

Benoît Roux

PROFESSIONAL ADDRESS:

Weill Medical College of Cornell University
Departments of Biochemistry and Physiology
1300 York Avenue
New York, NY 10021
Phone: (212) 746-6018
Fax: (212) 746-4843
Email: benoit.roux@med.cornell.edu

EDUCATION:

Ph.D. Biophysics. Committee on Higher Degree in Biophysics, Harvard University, Cambridge, MA. Advisor: Professor Martin Karplus. Dissertation title: "*Theoretical Study of Ion Transport in the Gramicidin A Channel*". Degree conferred: June 7, 1990

M.Sc. Biophysics. Physics Department, University of Montreal, Quebec, Canada. Advisor: Professor Rémy Sauvé. Dissertation title: "*Analysis of Patch Clamp Signals*". Degree conferred: September, 1984

B.Sc. Physics. Physics Department, University of Montreal, Québec, Canada. Degree conferred: December, 1981

PROFESSIONAL EXPERIENCE:

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| 1985-1990 | Research assistant in the laboratory of Martin Karplus in the Chemistry Department at Harvard University. |
| Summer 1989 | Visiting Researcher in the laboratory of Richard R. Ernst in the Department of Physical Chemistry at the ETH Zentrum, Zürich. |
| 1991 - 1992 | Invited Researcher in the laboratory of Dr. Jeremy Smith in the: Laboratoire d'Ingénierie des Protéines at the CEA in Saclay, France. |
| 1992 - 1996 | Assistant Professor in the Departments of Physics and Chemistry, Université de Montréal, Canada. |
| 1996 - 1999 | Associate Professor in the Departments of Physics and Chemistry, Université de Montréal, Canada. |
| 1999 | Visiting Professor, in the laboratory of Rod MacKinnon at The Rockefeller University (on sabbatical leave from the Université de Montréal). |
| 1999-present | Professor in the Department of Biochemistry and in the Department of Physiology & Biophysics, Weill Medical College of Cornell University. |

HONORS AND AWARDS:

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| 1998 | Rutherford Medal, The Royal Society of Canada |
| 1998 | Noranda Lecture Award, The Chemical Institute of Canada |
| 1996-1999 | MRC Research Fellow. |
| 1993-present | FRSQ Research Fellow. |
| 1990 | Medical Research Council of Canada, Post-Doctoral Fellowship. |
| 1983-1987 | Medical Research Council of Canada, Doctoral Fellowship. |
| 1986 | FCAR Doctoral Fellowship |
| 1985-1986 | FCAC Doctoral Fellowship |

CURRENT RESEARCH:

Grant NIH-GM 62342-01
Title: *Computational studies of ion channels*
Period January 1st 2001 until December 31st 2004

Grant NSF-0110847
Title: *Free Energy in biomolecular systems: development and application of computational approaches*
Period September 1st 2001 until August 31st, 2004

Grant NIH-CA 93577-01
Title: *Conformational flexibility in activation of Src-kinase*
Period April 1st 2002 until March 31st 2005

Grant Merck Research Laboratory
Title: *Structural models of K-channels/Toxins complexes*
Period 2001

Grant American Heart Association
Title: *Structural models of K-channels/Toxins complexes*
Period July 2002 until June 2005

OTHER ACTIVITIES:

Member of the Biophysical Society since 1985.

Member of the Editorial Board of the *Biophysical Journal* since 1995.

Member of the Editorial Board of *PROTEINS* since 2000.

Permanent member of the BBVA study section at NIH (2001-2005).

One of the current developers of the biomolecular simulation program CHARMM *Accelrys*.

Co-editor of the book "Computational Biochemistry and Biophysics" with Oren Becker, Alex MacKerell and Masa Watanabe (512 pages, including 21 chapters), Marcel Dekker Inc. Publisher (2001).

Co-editor with Thomas Simonson of the Special Issue of *Biophysical Chemistry* **78** (1999). on "Implicit Solvent for Biomolecular Simulations".

Co-editor of the book "Biological Membranes, A Perspective from Computation and Experiment" with Ken Merz, Jr. (587 pages, including 17 chapters), Birkhauser publisher (1996).

