular dynamics simulation of the Rieske subunit motion in the cytochrome *bc*<sub>1</sub> complex. *Biophys. J.*, 77:1753–1768, 1999.
- [103] A. Jack and M. Levitt. Refinement of large structures by simultaneous minimization of energy and R factor. *Acta Crystallogr.*, A34:931–935, 1978.
- [104] T. L. James, H. Liu, N. B. Ulyanov, S. Farr-Jones, H. Zhang, D. G. Donne, K. Kaneko, D. Groth, I. Mehlhorn, S. B. Prusiner, and F. E. Cohen. Solution structure of a 142-residue recombinant prion protein corresponding to the infectious fragment of the scrapie isoform. *Proc. Natl. Acad. Sci. USA*, 94:10086–10091, 1997.

- [105] M. Ø Jensen, E. Tajkhorshid, and K. Schulten. The mechanism of glycerol conduction in aquaglyceroporins. *Structure*, 9:1083–1093, 2001.
- [106] W. L. Jorgensen, J. Chandrasekar, J. Madura, R. Impey, and M. Klein. Comparison of simple potential functions for simulating liquid water. *J. Chem. Phys.*, 79:926–935, 1983.
- [107] H. F. Judson. *The Eighth Day of Creation. Makers of the Revolution in Biology*. Cold Spring Harbor Laboratory Press, Cold Spring Harbor, NY, 1996. (Expanded edition).
- [108] R. S. Kamath, A. G. Fraser, Y. Dong, G. Poulin, R. Durbin, M. Gotta, A. Kanapin, N. Le Bot, S. Moreno, M. Sohrmann, D. P. Welchman, P. Zipperlen, and J. Ahringer. Systematic functional analysis of the *Caenorhabditis elegans* genome using RNAi. *Nature*, 421:231–237, 2003.
- [109] P. Kapranov, S. E. Cawley, J. Drenkow, S. Bekiranov, R. L. Strausberg, S. P. A. Fodor, and T. R. Gingeras. Large-scale transcriptional activity in chromosomes 21 and 22. *Science*, 296:916–919, 2002.
- [110] J. Karle. Macromolecular structure from anomalous dispersion. *Phys. Today*, 42:20–22, 1989.
- [111] R. M. Karp. Mathematical challenges from genomics and molecular biology. *Notices Amer. Math. Soc.*, 49:544–553, 2002.
- [112] D. K. Klimov and D. Thirumalai. Stretching single-domain proteins: Phase diagram and kinetics of force-induced unfolding. *Proc. Natl. Acad. Sci. USA*, 96:6166–6170, 1999.
- [113] J. Kling. Out of Malaysia: Finding natural products to fight AIDS. *Mod. Drug Dis.*, 2:31–36, 1999.
- [114] P. Koehl and M. Levitt. A brighter future for protein structure prediction. *Nature Struc. Biol.*, 6:108–111, 1999.
- [115] J. H. Konnert and W. A. Hendrickson. A restrained-parameter thermal-factor refinement procedure. *Acta Crystallogr.*, A36:344–350, 1980.
- [116] E. V. Koonin, L. Aravind, and A. S. Kondrashov. The impact of comparative genomics on our understanding of evolution. *Cell*, 101:573–576, 2000.
- [117] A. Korostelev, R. Bertram, and M. S. Chapman. Simulated-annealing real-space refinement as a tool in model building. *Acta Cryst.*, D58:761–767, 2002.
- [118] D. Kosztin, T. C. Bishop, and K. Schulten. Binding of the estrogen receptor to DNA: The role of waters. *Biophys. J.*, 73:557–570, 1997.
- [119] P. D. Kwong, R. Wyatt, J. Robinson, R. W. Sweet, J. Sodroski, and W. A. Hendrickson. Structure of an HIV gp 120 envelope glycoprotein in complex with the CD4 receptor and a neutralizing human antibody. *Nature*, 393:648–659, 1998.
- [120] E. Lander. The new genomics: Global views of biology. *Science*, 274:536–539, 1996.
