

July, 2023

## CURRICULUM VITAE

### Richard W. Pastor, Ph.D.

Address: Laboratory of Membrane Biophysics  
National Heart, Lung and Blood Institute,  
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Date of Birth: June 21, 1951

Citizenship: United States

Education:

1984	Ph.D. Harvard University, Biophysics Dissertation Title: <i>Topics in Stochastic Dynamics of Polymers.</i> Preceptor: Martin Karplus
1977	M.S. Syracuse University, Chemistry Thesis Title: <i>Surface Tension Calculations for Molten Salts: Critique and Modification of the Kirkwood-Buff Model</i> Preceptor: Jerry Goodisman
1973	B.A. Hamilton College, Major in Philosophy

Employment:

2017-present	Chief, Laboratory of Membrane Biophysics, NHLBI/NIH
2006-2016	Principal Investigator, Laboratory of Computational Biology, NHLBI/NIH
1996-2006	Chief, Biophysics Laboratory, CBER/FDA
1998	Acting Chief, Laboratory of Immunobiochemistry, CBER/FDA
1990-1996	Research Chemist, Biophysics Lab, CBER/FDA
1984-1990	Senior Staff Fellow, Biophysics Lab, CBER/FDA
1984	Staff Fellow, Laboratory of Chemical Physics, National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health

Awards:

2021	<i>Avanti Award in Lipids</i> Biophysical Society
2019	<i>Orloff Award (Basic Science)</i> National Heart Lung Blood Institute
2013	<i>Director's Outstanding Basic Science Award</i> National Heart Lung Blood Institute
1997	<i>Center Director's Public Health Achievement Award</i> Center for Biologics Evaluation and Research
1996	<i>Scientific Achievement - Senior Investigator</i> Center for Biologics Evaluation and Research

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1996 *Excellence in Science by a Group*  
Food and Drug Administration

Research Area: The application of computer simulations and statistical mechanics to biophysics, with emphasis on membranes.

Scientific Review: Reviewer for numerous journals, including *Biophysical Journal*, *Journal of the American Chemical Society*, *Journal of Physical Chemistry*, *Journal of Chemical Physics*, *Journal of Computational Chemistry*, *Nature Communications*, and *Proceedings of the National Academy of Science*.

Guest editor for *Biophysical Journal*, and *PNAS*.

Ad Hoc reviewer for NIH (Biochemistry and Biophysics of Membranes Study Section, postdoctoral fellowships), NSF and PRF.

**Publications** (h=68, 34,000+ citations, Google Scholar, July 2023)

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2. Resonance Raman Studies of Macrocyclic Complexes. 2. Antiresonance and Selective Intensity Enhancement in Synthetic Metal (II) Porphrin Analogues, L.A. Nafie, R.W. Pastor, J.C. Dabrowiak, and W.H. Woodruff, *J. Am. Chem. Soc.* **98**, 8007-8014 (1976).
3. Surface Tension Calculations for Molten Salts: Critique and Modification of the Kirkwood-Buff Model, R.W. Pastor and J. Goodisman, *J. Chem. Phys.* **68**, 3654-3666 (1978).
4. A Model for the Surface of a Molten Salt, J. Goodisman and R.W. Pastor, *J. Phys. Chem.* **82**, 2078-2081 (1978).
5. A Recognition Site in Synthetic Helical Oligonucleotides for Monoclonal Anti-Native DNA Autoantibody, David Stollar, Gerald Zon, and Richard W. Pastor, *Proc. Natl. Acad. Sci. USA* **83**, 4469-2273 (1986).
6. Local Sequence Patterns of Hydrophobicity and Solvent Accessibility in Soluble Globular Proteins, David J. Lipman, Richard W. Pastor, and B. Lee, *Biopolymers* **26**, 17-26 (1987).
7. A Theoretically Determined Three-Dimensional Structure for the Repeating Tetrapeptide Unit of the Circumsporozoite Coat Protein of the Malaria Parasite *Plasmodium falciparum*, Bernard R. Brooks, Richard W. Pastor, and Frederick W. Carson, *Proc. Natl. Acad. Sci. USA* **84**, 4470-4474 (1987).
8. The Parametrization of the Friction Constant for Stochastic Simulations of Polymers, Richard W. Pastor and Martin Karplus, *J. Phys. Chem.* **92**, 2636-2641 (1988).
9. Frictional Models for Stochastic Simulations of Proteins, Richard M. Venable and Richard W. Pastor, *Biopolymers* **27**, 1001-1014 (1988).
10. Brownian Dynamics Simulation of a Lipid Chain in a Membrane Bilayer, Richard W. Pastor, Richard M. Venable, and Martin Karplus, *J. Chem. Phys.* **89**, 1112-1127 (1988).
11. A Simulation Based Model of NMR  $T_1$  Relaxation in Lipid Bilayer Vesicles, Richard W. Pastor, Richard M. Venable, Martin Karplus, and Attila Szabo, *J. Chem. Phys.* **89**, 1128-1140 (1988).