LIST OF PUBLICATIONS:

Articles in Refereed Journals

1. B. ROUX, and R. SAUVÉ, "A General Solution to the Time Intervale Omission Applied to Single Channel Analysis", *Biophys. J.* **48**, 149-158 (1985).
2. B. ROUX and M. KARPLUS, "The Normal Modes of the Gramicidin A Dimer", *Biophys. J.* **53**, 297-309 (1987).
3. B. ROUX, H.A. YU and M. KARPLUS, "Molecular Basis for the Born Model of Ion Solvation", *J. Phys. Chem.* **94**, 4683-4688 (1990).
4. H.A. YU, B. ROUX and M. KARPLUS, "Solvation Thermodynamics: An Approach From Analytic Temperature Derivatives", *J. Chem. Phys.* **92**, 5020-5033 (1990).
5. B. ROUX, R. BRÜSCHWEILER and R.R. ERNST, "The Structures of Gramicidin A in Dimethylsulphoxyde/acetone", *Eur. J. Biochem.* **194**, 57-60 (1990).
6. J.E. STRAUB, B.J. BERNE and B. ROUX, "Spatial Dependence of Time-Dependent Friction for Pair Diffusion in a Simple Fluid", *J. Chem. Phys.* **93**, 6804-6812 (1990).
7. B. ROUX and M. KARPLUS, "Ion Transport in a Gramicidin-like Channel: Structure and Thermodynamics", *Biophys. J.* **59**, 961-980 (1991).
8. B. ROUX and M. KARPLUS, "Ion Transport in a Gramicidin-like Channel: Dynamics and Mobility", *J. Phys. Chem.* **95**, 4856-4868 (1991).
9. R. BRÜSCHWEILER, B. ROUX, M. BLACKLEDGE, C. GRIESINGER, M. KARPLUS and R.R. ERNST, "Influence of Rapid Intramolecular Motions on NMR Cross-Relaxation Rates: A Molecular Dynamics Study of Antamanide in Solution", *J. Amer. Chem. Soc.* **114**, 2289-2302 (1992).
10. P. CALMETTES, B. ROUX, D. DURAND, M. DESMADRIL and J.C. SMITH, "Configurational Distribution of Denatured Phosphoglycerate Kinase", *J. Mol. Biol.* **231**, 840-848 (1993).
11. B. ROUX and M. KARPLUS, "Ion Transport in the Gramicidin Channel: Free Energy of the Solvated Right-Handed Dimer in a Model Membrane", *J. Am. Chem. Soc.* **115**, 3250-3262 (1993).
12. A. THOMAS, B. ROUX and J.C. SMITH, "Computer Simulations of the Flexibility of a Series of Synthetic Peptide Analogues", *Biopolymers* **33**, 1249-1270 (1993).
13. M. FERRAND, G. ZACCAI, M. NINA, J.C. SMITH, C. ETCHEBEST and B. ROUX, "Structure and Dynamics of Bacteriorhodopsin - Comparison of Simulation and Experiment", *FEBS* **327**, 256-260 (1993).
14. M. NINA, J.C. SMITH and B. ROUX, "Ab Initio Quantum Chemical Analysis of Water-Schiff Base Interactions in Bacteriorhodopsin", *J. Mol. Struct. (Theochem.)* **286**, 231-245 (1993).
15. B. ROUX, "Nonadditivity in Cation-Peptide Interactions: A Molecular Dynamics and Ab Initio Study of Na⁺ in the Gramicidin Channel", *Chem. Phys. Lett.* **212**, 231-240 (1993).
16. B. ROUX and M. KARPLUS, "Molecular Dynamics Simulations of the Gramicidin Channel", *Ann. Rev. Biomol. Struct. Dyn.* **23**, 731-761 (1994).