- [121] B. A. Larder and D. K. Stammers. Closing in on HIV drug resistance. *Nature Struc. Biol.*, 6:103–106, 1999.
- [122] T. Lazaridis and M. Karplus. “New view” of protein folding reconciled with the old through multiple unfolding simulations. *Science*, 278:1928–1931, 1997.
- [123] C. Levinthal. Are there pathways for protein folding? *J. Chim. Physique*, 65:44–45, 1969.

- [124] C. Levinthal. How to fold graciously. In P. Debrunner, J. C. M. Tsibris, and E. Münch, editors, *Mossbauer Spectroscopy in Biological Systems, Proceedings of a Meeting held at Allerton House, Monticello, Illinois*, page 22, Urbana, Illinois, 1969. University of Illinois Press.
- [125] M. Levitt. Computer simulation of DNA double-helix dynamics. *Cold Spring Harbor Symp. Quant. Biol.*, 47:251–275, 1983.
- [126] M. Levitt. The birth of computational structural biology. *Nat. Struc. Biol.*, 8:392–393, 2001.
- [127] R. M. Levy, R. P. Sheridan, J. W. Keepers, G. S. Dubey, S. Swaminathan, and M. Karplus. Molecular dynamics of myoglobin at 298°K. Results from a 300-ps computer simulation. *Biophys. J.*, 48:509–518, 1985.
- [128] H. Liu, S. Farr-Jones, N. B. Ulyanov, M. Llinas, S. Marqusee, D. Groth, F. E. Cohen, S. B. Prusiner, and T. L. James. Solution structure of a syrian hamster prion protein rPrP(90–231). *Biochemistry*, 38:5362–5377, 1999.
- [129] O. Llorca, E. A. McCormack, G. Hynes, J. Grantham, J. Cordell, J. L. Carrascosa, K. R. Willison, J. J. Fernandez, and J. M. Valpuesta. Eukaryotic type II chaperonin CCT interacts with actin through specific subunits. *Nature*, 402:693–696, 1999.
- [130] L. L. Looger, M. A. Dwyer, J. J. Smith, and H. W. Hellinga. Computational design of receptor and sensor proteins with novel functions. *Nature*, 423:185–190, 2003.
- [131] K. Luger, A. W. Mäder, R. K. Richmond, D. F. Sargent, and T. J. Richmond. Crystal structure of the nucleosome core particle at 2.8 Å resolution. *Nature*, 389:251–260, 1997.
- [132] R. MacKinnon, S. L. Cohen, A. Kuo, A. Lee, and B. T. Chait. Structural conservation in prokaryotic and eukaryotic potassium channel. *Science*, 280:106–109, 1998.
- [133] B. Maddox. *Rosalind Franklin. The Dark Lady of DNA*. HarperCollins, New York, NY, 2002.
- [134] M. A. Marti-Renom, M. S. Madhusudhan, A. Fiser, B. Rost, and A. Sali. Reliability of assessment of protein structure prediction methods. *Structure*, 10:435–440, 2002.
- [135] J. S. Mattick. Non-coding RNAs: The architects of eukaryotic complexity. *EMBO Rep.*, 2:986–991, 2001.
- [136] J. A. McCammon, B. R. Gelin, and M. Karplus. Dynamics of folded proteins. *Nature*, 267:585–590, 1977.
- [137] J. A. McCammon and S. C. Harvey. *Dynamics of Proteins and Nucleic Acids*. Cambridge University Press, Cambridge, MA, 1987.
- [138] J. J. McCarthy and R. Hilfiker. The use of single-nucleotide polymorphism maps in pharmacogenomics. *Nature Biotech.*, 18:505–508, 2000.
- [139] A. McPherson. Macromolecular crystals. *Sci. Amer.*, 260:62–69, 1989.
- [140] D. A. McQuarrie. *Statistical Mechanics*. Harper & Row, New York, NY, 1976. Chapters 20–21.
- [141] L. Mirny and E. Shakhnovich. Protein folding theory: From lattice to all-atom models. *Ann. Rev. Biophys. Biomol. Struc.*, 30:361–396, 2001.