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12. An Analysis of the Accuracy of Langevin and Molecular Dynamics Algorithms, Richard W. Pastor, Bernard R. Brooks, and Attila Szabo, *Mol. Phys.* **65**, 1409-1419 (1988).
13. Theoretically Determined Three-Dimensional Structures for Amphipathic Segments of the HIV-1 gp41 Envelope Protein, Richard M. Venable, Richard W. Pastor, Bernard R. Brooks, and Frederick W. Carson, *AIDS Research and Human Retroviruses* **5**, 7-21 (1989).
14. Anisotropic Bead Models for Molecular Hydrodynamics, Richard W. Pastor and Robert Zwanzig, *J. Chem. Phys.* **90**, 5729-5734 (1989).
15. Inertial Effects in Butane Stochastic Dynamics, Richard W. Pastor and Martin Karplus, *J. Chem. Phys.* **91**, 211-218 (1989).
16. Determination of Chain Conformations in the Membrane Interior by Brownian Dynamics Simulations, Richard W. Pastor, in *Molecular Description of Biological Membrane Components by Computer Aided Conformational Analysis*, Vol. I, (ed. R. Brasseur, CRC Press, Boca Raton, 1990), pp. 171-201.
17. Model for the Structure of the Lipid Bilayer, Richard W. Pastor, Richard M. Venable, and Martin Karplus, *Proc. Natl. Acad. Sci. USA* **88**, 892-896 (1991).
18. Mean Field Stochastic Boundary Molecular Dynamics Simulation of a Phospholipid in a Membrane, Hans De Loof, Stephen C. Harvey, Jere P. Segrest, and Richard W. Pastor, *Biochemistry* **30**, 2099-2113 (1991).
19. Molecular Dynamics Simulation of Methyl Group Relaxation in Water, Goran Widmalm, Richard W. Pastor and Thomas E. Bull, *J. Chem. Phys.* **94**, 4097-4098 (1991).
20. Analyses of Statistical Errors in Dynamics Simulations, Richard W. Pastor, in *Proteins: Structure, Dynamics, Design* (ed. V. Renugopalakrishnan, P.R. Carey, I.C.P. Smith, S.G. Huang, and A.C. Storer, ESCOM Science Publishers, The Netherlands, 1991), pp. 229-233.
21. Synexin: Molecular Mechanism of Calcium-Dependent Membrane Fusion and Voltage-Dependent Calcium Channel Activity, Harvey B. Pollard, Eduardo Rojas, Richard W. Pastor, Eduardo M. Rojas, H. Robert Guy, and A. Lee Burns, *Ann. New York Acad. Sci.* **635**, 328-351 (1991).
22. Langevin Dynamics of Peptides: the Frictional Dependence of Isomerization Rates of N-Acetylalanyl-N'-Methylamide, Richard J. Loncharich, Bernard R. Brooks, and Richard W. Pastor, *Biopolymers* **32**, 523-535 (1992).
23. Backbone Dynamics of Calmodulin Studied by <sup>15</sup>N Relaxation Using Inverse Detected Two-Dimensional NMR Spectroscopy: The Central Helix is Flexible, Gaetano Barbato, Mitsuhiro Ikura, Lewis E. Kay, Richard W. Pastor, and Ad Bax, *Biochemistry* **31**, 5269-5278 (1992).
24. Conformational States of a TT Mismatch from Molecular Dynamics Simulation of d(CGCGATTCGCG), Richard M. Venable, Goran Widmalm, Bernard R. Brooks, William Egan, and Richard W. Pastor, *Biopolymers* **32**, 783-794 (1992).
25. A Comparison of Langevin and Molecular Dynamics Simulations: Equilibrium and Dynamics of Ethylene Glycol in Water, Goran Widmalm and Richard W. Pastor, *J. Chem. Soc. Faraday Trans.* **88**, 1747-1754 (1992).
26. Langevin Dynamics of a Linear Rotor in a Maier-Saupe Potential: Kramers Turnover of the Flipping Rate, Richard W. Pastor and Attila Szabo, *J. Chem. Phys.* **97**, 5098-5100 (1992).
27. Positional Time Correlation Function for One-Dimensional Systems with Barrier Crossing: Memory Function Corrections to the Optimized Rouse-Zimm Approximation, Angelo Perico, Roberto Pratolongo, Karl F. Freed, Richard W. Pastor, and Attila Szabo, *J. Chem. Phys.* **98**, 564-573 (1993).