17. T.B. WOOLF and B. ROUX, "The Conformational Flexibility of o-Phosphorylcholine and o-Phosphorethanolamine: A Molecular Dynamics Study of Solvation Effects", *J. Amer. Chem. Soc.* **116**, 5916-5926 (1994).
18. D. BEGLOV and B. ROUX, "Finite Representation of an Infinite Bulk System: Solvent Boundary Potential for Computer Simulations", *J. Chem. Phys.* **100**, 9050-9063 (1994).
19. S. CROUZY, T.B. WOOLF and B. ROUX, "Gating of an Ion Channel: A Molecular Dynamics Study of Dioxolane-Linked Gramicidin A Channels", *Biophys. J.* **67**, 1370-1386 (1994).
20. T.B. WOOLF and B. ROUX, "Molecular Dynamics Simulation of the Gramicidin A Channel in a Phospholipid Bilayer", *Proc. Natl. Acad. Sci. USA* **91**, 11631-11635 (1994).
21. M. NINA, B. ROUX and J.C. SMITH, "Functional Interactions in Bacteriorhodopsin: A Theoretical Analysis of Retinal Hydrogen Bonding With Water", *Biophys. J.* **68**, 25-39 (1995).
22. D. BEGLOV and B. ROUX, "Dominant Solvation Effects from Primary Shell of Hydration: Approximation for Molecular Dynamics Simulations", *Biopolymers* **35**, 171-178 (1995).
23. B. ROUX and M. KARPLUS, "Potential Energy Function For Cations-Peptide Interactions: An Ab Initio Study", *J. Comp. Chem.* **16**, 690-704 (1995).
24. B. ROUX, B. PROD'HOM and M. KARPLUS, "Ion Transport in the Gramicidin Channel: Molecular Dynamics Study of Single and Double Occupancy", *Biophys. J.* **68**, 876-892 (1995).
25. R. POMES and B. ROUX, "Quantum Effects on the Structure and Energy of a Protonated Linear Chain of Hydrogen-Bonded Water Molecules", *Chem. Phys. Lett.* **234**, 416-624 (1995).
26. T.B. WOOLF, V. MALKIN, O. MALKIN, D.R. SALAHUB and B. ROUX, "A Molecular Dynamics and Ab Initio Study of the Backbone ^{15}N Chemical Shift Tensor of the Gramicidin Channel. Consequences for Structure Determination by Solid State NMR", *Chem. Phys. Lett.* **239**, 186-194 (1995).
27. B. ROUX, "The Calculation of the Potential of Mean Force Using Computer Simulations", *Comp. Phys. Comm.*, 1-8 (1995).
28. D. BEGLOV and B. ROUX, "Numerical Solution of the HNC Equation for Solute of Arbitrary Geometry in Three-Dimensions", *J. Chem. Phys.* **103**, 360-364 (1995).
29. T.B. WOOLF and B. ROUX, "Molecular Dynamics Simulation of the Gramicidin A Channel in a Phospholipid Bilayer", *PROT: Struc. Funct. Gen.*, **24**, 92-114 (1996).
30. R. POMES and B. ROUX, "Theoretical Study of H^+ Translocation Along a Model Proton Wire", *J. Chem. Phys.* **100**, 2519-2527 (1996).
31. R. POMES and B. ROUX, "Structure and Dynamics of a Proton Wire: A Theoretical Study of H^+ Translocation Along the Single-File Water Chain in the Gramicidin A Channel", *Biophys. J.*, **71**, 19-39 (1996).
32. D. BEGLOV and B. ROUX, "Solvation of Complex Molecules in a Polar Liquid: An Integral Equation Theory", *J. Chem. Phys.* **104**, 8678-8689 (1996).
33. B. ROUX, M. NINA, R. POMES and J.C. SMITH, "Thermodynamics Stability of Water Molecules in the Bacteriorhodopsin Proton Channel: A Molecular Dynamics Free Energy Perturbation Study", *Biophys. J.* **72**, 670-681 (1996).