- [142] P. R. E. Mittl and M. G. Grütter. Structural genomics: Opportunities and challenges. *Curr. Opin. Chem. Biol.*, 5:402–408, 2001.



- [143] K. Moffat. Time-resolved biochemical crystallography: A mechanistic perspective. *Chem. Rev.*, 101:1569–1581, 2001.
- [144] G. T. Montelione and S. Anderson. Structural genomics: Keystone for a human proteome project. *Nature Struct. Biol.*, 6:11–12, 1999.
- [145] J. H. Morais-Cabral, Y. Zhou, and R. MacKinnon. Energetic optimization of ion conduction rate by the K<sup>+</sup> selectivity filter. *Nature*, 414:37–42, 2001.
- [146] J. Moult, K. Fidelis, A. Zemla, and T. Hubbard. Critical assessment of methods of protein structure prediction (CASP): Round IV. *Proteins: Struct. Func. Gen.*, Suppl. 5:2–7, 2001.
- [147] J. Moult, K. Fidelis, A. Zemla, T. Hubbard, and A. Tramontano. The significance of performance ranking in CASP—Response to Marti-Renom et al. *Structure*, 10:291–292, 2002.
- [148] D. W. Mount. *Bioinformatics. Sequence and Genome Analysis*. Cold Spring Harbor Laboratory Press, Cold Spring Harbor, NY, 2001.
- [149] K. B. Mullis. *Dancing Naked in the Mind Field*. Pantheon Books, New York, NY, 1998.
- [150] E. W. Myers, G. G. Sutton, H. O. Smith, M. D. Adams, and J. C. Venter. On the sequencing and assembly of the human genome. *Proc. Natl. Acad. Sci. USA*, 99:4145–4146, 2002.
- [151] X. Nassif. A furtive pathogen revealed. *Science*, 287:1767–1768, 2000.
- [152] S. Neidle. New insights into sequence-dependent DNA structure. *Nature Struct. Biol.*, 5:754–756, 1998.
- [153] P. Nissen, J. Hansen, N. Ban, P. B. Moore, and T. A. Steitz. The structural basis of ribosome activity in peptide bond synthesis. *Science*, 289:920–930, 2000.
- [154] S. Normark. Anfinsen comes out of the cage during assembly of the bacterial pilus. *Proc. Natl. Acad. Sci. USA*, 97:7670–7672, 2000.
- [155] K. Okada and S. Okada. X-ray crystallographic analysis and semiempirical computations. In P. von Ragué Schleyer (Editor-in Chief), N. L. Allinger, T. Clark, J. Gasteiger, P. A. Kollman, and H. F. Schaefer, III, editors, *Encyclopedia of Computational Chemistry*, volume 5, pages 3223–3247. John Wiley & Sons, West Sussex, England, 1998.
- [156] S. Oliver. Proteomics: Guilt-by-association goes global. *Nature*, 403:601–602, 2000.
- [157] J. N. Onuchic. Contacting the protein folding funnel with NMR. *Proc. Natl. Acad. Sci. USA*, 94:7129–7131, 1997.
- [158] J. N. Onuchic, Z. Luthey-Schulten, and P. G. Wolynes. Theory of protein folding: The energy landscape perspective. *Annu. Rev. Phys. Chem.*, 48:545–600, 1997.
- [159] E. V. Orlova, M. A. Rahman, B. Gowen, K. E. Volynski, A. C. Ashton, C. Manser, M. van Heel, and Y. A. Ushkaryov. Structure of  $\alpha$ -latrotoxin oligomers reveals that divalent cation-dependent tetramers form membrane pores. *Nat. Struct. Biol.*, 7:48–53, 2000.
- [160] R. V. Pappu. Review of the fourth Johns Hopkins protein folding meeting. *Proteins: Struct. Func. Gen.*, 36:263–269, 1999.

