

Appendix B

Article Reading List

Before 1970

1. B. J. Alder and T. E. Wainwright, "Studies in Molecular Dynamics. I. General Method", *J. Chem. Phys.* **31**, 459–466 (1959).
2. G. Némethy and H. A. Scheraga, "Theoretical Determination of Sterically Allowed Conformations of a Polypeptide Chain by a Computer Method", *Biopolymers* **3**, 155–184 (1965).

1970s

3. A. Rahman and F. H. Stillinger, "Molecular Dynamics Study of Liquid Water", *J. Chem. Phys.* **55**, 3336–3359 (1971).
4. P. Y. Chou and G. D. Fasman, "Prediction of Protein Conformation", *Biochemistry* **13**, 222–245 (1974).
5. M. Levitt and A. Warshel, "Computer Simulation of Protein Folding", *Nature* **253**, 694–698 (1975).
6. M. Levitt and C. Chothia, "Structural Patterns in Globular Proteins", *Nature* **261**, 552–558 (1976).

1980s

7. S. Lifson, "Potential Energy Functions for Structural Molecular Biology", in *Methods in Structural Molecular Biology*, pp. 359–385, D. B. Davies, W. Saenger, and S. S. Danyluk, Eds., Plenum Press, London (1981).
8. M. Karplus and J. A. McCammon, "The Dynamics of Proteins", *Sci. Amer.* **254**, 42–51 (1986).
9. M. S. Friedrichs and P. G. Wolynes, "Toward Protein Tertiary Structure Recognition by Means of Associative Memory Hamiltonians", *Science* **246**, 371–373 (1989).
10. I. K. Roterman, M. H. Lambert, K. D. Gibson, and H. A. Scheraga, "Comparison of the CHARMM, AMBER and ECEPP Potentials for Peptides. I. Conformational Predictions for the Tandemly Repeated Peptide (Asn-Ala-Asn-Pro)₉", *J. Biomol. Struct. Dyn.* **7**, 391–419 (1989a).
11. I. K. Roterman, M. H. Lambert, K. D. Gibson, and H. A. Scheraga, "Comparison of the CHARMM, AMBER and ECEPP Potentials for Peptides. II. ϕ - ψ Maps

for N-Methyl Amide: Comparisons, Contrasts and Simple Experimental Tests”, *J. Biomol. Struct. Dyn.* **7**, 421–453 (1989b).

1990–1992

12. M. Karplus and G. A. Petsko, “Molecular Dynamics Simulations in Biology”, *Nature* **347**, 631–639 (1990).
13. J. Skolnick and A. Kolinski, “Simulations of the Folding of a Globular Protein”, *Science* **250**, 1121–1125 (1990).
14. F. M. Richards, “The Protein Folding Problem” *Sci. Amer.* **264**, 54–63 (1991).
15. P. A. Kollman and K. A. Dill, “Decisions in Force Field Development: An Alternative to Those Described by Roterman *et al.*”, *J. Biomol. Struct. Dyn.* **8**, 1103–1107 (1991).
16. K. B. Gibson and H. A. Scheraga”, “Decisions in Force Field Development: Reply to Kollman and Dill”, *J. Biomol. Struct. Dyn.* **8**, 1109–1111 (1991).
17. H. A. Scheraga, “Predicting Three-Dimensional Structures of Oligopeptides”, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Editors, Vol. 3, pp. 73–142, VCH Publishers, New York (1992).
18. T. Schlick, “Optimization Methods in Computational Chemistry”, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Editors, Vol. 3, pp. 1–71, VCH Publishers, New York (1992). See also T. Schlick, “Geometry Optimization”, in the *Encyclopedia of Computational Chemistry*, P. von Ragué Schleyer (Editor-in-Chief) and N. L. Allinger and T. Clark and J. Gasteiger and P. A. Kollman and Schaefer, III, H. F., Editors, Vol. 3, pp. 1136–1157, John Wiley & Sons, West Sussex, England (1998).