34. K. HINSEN and B. ROUX, "A Potential Function for Computer Simulation Studies of Proton Transfer in Acetylacetone", *J. Comp. Chem.* **106**, 3567-3577 (1997).
35. B. ROUX, "Comentary: Surface Tension of Biomembranes", *Biophys. J.*, **71**, 1346-1347 (1996).
36. J.M. PETIT, B. ROUX, X.X. Zhu and P.M. MACDONALD, "A New Physical Model for the Diffusion of Solvents and Solute Probes in Polymer Solutions", *Macromol.* **29**, 6031-6036 (1996).
37. K. HINSEN and B. ROUX, "Potential of Mean Force and Reaction Rates for Proton Transfer in Acetylacetone", *J. Chem. Phys.* **106**, 3567-3577 (1997).
38. B. ROUX, "The Molecular Basis of the Valence Selectivity of the Gramicidin Channel: A Molecular Dynamics Free Energy Perturbation Study", *Biophys. J.* **71**, 3177-3187 (1996).
39. A.J. PETRESCU, P. CALMETTES, D. DURAND, V. RECEVEUR, M. DESMADRIL, B. ROUX and J.C. SMITH, "Small Angle Neutron Scattering of a Strongly Denatured Protein: Analysis Using Random Polymer Theory", *Biophys. J.* **72**, 335-342 (1997).
40. T.B. WOOLF and B. ROUX, "The Binding Site of Sodium in the Gramicidin A Channel: A Comparison of Molecular Dynamics Simulations with Solid State NMR Data", *Biophys. J.*, **72**, 1930-1945 (1997).
41. O. SHARAFEDDIN, K. HINSEN, T. CARRINGTON and B. ROUX, "Mixed Quantum-Classical Simulation Methods Applied to Intramolecular Proton Transfer in Acetylacetone", *J. Comp. Chem.* **18**, 1760-1772 (1997).
42. M. NINA, D. BEGLOV and B. ROUX, "Atomic Radii for Continuum Electrostatic Calculations Based on Molecular Dynamics Free Energy Simulations", *J. Phys. Chem.* **101**, 5239-5248 (1997).
43. I. GAMBU and B. ROUX, "The Interaction of K⁺ with a Phospholipid Bilayer: A Molecular Dynamics Study", *J. Phys. Chem.* **101**, 6066-6072 (1997).
44. D. BEGLOV and B. ROUX, "An Integral Equation to Describe the Solvation of Polar Molecules in Liquid Water", *J. Phys. Chem.* **101**, 7821-7826 (1997).
45. D. MOHANTY, R. ELBER, D. THIRUMALAI, D. BEGLOV and B. ROUX, "Kinetic of Peptide Folding: Computer Simulations of SYPFDV and Peptide Variants in Water", *J. Mol. Biol.* **272**, 423-442 (1997).
46. B. ROUX, "The Influence of the Membrane Potential on the Free Energy of an Intrinsic Protein", *Biophys. J.* **73**, 2980-2989 (1997).
47. K. BELOHORCOVA, J.H. DAVIS, T.B. WOOLF and B. ROUX, "Structure and Dynamics of an Amphiphilic Peptide in a Phospholipid Bilayer: A Molecular Dynamics Study", *Biophys. J.* **73**, 3039-3055 (1997).
48. J. BAUDRY, S. CROUZY, B. ROUX and J.C. SMITH, "Quantum Chemical and Free Energy Simulation Analysis of Reinal Conformational Energetics", *J. Chem. Inf. Comp. Sci.* **37**, 1018-1024 (1997).
49. R.R. KETCHEM, B. ROUX and T.A. CROSS, "High Resolution Refinement of a Solid-State NMR-Derived Structure of Gramicidin A in a Lipid Bilayer Environment", *Prot. Sci.* **5**, 1655-1669 (1997).