- [161] G. A. Patikoglou, J. L. Kim, L. Sun, S.-H. Yang, T. Kodadek, and S. K. Burley. TATA element recognition by the TATA box-binding protein has been conserved throughout evolution. *Genes & Devt.*, 13:3217–3230, 1999.
- [162] L. Pauling and R. B. Corey. Configurations of polypeptide chains with favored orientations around single bonds: Two new pleated sheets. *Proc. Natl. Acad. Sci. USA*, 37:729–740, 1951.
- [163] L. Pauling, R. B. Corey, and H. R. Branson. The structure of proteins: Two hydrogen-bonded helical configurations of the polypeptide chain. *Proc. Natl. Acad. Sci. USA*, 37:205–211, 1951.
- [164] M. B. Pepys, J. Herbert, W. L. Hutchinson, G. A. Tennent, H. J. Lachmann, J. R. Gallimore, L. B. Lovat, T. Bartfai, A. Alanine, C. Hertel, T. Hoffmann, R. Jakob-Roetne, R. D. Norcross, J. A. Kemp, K. Yamamura, M. Suzuki, G. W. Taylor, S. Murray, D. Thompson, A. Purvis, S. Kolstoe, S. P. Wood, and P. N. Hawkins. Targeted pharmacological depletion of serum amyloid P component for treatment of human amyloidosis. *Nature*, 417:254–259, 2002.
- [165] G. A. Petsko and D. Ringe. Observation of unstable species in enzyme-catalyzed transformations using protein crystallography. *Curr. Opin. Chem. Biol.*, 4:89–94, 2000.
- [166] M. Pizza, V. Scarlato, V. Masignani, M. M. Giuliani, B. Aricó, M. Comanducci, G. T. Jennings, L. Baldi, E. Bartolini, B. Capecchi, C. L. Galeotti, E. Luzzi, R. Manetti, E. Marchetti, M. Mora, S. Nuti, G. Ratti, L. Santini, S. Savino, M. Scarselli, E. Storni, P. Zuo, M. Broecker, E. Hundt, B. Knapp, E. Blair, T. Mason, H. Tettelin, D. W. Hood, A. C. Jeffries, N. J. Saunders, D. M. Granoff, J. C. Venter, E. R. Moxon, G. Grandi, and R. Rappuoli. Identification of vaccine candidates against serogroup B meningococcus by whole-genome sequencing. *Science*, 287:1816–1820, 2000.
- [167] S. L. Pomeroy, P. Tamayo, M. Gaasenbeek, L. M. Sturla, M. Angelo, M. E. McLaughlin, J. Y. H. Kim, L. C. Goumnerova, P. M. Black, C. Lau, J. C. Allen, D. Zagzag, J. M. Olson, T. Curran, C. Wetmore, J. A. Biegel, T. Poggio, S. Mukherjee, R. Rifkin, A. Califano, G. Stolovitzky, D. N. Louis, J. P. Mesirov, E. S. Lander, and T. R. Golub. Prediction of central nervous system embryonal tumour outcome based on gene expression. *Nature*, 415:436–442, 2002.
- [168] M. Prabhakaran, S. C. Harvey, B. Mao, and J. A. McCammon. Molecular dynamics of phenylalanine transfer RNA. *J. Biomol. Struct. Dynam.*, 1:357–369, 1983.
- [169] A. Rahman and F. H. Stillinger. Molecular dynamics study of liquid water. *J. Chem. Phys.*, 55:3336–3359, 1971.
- [170] A. Rahman and F. H. Stillinger. Improved simulation of liquid water by molecular dynamics. *J. Chem. Phys.*, 60:1545–1557, 1974.
- [171] D.C. Rapaport. *The Art of Molecular Dynamics Simulation*. Cambridge University Press, Cambridge, England, 1995.
- [172] P. R. Reilly. *Abraham Lincoln's DNA and Other Adventures in Genetics*. Cold Spring Harbor Laboratory Press, Cold Spring Harbor, NY, 2000.