1993–1995

19. R. A. Abagyan and M. M. Totrov, “Biased Probability Monte Carlo Conformational Searches and Electrostatic Calculations for Peptides and Proteins”, *J. Mol. Biol.* **235**, 983–1002 (1994).
20. J. A. Board, Jr., L. V. Kalé, K. Schulten, R. D. Skeel, and T. Schlick, “Modeling Biomolecules: Larger Scales, Longer Durations”, *IEEE Comp. Sci. Eng.* **1**, 19–30 (Winter 1994).
21. K. B. Lipkowitz, “Abuses of Molecular Mechanics. Pitfalls to Avoid”, *J. Chem. Educ.* **72**, 1070–1075 (1995).
22. B. Honig and A. Nicholls, “Classical Electrostatics in Biology and Chemistry”, *Science* **268**, 1144–1149 (1995).

1996–1998

23. B. Cipra, “Computer Science Discovers DNA”, in *What’s Happening in the Mathematical Sciences*, pp. 26–37 (P. Zorn, Ed.), American Mathematical Society, Colonial Printing, Cranston, RI (1996).
24. A. Neumaier, “Molecular Modeling of Proteins and Mathematical Prediction of Protein Structure”, *SIAM Review* **39**, 407–460 (1997).

25. K. A. Dill and H. S. Chan, "From Levinthal to Pathways to Funnels", *Nature Struct. Biol.* **4**, 10–19 (1997).
 26. T. Lazaridis and M. Karplus, " 'New View' of Protein Folding Reconciled with the Old Through Multiple Unfolding Simulations", *Science* **278**, 1928–1931 (1997).
 27. T. Schlick, E. Barth, and M. Mandziuk, "Biomolecular Dynamics at Long Time-steps: Bridging the Timescale Gap Between Simulation and Experimentation", *Ann. Rev. Biophys. Biomol. Struct.* **26**, 179–220 (1997).
 28. E. Barth and T. Schlick, "Overcoming Stability Limitations in Biomolecular Dynamics: I. Combining Force Splitting via Extrapolation with Langevin Dynamics in LN", *J. Chem. Phys.* **109**, 1617–1632 (1998).
 29. M. Gerstein and M. Levitt, "Simulating Water and the Molecules of Life", *Sci. Amer.* **279**, 101–105 (1998).
 30. 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 (1998).
 31. H. J. C. Berendsen, "A Glimpse of the Holy Grail", *Science* **282**, 642–643 (1998).
 32. L. S. D. Caves, J. D. Evanseck, and M. Karplus, "Locally Accessible Conformations of Proteins: Multiple Molecular Dynamics Simulations of Crambin", *Prot. Sci.* **7**, 649–666 (1998).
 33. W. F. van Gunsteren and A. E. Mark, "Validation of Molecular Dynamics Simulation", *J. Chem. Phys.* **108**, 6109–6116 (1998).
 34. X. Daura, B. Juan, 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).
- 1999–2003
35. A. L. Delcher, S. Kasif, R. D. Fleischmann, J. Peterson, O. White, and S. L. Salzberg, "Alignment of Whole Genomes", *Nuc. Acids Res.* **27**, 2369–2376 (1999).
 36. D. Baker and A. Sali, "Protein Structure Prediction and Structural Genomics", *Science* **294**, 93–96 (2001).
 37. R. Bonneau and D. Baker, "Ab Initio Protein Structure Prediction: Progress and Prospects", *Annu. Rev. Biophys. Struct.* **30**, 173–189 (2001).
 38. J. C. Whisstock and A. M. Lesk, "Prediction of Protein Function from Protein Sequence and Structure", *Quart. Rev. Biophys.* **36**, 173–189 (2001).
 39. H. Kitano, "Systems Biology: A Brief Overview", *Science* **295**, 1662–1664 (2002).
 40. R. M. Karp, "Mathematical Challenges from Genomics and Molecular Biology", *Notices Amer. Math. Soc.* **49**, 544–553 (2002).
 41. M. Karplus and J. A. McCammon, "Molecular Dynamics simulations of Biomolecules", *Nat. Struct. Biol.* **9**, 307–340 (2003).
 42. J. Norberg and L. Nilsson, "Advances in Biomolecular Simulations: Methodology and Applications", *Quart. Rev. Biophys.* **36**, 257–306 (2003).