50. W. IM, D. BEGLOV and B. ROUX, "Continuum Solvation Model: Electrostatic Forces From Numerical Solutions to the Poisson-Boltzmann Equation", *Comp. Phys. Comm.* **111**, 59-75 (1998).
51. A.D MACKERELL, D. BASHFORD, M BELLOT, R.L. DUNBRACK, J.D. EVANSECK, M.J. FIELD, J. GAO, H. GUO, S. HA, D. JOSEPH-MCARTHY, L. KUCHNIR, K. KUCZERA, F.T.K. LAU, C. MATTOS, S. MICHNICK, T. NOG, D.T. NGUYEN, B. PRODHOM, W.E. REIHER, B. ROUX, M. SCHLENKRICH, J.C. SMITH, R. STOTE, J. STRAUB, M. WATANABE, J. WIORKIEWICZ-KUCZERA and M. KARPLUS, "All-Atom Empirical Potential for Molecular Modeling and Dynamics Studies of Proteins", *J. Phys. Chem. B.* **102**, 3586-3616 (1998).
52. B. ROUX, "Molecular dynamics Simulations of Ion Channels: How Far We Have Gone and Where are We Heading?", *Biophys. J.* **74**, 2744-2745 (1998).
53. R. POMES and B. ROUX, "Free Energy Profiles for H⁺ Conduction Along Hydrogen-Bonded Chains of Water Molecules", *Biophys. J.* **75**, 33-40 (1998).
54. S. BERNECHE, M. NINA and B. ROUX, "Molecular Dynamics of Melittin in a Dimyristoyl Phosphatidylcholine Bilayer Membrane", *Biophys. J.* **75**, 1603-1618 (1998).
55. S. MARCHAND and B. ROUX, "Molecular Dynamics Study of Calbindin D9K in the Apo, Singly and Doubly Calcium-Loaded States", *PROT. Struct. Func. Gen.* **33** (1998).
56. N. CHAKRABARTI, T. CARRINGTON and B. ROUX, "Rigorous Quantum Mechanical Formulation of Transition Rates Based on Feynman Path Integral for Computer Simulations", *Chem. Phys. Lett.* **293**, 209-220 (1998).
57. B. ROUX and T. SIMONSON, "Implicit Solvent Models", *Biophys. Chem.* **78**, 1-20 (1999).
58. B. ROUX, D. BEGLOV, W. IM and M. NINA, "Optimized Radii for Protein Solvation Forces Based on Continuum Electrostatics", *Biophys. Chem.* **78**, 89-96 (1999).
59. P. LAGUE, M.J. ZUCKERMANN and B. ROUX, "Protein Inclusions in Lipid Membranes: A Theory Based on the Hypernetted Chain Integral Equation", *J. Chem. Soc. Farad. Trans.* **111**, 165-172 (1999).
60. J. BAUDRY, S. CROUZY, B. ROUX and J.C. SMITH, "Simulation Analysis of the Retinal Conformational Equilibrium in Dark-Adapted Bacteriorhodopsin", *Biophys. J.* **76**, 1909-2927 (1999).
61. B. ROUX, "Statistical Mechanical Equilibrium Theory of Selective Ion Channels", *Biophys. J.* **77**, 139-153 (1999).
62. B. ROUX and R. MACKINNON, "The Cavity and Pores Helices in the KcsA K⁺ Channel: Electrostatic Stabilization of Monovalent Cations", *Science* **285**, 100-102 (1999).
63. S. CROUZY, J. BAUDRY, J.C. SMITH and B. ROUX, "Efficient Calculation of 2-Dimensional Adiabatic and Free Energy Maps: Application to the Isomerization of the C13=C14 and C15=N16 Bonds in the Retinal of Bacteriorhodopsin", *J. Comp. Chem.* **20** (15), 1644-1658 (1999).
64. R. POMES, E. EISENMESSER, C.B. POST and B. ROUX, "Calculating Excess Chemical Potentials Using Dynamical Simulations in the Fourth Dimension", *J. Chem. Phys.* **111**, 3387-3395 (1999).
65. Q. Du, D. BEGLOV and B. ROUX, "Solvation Free Energy of Polar and Non-Polar Molecules in Water: An Extended Site-Reduced Integral Equation Theory", *J. Phys. Chem. B.* **104**, 796-805 (1999).