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28. Molecular Dynamics Simulations of a Lipid Bilayer and of Hexadecane: An Investigation of Membrane Fluidity, Richard M. Venable, Yuhong Zhang, Barry J. Hardy, and Richard W. Pastor, *Science* **262**, 223-226 (1993).
29. Molecular and Stochastic Dynamics Simulation of Lipid Membranes, Richard W. Pastor and Richard M. Venable, in *Computer Simulation of Biomolecular Systems: theoretical and experimental applications* (ed. Wilfred F. van Gunsteren, Paul K. Weiner, and Anthony K. Wilkinson, ESCOM Science Publishers, Leiden, 1993), pp. 443-463.
30. Conformational Sampling of Hydrocarbon and Lipid Chains in an Ordering Potential, Barry J. Hardy, and Richard W. Pastor, *J. Comput. Chem.* **15**, 208-226 (1994).
31. A Comparison of Methods for Computing Transition Rates from Molecular Dynamics Simulation, Yuhong Zhang and Richard W. Pastor, *Molecular Simulation*, **13**, 25-38 (1994).
32. Techniques and Applications of Langevin Dynamics Simulations, Richard W. Pastor, in *The Molecular Dynamics of Liquid Crystals* (eds. G.R. Luckhurst and C.A. Veracini, Kluwer Academic Publishers, The Netherlands, 1994), pp. 85-138.
33. Molecular Dynamics and Monte Carlo Simulations of Lipid Bilayers, Richard W. Pastor, *Current Opinion in Structural Biology* **4**, 486-492 (1994).
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35. Constant Pressure Molecular Dynamics Simulation: The Langevin Piston Method, Scott E. Feller, Yuhong Zhang, Richard W. Pastor, and Bernard R. Brooks, *J. Chem. Phys.* **103**, 4613-4621 (1995).
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40. Time Scales of Lipid Dynamics and Molecular Dynamics, Richard W. Pastor and Scott E. Feller, in *Membrane Structure and Dynamics* (ed. K.M. Merz and B. Roux, Birkhauser, Boston, 1996), pp. 3-29.
41. On Simulating Lipid Bilayers with an Applied Surface Tension: Periodic Boundary Conditions and Undulations, Scott E. Feller and Richard W. Pastor, *Biophysical Journal* **71**, 1350-1355 (1996).
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45. Molecular Dynamics Simulation of Unsaturated Lipid Bilayers at Low Hydration: Parametrization and Comparison with Diffraction Studies, Scott E. Feller, Daxu Yin, Richard W. Pastor, and Alexander D. MacKerell, Jr. *Biophysical Journal*, **73**, 2269-2279 (1997).
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48. Solution Structure of the Linked Cell Attachment Modules of Mouse Fibronectin Containing the RGD and Synergy Regions: Comparison with the Human Fibronectin Crystal Structure, Valerie Copie, York Tomita, Steven K. Akiyama, Shin-ichi Aota, Kenneth M. Yamada, Richard M. Venable, Richard W. Pastor, Susan Krueger, and Dennis A. Torchia, *J. Mol. Biol.* **277**, 663-682 (1998).
49. Constant Surface Tension Simulations of Lipid Bilayers: The Sensitivity of Surface Areas and Compressibilities, Scott E. Feller, and Richard W. Pastor, *J. Chem. Phys.* **111**, 1281-1287 (1999).
50. Distinguishing Anisotropy and Flexibility of the Pentasaccharide LNF-1 in Solution by Carbon-13 NMR Relaxation and Hydrodynamic Modeling, Torgny Rundlöf, Richard M. Venable, Richard W. Pastor, Jozef Kowalewski, and Göran Widmalm, *J. Am. Chem. Soc.* **121**, 11847-11854 (1999).
51. Statistical Considerations in the Establishment of Release Criteria for Allergen Vaccines, Jay E. Slater, Albert A. Gam, Maneesha D. Solanki, Suzann H. Burk, Faith M. May, and Richard W. Pastor in *Proceedings of the 1999 Paul Ehrlich Symposium*, (ed. R. Kurth and D. Haustein, GIT VERLAG, Darmstadt, 2000), pp. 47-56.
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54. Molecular Dynamics Simulations of Gel ( $L_{\beta 1}$ ) Phase Lipid Bilayers in Constant Pressure and Constant Surface Tension Ensembles, Richard M. Venable, Bernard R. Brooks, and Richard W. Pastor, *J. Chem. Phys.* **112**, 4822-4832 (2000).
55. Molecular Dynamics Simulations of Octyl Glucoside Micelles: Structural Properties, Stephen Bogusz, Richard M. Venable, and Richard W. Pastor, *J. Phys. Chem. B* **104**, 5462-5470 (2000).
56. ICAM-1 Enhances MHC-peptide Activation of CD8<sup>+</sup> T-cells without an Organized Immunological Synapse, Julia S. Goldstein, Trina Chen, Elena Gubina, Richard W. Pastor, and Steven Kozlowski, *European J. Immunology*, **30**, 3266-3279 (2000).
57. Molecular Dynamics Simulations of Octyl Glucoside Micelles: Dynamic Properties, Stephen Bogusz, Richard M. Venable, and Richard W. Pastor, *J. Phys. Chem. B* **105**, 8312-8321 (2001).
58. Molecular Dynamics Simulations of Water Wires and Water/Octane Model Systems, Richard M. Venable, and Richard W. Pastor, *J. Chem. Phys.* **116**, 2663-2664 (2002).
59. Simulations of Membranes and Other Interfacial Systems Using P2<sub>1</sub> and P<sub>6</sub> Periodic Boundary Conditions, Elizabeth A. Dolan, Richard M. Venable, Richard W. Pastor, and Bernard R. Brooks, *Biophysical Journal* **85**, 2317-2325 (2002).
60. Lipid Bilayers, NMR Relaxation, and Computer Simulations, Richard W. Pastor, Richard M. Venable, and Scott E. Feller, *Accounts of Chemical Research* **35**, 438-446 (2002).