43. J. D. Storey and R. Tibshirani, "Statistical Significance for Genomewide Studies", *Proc. Natl. Acad. Sci. USA* **100**, 9440–9445 (2003).
 44. F. S. Collins, E. D. Green, A. E. Guttmacher, and M. S. Guyer, "A Vision for the Future of Genomics Research", *Nature* **422**, 835–847 (2003).
 45. T. Ideker and D. Lauffenburger, "Building with a Scaffold: Emerging Strategies for High- to Low-Level Cellular Modeling", *Trends Biotech.* **21**: 255–262 (2003).
 46. R. Jansen, H. Yu, D. Greenbaum, Y. Kluger, N. J. Krogan, S. Chung, A. Emili, M. Snyder, J. F. Greenblatt, and M. Gerstein, "A Bayesian Networks Approach for Predicting Protein-Protein Interactions from Genomic Data", *Science* **17**, 449–453 (2003).
- 2004–
47. J. E. Cohen, "Mathematics is Biology's Next Microscope, Only Better; Biology is Mathematics' Next Physics, Only Better", *PLoS Biology* **2** (e439), 2017–2023 (2004).
 48. M. Kellis, N. Patterson, B. Birren, B. Berger, and E. S. Lander, "Methods in Comparative Genomics: Genome Correspondence, Gene Identification and Regulatory Motif Discovery", *J. Comp. Biol.* **11**, 319–355 (2004).
 49. W. C. Winkler, A. Nahvi, A. Roth, J. A. Collins and R. R. Breaker, "Control of Gene Expression by a Natural Metabolite-Responsive Ribozyme", *Nature* **428**, 281–286 (2004).
 50. A. Hastings et al., "Quantitative Bioscience for the 21st Century", *Bioscience* **55**, 511–517 (2005).
 51. J. C. Phillips, R. Braun, W. Wang, J. Gumbart, E. Tajkhorshid, E. Villa, C. Chipot, R. D. Skeel, L. Kalé and K. Schulten, "Scalable Molecular Dynamics with NAMD", *J. Comp. Chem.* **26**, 1781–1802 (2005).
 52. T. Schlick, "The Critical Collaboration Between Art and Science: Applying *An Experiment on a Bird in an Air Pump* to the Ramifications of Genomics on Society", *Leonardo* **38** (4), 323–329 (2005).
 53. M. Karplus and J. Kuriyan, "Molecular Dynamics and Protein Function", *Proc. Natl. Acad. Sci. USA* **102**, 6679–6685 (2005).
 54. W. F. van Gunsteren et al., "Biomolecular Modeling: Goals, Problems, Perspectives", *Angew. Chem. Int. Ed.* **45**, 4064–4092 (2006).
 55. E. Segal, Y. Fondufe-Mittendorf, L. Chen, A. Thåström, Y. Field, I. K. Moore, J.-P. Z. Wang, and J. Widom, "A Genomic Code for Nucleosome Positioning", *Nature* **442**, 772–778 (2006).
 56. J.-M. Chandonia and S. E. Brenner, "The Impact of Structural Genomics: Expectations and Outcomes", *Science* **311**, 347–351 (2006).
 57. S. A. Adcock and J. A. McCammon, "Molecular dynamics: survey of methods for simulating the activity of proteins", *Chem. Rev.* **106**: 1589–1615 (2006).
 58. M. A. Gerstein et al., "What is a Gene, post ENCODE? History and Updated Definition", *Genome Research* **17**, 669–681 (2007).

59. E. H. Lee, J. Hsin, M. Sotomayor, G. Comellas, and K. Schulten, “Discovery Through the Computational Microscope”, *Structure* **17**: 1295–1306 (2009).