- [173] J. Ren, R. M. Esnouf, A. L. Hopkins, E. Y. Jones, I. Kirby, J. Keeling, C. K. Ross, B. A. Larder, D. I. Stuart, and D. K. Stammers. 3'-Azido-3'-deoxythymidine drug resistance mutations in HIV-1 reverse transcriptase can induce long range

- conformational changes resistance. *Proc. Natl. Acad. Sci. USA*, 95:9518–9523, 1998.
- [174] G. Rhodes. *Crystallography Made Crystal Clear: A Guide for Users of Macromolecular Models*. Academic Press, San Diego, CA, second edition, 2000.
- [175] J. B. Ristaino, C. T. Groves, and G. R. Parra. PCR amplification of the Irish potato famine pathogen from historic specimens. *Nature*, 411:695–697, 2001.
- [176] N. A. Roberts, J. A. Martin, D. Kinchington, A. V. Broadhurst, J. C. Craig, I. B. Duncan, S. A. Galpin, B. K. Handa, J. Kay, A. Kröhn, R. W. Lambert, J. H. Merrett, J. S. Mills, K. E. B. Parkes, S. Redshaw, A. J. Ritchie, D. L. Taylor, G. J. Thomas, and P. J. Machin. Rational design of peptide-based HIV proteinase inhibitors. *Science*, 248:358–361, 1990.
- [177] G. Rose. Protein folding and the Paracelsus challenge. *Nature Struct. Biol.*, 4:512–514, 1997.
- [178] S. M. Ross. *A Course in Simulation*. Macmillan Publishing Company, New York, NY, 1990.
- [179] E. Rothstein. DNA teaches history a few lessons of its own. *New York Times*, 1998. Sunday, May 24 (under Ideas & Trends of the Week in Review).
- [180] J. P. Ryckaert, G. Ciccotti, and H. J. C. Berendsen. Numerical integration of the Cartesian equations of motion of a system with constraints: Molecular dynamics of n-alkanes. *J. Comput. Phys.*, 23:327–341, 1977.
- [181] S. Saha, A. B. Sparks, C. Rago, V. Akmaev, C. J. Wang, B. Vogelstein, K. W. Kinzler, and V. E. Velculescu. Using the transcriptome to annotate the genome. *Nat. Biotech.*, 19:508–512, 2002.
- [182] A. Sali, M. A. Marti-Renom, M. S. Madhusudhan, A. Fiser, and B. Rost. Reply to Moulton et al. *Structure*, 10:292–293, 2002.
- [183] R. Sánchez and A. Šali. Advances in comparative protein-structure modelling. *Curr. Opin. Struct. Biol.*, 7:206–214, 1997.
- [184] R. Sánchez and A. Šali. Large-scale protein structure modeling of the *saccharomyces cerevisiae* genome. *Proc. Natl. Acad. Sci. USA*, 95:13597–13602, 1998.
- [185] T. Schlick, R. D. Skeel, A. T. Brünger, L. V. Kalé, J. A. Board, Jr., J. Hermans, and K. Schulten. Algorithmic challenges in computational molecular biophysics. *J. Comput. Phys.*, 151:9–48, May 1999. (Special Volume on Computational Biophysics).
- [186] F. Schluenzen, A. Tocilj, R. Zarivach, J. Harms, M. Gluehmann, D. Janell, A. Bashan, H. Bartels, I. Agmon, F. Franceschi, and A. Yonath. Structure of functionally activated small ribosomal subunit at 3.3 Å resolution. *Cell*, 102:615–623, 2000.
- [187] M. R. Scott, R. Will, J. Ironside, H.-Oanh B. Nguyen, P. Tremblay, S. J. DeArmond, and S. B. Prusiner. Compelling transgenic evidence for transmission of bovine spongiform encephalopathy prions to humans. *Proc. Natl. Acad. Sci. USA*, 96:15137–15142, 1999.
- [188] W. G. Scott and A. Klug. Ribozymes: Structure and mechanism in RNA catalysis. *Trends Bio. Sci.*, 21:220–224, 1996.