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61. Micelle-Bound Conformation of a Hairpin-Forming Peptide: A Combined NMR and Molecular Dynamics Study, Ann M. Dixon, Richard M. Venable, Richard W. Pastor, and Thomas E. Bull, *Biopolymers* **65**, 284-298 (2002).
62. Application of NMR, Molecular Simulation and Hydrodynamics to Conformational Analysis of Trisaccharides, Ann M. Dixon, Richard M. Venable, Göran Widmalm, Thomas E. Bull, and Richard W. Pastor, *Biopolymers* **69**, 448-460 (2003).
63. Sample Size Considerations for Establishing Clinical Bioequivalence of Allergen Formulations, Ronald L. Rabin, Jay E. Slater, Peter Lachenbruch, and Richard W. Pastor in *Proceedings of the 2002 Paul Ehrlich Symposium*, (ed. J. Lower, W. Becker and S. Vieths, Druck und Verlagshaus Sperllich, Frankfurt, 2003), pp. 24-33.
64. A Pressure-Based Long-Range Correction for Lennard Jones Interactions In Molecular Dynamics Simulations: Application To Alkanes and Interfaces, Patrick Lague, Richard W. Pastor, Bernard Brooks, *J. Phys. Chem. B* **108**, 363-368 (2004).
65. Discriminating the Helical Forms of Peptides by NMR and Molecular Dynamics Simulation, Darón I. Freedberg, Richard M. Venable, Angelo Rossi, Thomas E. Bull, and Richard W. Pastor, *J. Am. Chem. Soc.* **126**, 10478-10484 (2004).
66. An Ab Initio Study on the Torsional Surface of Alkanes and its Effect on Molecular Simulations of Alkanes and a DPPC Bilayer, Jeffery B. Klauda, Bernard R. Brooks, Alexander D. MacKerell, Jr., Richard M. Venable, and Richard W. Pastor, *J. Phys. Chem. B.* **109**, 5300-5311 (2005).
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69. Molecular Dynamics Simulations of the Influenza Hemagglutinin Fusion Peptide in Micelles and Bilayers: Conformational Analysis of Peptide and Lipids. Patrick Lagüe, Benoît Roux, and Richard W. Pastor, *J. Mol. Biol.*, **354**, 1129-1141 (2005).
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71. Simulation-based Methods for Interpreting X-ray Data from Lipid Bilayers, Jeffery B. Klauda, Norbert Kučerka, Bernard R. Brooks, Richard W. Pastor, and John F. Nagle, *Biophysical Journal*, **90**, 2796-2807 (2006).
72. Constant Surface Tension Molecular Dynamics Simulations of Lipid Bilayers with Trehalose, Richard M. Venable, Anna Skibinsky, and Richard W. Pastor, *Molecular Simulation*, **32**, 849-855 (2006).
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74. Long-range Lennard-Jones and Electrostatic Interactions in Interfaces: Application of the Isotropic Periodic Sum Method, Jeffery B. Klauda, Xiongwu Wu, Richard W. Pastor, and Bernard R. Brooks, *J. Phys. Chem., B*, **111**, 4393-4400 (2007).
75. Additive and Classical Drude Polarizable Force Fields for Linear and Cyclic Ethers, Igor Vorobyov, Victor M. Anisimov, Shannon Greene, Richard M. Venable, Adam Moser, Richard W. Pastor, and Alexander D. MacKerell, Jr., *J. Chemical Theory and Computation*, **3**, 1120-1133 (2007).

