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# CURRICULUM VITAE

## Richard W. Pastor, Ph.D.


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Date of Birth: June 21, 1951

Citizenship: United States

Education:

1984 Ph.D. Harvard University, Biophysics
Dissertation Title: *Topics in Stochastic Dynamics of Polymers.*
Preceptor: Martin Karplus

1977 M.S. Syracuse University, Chemistry
Thesis Title: *Surface Tension Calculations for Molten Salts: Critique and Modification of the Kirkwood-Buff Model*
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 *Avanti Award in Lipids*
Biophysical Society

2019 *Orloff Award* (Basic Science)
National Heart Lung Blood Institute

2013 *Director's Outstanding Basic Science Award*
National Heart Lung Blood Institute

1997 *Center Director's Public Health Achievement Award*
Center for Biologics Evaluation and Research

1996 *Scientific Achievement - Senior Investigator*
Center for Biologics Evaluation and Research

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 *Biochemistry*

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

**Publications**


1. Resonance Raman Studies of Macrocyclic Complexes. 1. Structural and Electronic Effects in Synthetic Metal (II) Porphrin Analogues. W.H. Woodruff, R.W. Pastor and J.C. Dabrowiak, *J. Am. Chem. Soc.* **98**, 7999-8006 (1976).

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).

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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).

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.

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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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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).

67. Adjacent Gauche Stabilization in Linear Alkanes: Implications for Polymer Models and Conformational Analysis, Jeffery B. Klauda, Richard W. Pastor, and Bernard R. Brooks, *J. Phys. Chem B.* **109**, 16584-15686 (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).

70. Importance of the CMAP Correction to the CHARMM22 Protein Force Field. Dynamics of Hen Lysozyme, Matthias Buck, Sabine Bouguet-Bonnet, Richard W. Pastor, and Alexander D. MacKerell, Jr, *Biophysical Journal*, **90**, L36-L38 (2006).

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Mondragon-Ramirez, Igor Vorobyov, Alexander D. MacKerell, Jr., and Richard W. Pastor, *J. Phys. Chem. B.,***114**, 7830-7843 (2010).

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