- [189] G. L. Seibel, U. C. Singh, and P. A. Kollman. A molecular dynamics simulation of double-helical B-DNA including counterions and water. *Proc. Natl. Acad. Sci. USA*, 82:6537–6540, 1985.
- [190] J.-E. Shea and C. L. Brooks, III. From folding theories to folding proteins: A review and assessment of simulation studies of protein folding and unfolding. *Annu. Rev. Phys. Chem.*, 52:499–535, 2001.
- [191] M. Shirts and V. Pande. Screen savers of the world unite! *Science*, 290:1903–1904, 2000.
- [192] M. Shtilerman, G. H. Lorimer, and S. W. Englander. Chaperonin function: Folding by forced unfolding. *Science*, 284:822–825, 1999.
- [193] G. Siegal, J. van Duynhoven, and M. Baldus. Biomolecular NMR: Recent advances in liquids, solids and screening. *Curr. Opin. Chem. Biol.*, 3:530–536, 1999.
- [194] B. Simon and M. Sattler. De novo structure determination from residual dipolar couplings by NMR spectroscopy. *Angew. Chem. Int. Ed.*, 41:437–440, 2002.
- [195] C. D. Snow, H. Nguyen, V. S. Pande, and M. Gruebele. Absolute comparison of simulated and experimental protein folding dynamics. *Nature*, 420:102–106, 2002.
- [196] C. M. T. Spahn, P. A. Penczek, A. Leith, and J. Frank. A method for differentiating proteins from nucleic acids in intermediate-resolution density maps: Cryo-electron microscopy defines the quaternary structure of the *Escherichia coli* 70S ribosome. *Structure*, 8:937–948, 2000.
- [197] D. K. Stammers, D. O’N. Somers, C. K. Ross, I. Kirby, P. H. Ray, J. E. Wilson, M. Norman, J. S. Ren, R. M. Esnouf, E. F. Garman, E. Y. Jones, and D. I. Stuart. Crystals of HIV-1 reverse transcriptase diffracting to 2.2 Å resolution. *J. Mol. Biol.*, 242:586–588, 1994.
- [198] S. D. Stellman, B. Hingerty, S. B. Broyde, E. Subramanian, T. Sato, and R. Langridge. Structure of guanosine-3’, 5’-cytidine monophosphate. I. Semi-empirical potential energy calculations and model-building. *Biopolymers*, 12:1731–2750, 1973.
- [199] T. Strick, J.-F. Allemand, V. Croquette, and D. Bensimon. The manipulation of single biomolecules. *Physics Today*, 54:46–51, October 2001.
- [200] R. S. Struthers, J. Rivier, and A. T. Hagler. Theoretical simulation of conformation, energetics, and dynamics in the design of GnRH analogs. *Trans. Amer. Cryst. Assoc.*, 20:83–96, 1984. Proceedings of the Symposium on Molecules in Motion, University of Kentucky, Lexington, Kentucky, May 20–21, 1984.
- [201] L. Stryer. *Biochemistry*. W. H. Freeman, New York, NY, 5 edition, 2001.
- [202] J. Sulston and G. Ferry. *The Common Thread: A Story of Science, Politics, Ethics and the Human Genome*. Joseph Henry Press, Washington D. C., 2002.
- [203] E. Tajkhorshid, P. Nollert, M. Ø Jensen, L. J. W. Miercke, J. O’Connell, R. M. Stroud, and K. Schulten. Control of the selectivity of the aquaporin water channel family by global orientational tuning. *Science*, 296:525–530, 2002.
- [204] Y. Tao and W. Zhang. Recent developments in cryo-electron microscopy reconstruction of single particles. *Structure*, 10:616–622, 2000.
- [205] D. Thirumalai and G. H. Lorimer. Chaperonin-mediated protein folding. *Ann. Rev. Biophys. Biomol. Struct.*, 30:245–269, 2001.

- [206] J. T. Thomas. The scientific and humane legacy of Max Perutz (1914 – 2002). *Angew. Chem. Int. Ed.*, 41:3155–3166, 2002.