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77. Rotation of Lipids in Membranes: MD Simulation,<sup>31</sup>P Spin-Lattice Relaxation, and Rigid-Body Dynamics, Jeffrey B. Klauda, Mary F. Roberts, Alfred G. Redfield, Bernard R. Brooks, and Richard W. Pastor, *Biophysical Journal*, **94**, 3074-3083 (2008).
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83. Additive Empirical Force Field for Hexopyranose Monosaccharides, Olgun Guvench, Shannon N. Greene, Ganesh Kamath, John W. Brady, Richard M. Venable, Richard W. Pastor, and Alexander D. MacKerell, Jr., *J. Comp. Chem.*, **29**, 2543-2564 (2008).
84. Structure and Dynamics of Helix-0 of the N-BAR Domain in Lipid Micelles and Bilayers, Christian Löw, Ulrich Weininger, Hwanky Lee, Kristian Schweimer, Ines Neundorf, Annette G. Beck-Sickinger, Richard W. Pastor, and Jochen Balbach, *Biophysical Journal*, **95**, 4315-4323 (2008).
85. Comparison of the Extended Isotropic Periodic Sum and Particle Mesh Ewald Methods for Simulations of Lipid Bilayers and Monolayers, Richard M. Venable, Linda E. Chen, and Richard W. Pastor, *J. Phys. Chem. B.*, **113**, 5855-5862 (2009).
86. CHARMM: The Biomolecular Simulation Program, B.R. Brooks, C.L. Brooks III, A.D. MacKerell, Jr., L. Nilsson, R.J. Petrella, B. Roux, Y. Won, G. Archontis, C. Bartels, S. Boresch, A. Caffisch, L. Caves, Q. Cui, A.R. Dinner, M. Feig, S. Fischer, J. Gao, M. Hodoscek, W. Im, K. Kuczera, T. Lazaridis, J. Ma, V. Ovchinnikov, E. Paci, R.W. Pastor, C.B. Post, J.Z. Pu, M. Schaefer, B. Tidor, R. M. Venable, H. L. Woodcock, X. Wu, W. Yang, D.M. York, and M. Karplus, *J. Comp. Chem.*, **30**, 1545-1614 (2009).
87. Molecular Dynamics Simulations of PIP<sub>2</sub> and PIP<sub>3</sub> in Lipid Bilayers: Determination of Ring Orientation, and the Effects of Surface Roughness on a Poisson-Boltzmann Description, Zheng Li, Richard M. Venable, Laura A. Rogers, Diana Murray, and Richard W. Pastor, *Biophysical Journal*, **97**, 155-163 (2009).
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89. A Coarse-Grained Model for Polyethylene Oxide and Polyethylene Glycol: Conformation and Hydrodynamics, Hwanky Lee, Alex H. de Vries, Siewert-Jan Marrink, and Richard W. Pastor, *J. Phys. Chem. B.*, **113**, 13186-13194 (2009).

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96. A coarse-grained model for PEGylated lipids: the effect of PEGylation on size and shape of self-assembled structures, Hwankyu Lee, and Richard W. Pastor, *J. Phys. Chem. B.*, **115**, 7830-7837 (2011).
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