- [207] B. Tidor, K. K. Irikura, B. R. Brooks, and M. Karplus. Dynamics of DNA oligomers. *J. Biomol. Struct. Dynam.*, 1:231–252, 1983.
- [208] J. R. Tolman. Dipolar couplings as a probe of molecular dynamics and structure in solution. *Curr. Opin. Struct. Biol.*, 11:532–539, 2001.
- [209] A. Tramontano. Of men and machines. *Nat. Struct. Biol.*, 10:87–90, 2003.
- [210] P. Uetz, L. Giot, G. Cagney, T. A. Mansfield, R. S. Judson, J. R. Knight, D. Lockshon, V. Narayan, M. Srinivasan, P. Pochart, A. Qureshi-Emili, Y. Li, B. Godwin, D. Conover, T. Kalbfleisch, G. Vijayadamodar, M. Yang, M. Johnston, S. Fields, and J. M. Rothberg. A comprehensive analysis of protein-protein interactions in *Saccharomyces cerevisiae*. *Nature*, 403:623–627, 2000.
- [211] V. M. Unger. Electron cryomicroscopy. *Curr. Opin. Struct. Biol.*, 11:548–554, 2001.
- [212] I. Usón and G. M. Sheldrick. Advances in direct methods for protein crystallography. *Curr. Opin. Struct. Biol.*, 9:643–648, 1999.
- [213] W. F. van Gunsteren, R. Bürgi, C. Peter, and X. Daura. The key to solving the protein-folding problem lies in an accurate description of the denatured state. *Angew. Chem. Int. Ed.*, 40:352–355, 2001.
- [214] W. F. van Gunsteren, R. Bürgi, C. Peter, and X. Daura. Reply. *Angew. Chem. Int. Ed.*, 40:4616–4618, 2001.
- [215] J. Vrebalov, D. Ruezinsky, V. Padmanabhan, R. White, D. Medrano, R. Drake, W. Schuch, and J. Giovannoni. A MADS-box gene necessary for fruit ripening at the tomato ripening-inhibitor (*Rin*) locus. *Science*, 296:343–346, 2002.
- [216] D. M. Walsh, I. Klyubin, J. V. Fadeeva, W. K. Cullen, R. Anwyl, M. S. Wolfe, M. J. Rowan, and D. J. Selkoe. Naturally secreted oligomers of amyloid  $\beta$  protein potently inhibit hippocampal long-term potentiation *in vivo*. *Nature*, 416:535–539, 2002.
- [217] S. Walter and J. Buchner. Molecular chaperones—Cellular machines for protein folding. *Angew. Chem. Int. Ed.*, 41:1098–1113, 2002.
- [218] W. Wang, O. Donini, C. M. Reyes, and P. A. Kollman. Biomolecular simulations: Recent developments in force fields, simulations of enzyme catalysis, protein-ligand, protein-protein, and protein-nucleic acid noncovalent interactions. *Ann. Rev. Biophys. Biomol. Struct.*, 30:211–243, 2001.
- [219] R. H. Waterston, E. S. Lander, and J. E. Sulston. On the sequencing of the human genome. *Proc. Natl. Acad. Sci. USA*, 99:3712–3716, 2002.
- [220] J. Wehrle and D. Barrick. Review of the fifth annual Johns Hopkins protein folding meeting. *Proteins: Struct. Func. Gen.*, 42:141–147, 2001.
- [221] J. J. Wendoloski, S. J. Kimatian, C. E. Schutt, and F. R. Salemme. Molecular dynamics simulation of a phospholipid micelle. *Science*, 243:636–638, 1989.
- [222] B. Werth. *The Billion-Dollar Molecule: One Company's Quest for the Perfect Drug*. Simon & Schuster, New York, NY, 1994.
- [223] H. Wille, M. D. Michelitsch, V. Guénebaut, S. Supattapone, A. Serban, F. E. Cohen, D. A. Agard, and S. B. Prusiner. Structural studies of the scrapie prion protein by electron crystallography. *Proc. Natl. Acad. Sci. USA*, 99:3563–3568, 2002.

- [224] J. R. Williamson. Small subunit, big science. *Nature*, 407:306–307, 2000.
- [225] E. O. Wilson. *Consilience. The Unity of Knowledge*. Alfred A. Knopf, New York, NY, 1998.
- [226] M. Wilson, J. DeRisi, H. H. Kristensen, P. Imboden, S. Rane, P. O. Brown, and G. K. Schoolnik. Exploring drug-induced alterations in gene expression in *Mycobacterium tuberculosis* by microarray hybridization. *Proc. Natl. Acad. Sci. USA*, 96:12833–12838, 1999.
- [227] B. T. Wimberly, D. E. Brodersen, W. M. Clemons Jr., R. J. Morgan-Warren, A. P. Carter, C. Vornrhein, T. Hartsch, and V. Ramakrishnan. Structure of the 30S ribosomal subunit. *Nature*, 407:327–339, 2000.
- [228] P. G. Wolynes. Folding funnels and energy landscapes of larger proteins within the capillarity approximation. *Proc. Natl. Acad. Sci. USA*, 94:6170–6175, 1997.
- [229] K. Wong. The mammals that conquered the seas. *Sci. Amer.*, 286:70–79, 2002.
- [230] P. E. Wright and H. J. Dyson. Intrinsically unstructured proteins: Reassessing the protein structure-function paradigm. *J. Mol. Biol.*, 293:321–331, 1999.
- [231] K. Wüthrich. *NMR of Proteins and Nucleic Acids*. (The George Fisher Baker Non-Resident Lectureship in Chemistry at Cornell University series). Wiley Interscience, New York, NY, 1986.
- [232] R. Xu, B. Ayers, D. Cowburn, and T. W. Muir. Chemical ligation of folded recombinant proteins: Segmental isotopic labeling of domains for NMR studies. *Proc. Natl. Acad. Sci. USA*, 96:388–393, 1999.
- [233] Z. Xu, A. L. Horwich, and P. B. Sigler. The crystal structure of the asymmetric GroEL-GroES-(ADP)<sub>7</sub> chaperonin complex. *Nature*, 388:741–750, 1997.
- [234] B. I. Yakobson and R. E. Smalley. Fullerene nanotubes: C<sub>1,000,000</sub> and beyond. *American Scientist*, 85(4):324–337, 1997.
- [235] M. A. Young and D. L. Beveridge. Molecular dynamics simulations of an oligonucleotide duplex with adenine tracts phased by a full helix turn. *J. Mol. Biol.*, 281:675–687, 1998.
- [236] H. Yu. Extending the size limit of protein nuclear magnetic resonance. *Proc. Natl. Acad. Sci. USA*, 96:332–334, 1999.
- [237] M. M. Yusupov, G. Zh. Yusupova, A. Baucom, K. Lieberman, T. N. Earnest, J. H. D. Cate, and H. F. Noller. Crystal structure of the ribosome at 5.5 Å resolution. *Science*, 292:883–896, 2001.
- [238] B. Zagrovic, E. J. Sorin, and V. Pande.  $\beta$ -hairpin folding simulations in atomistic detail using an implicit solvent model. *J. Mol. Biol.*, 313:151–169, 2001.
- [239] R. Zahn, A. Liu, T. Lühns, R. Riek, C. von Schroetter, F. López Garcia, M. Billeter, L. Calzolari, G. Wider, and Kurt Wüthrich. NMR solution structure of the human prion protein. *Proc. Natl. Acad. Sci. USA*, 97:145–150, 2000.
- [240] F. N. Zaidi, U. Nath, and J. B. Udgaonkar. Multiple intermediates and transition states during protein unfolding. *Nature Struc. Biol.*, 4:1016–1024, 1997.
- [241] Y. Zhou, J. H. Morais-Cabral, A. Kaufman, and R. MacKinnon. Chemistry of ion coordination and hydration revealed by a K<sup>+</sup> channel-Fab complex at 2.0 Å resolution. *Nature*, 414:43–48, 2001.