66. B. ROUX, "Theories of Ion Permeation: A Chaser", *J. Gen. Physiol.* **114**, 605-608 (1999).
67. B. ROUX, "Proton Wires are Different", *Biophys. J.* **77**, 2331-2332 (1999).
68. S. BERNÈCHE and B. ROUX, "Molecular Dynamics of the KcsA K⁺ Channel in a Bilayer Membrane", *Biophys. J.* **78**, 2900-2917 (2000).
69. W. IM, S. SEEFELD and B. ROUX, "A Grand Canonical Monte Carlo - Brownian Dynamics Algorithm for Simulating Ion Channels", *Biophys. J.* **79**, 788-801 (2000).
70. S.S. SHOBANA, B. ROUX and O.S. ANDERSEN, "Free Energy Simulations: Thermodynamics Reversibility and Variability", *J. Phys. Chem. B.* **104**, 5179-5190 (2000).
71. M. NINA, S. BERNÈCHE and B. ROUX, "Anchoring of a Monotopic Membrane Protein: The Binding of Prostaglandin H2 Synthase-1 to the Surface of a Phospholipid Bilayer", *Europ. Biophys. J.* **29**, 439-454 (2000).
72. B. ROUX, S. BERNÈCHE and W. IM, "Ion Channels, Permeation, and Electrostatics: Insight into the Function of KcsA", *Biochem.* **39**, 13295-13306 (2000).
73. P. LAGUE, M.J. ZUCKERMANN and B. ROUX, "Lipid-Mediated Interactions Between Intrinsic Membrane Proteins: A Theoretical Study Based on Integral Equations", *Biophys. J.* **79**, 2867-2879 (2000).
74. M.F. SCHUMAKER, R. POMES and B. ROUX, "A Combined Molecular Dynamics Diffusion Model of Single Proton Conduction Through Gramicidin", *Biophys. J.* **79**, 2840-2857 (2000).
75. M. SQUAILLE and B. ROUX, "Extension to the Weighted Histogram Analysis Method: Combining Umbrella Sampling with Free Energy Calculations", *Comput. Phys. Comm.* **135**, 40-57 (2001).
76. M.F. SCHUMAKER, R. POMES and B. ROUX, "Framework Model for Single Proton Conduction Through Gramicidin", *Biophys. J.* **80**, 12-30 (2001).
77. P. LAGUE, M.J. ZUCKERMAN and B. ROUX, "Lipid-Mediated Interactions Between Intrinsic Membrane Proteins: Dependence on Protein Size and Lipid Composition", *Biophys. J.* **81**, 276-284 (2001).
78. M.A. YOUNG, S. GONFLONI, G. SUPERTI-FURGA, B. ROUX and J. KURIYAN, "Dynamic Coupling Between the SH2 and SH3 Domains of c-Rc and Hck Underlies Their Inactivation by C-terminal Tyrosine Phosphorylation", *Cell* **105**(1), 115-126 (2001).
79. W. IM, S. BERNÈCHE and B. ROUX, "Generalized Solvent Boundary Potential for Computer Simulations", *J. Chem. Phys.* **114**, 2924-2937 (2000).
80. S. CROUZY, S. BERNÈCHE and B. ROUX, "Extracellular Blockade of K⁺ Channels by TEA: Results from Molecular Dynamics Simulations of the KcsA Channel", *J. Gen. Physiol.* **118**, 207-216 (2001).
81. W. IM and B. ROUX, "Brownian Dynamics Solutions of Ions Channels: A General Treatment of Electrostatic Reaction Fields for Molecular Pores of Arbitrary Geometry", *J. Chem. Phys.* **115**, 4850-4861 (2001).
82. S. BERNÈCHE and B. ROUX, "Energetics of Ion Conduction Through the K⁺ Channel", *Nature* **414**, 73-77 (2001).

83. S. BERNÈCHE and B. ROUX, "The Ionization State and the Conformation of Glu-71 in the KcsA K(+) Channel", *Biophys J.* **82**, 772-780 (2002).
84. A. PHILIPPSEN, W. IM, A. ENGEL, T. SCHIRMER, B. ROUX, DJ MULLER, "Imaging the Electrostatic Potential of Transmembrane Channels: Atomic Probe Microscopy of OmpF Porin", *Biophys. J.* **82**, 1667-1676 (2002).
85. B. ROUX and S. BERNÈCHE, "On the potential functions used in molecular dynamics simulations of ion channels", *Biophys. J.* **82**, 1681-1684 (2002).
86. B. ROUX, "Theoretical and Computational Models of Ion Channels", *Current Opinion in Structural Biology*, (in press, 2002).
87. B. ROUX, "Computational Studies of the Gramicidin Channel", *Account of Chemical Research*, (in press, 2002).

Book Chapters

- B1. R. SAUVÉ and B. ROUX, "Comparison Between Noise and Time Interval Analysis in the Study of Single Channel Fluctuations", *9th International Conference on Noise in Physical Systems*, 255-264, C.M. Van Vliet, Ed., World Scientific (1987).
- B2. B. ROUX and R. SAUVÉ, "Ionic Channels Transitions in Patch Clamp: Effects of Noise", *Cahiers de l'atelier de Grenoble*, **1**, 170 (1984).
- B3. M. NINA, B. ROUX, J.C. SMITH, "Ground State Potential Surface Calculations for Butadiene and Retinal Structure and Function of Retinal Proteins", J.L. Rigaud, Ed., Colloque INSERM, John Libbey Eurotext Ltd., **221**, 17-20 (1992).
- B4. J.C. SMITH, P. CALMETTES, D. DURAND, M. DESMADRIL, S. FUROIS-CORBIN, G.R. KNELLER and B. ROUX, "On the Configurations Accessible to Folded and to Denatured Proteins", *NATO Advanced Research Workshop on Statistical Mechanics, Protein Structure & Substrate Interactions*, S. Doniac, Ed., Plenum Press, 135-145 (1994).
- B5. J.C. SMITH, D. DURAND, M. FIELD, S. FUROIS-CORBIN, G.R. KNELLER, M. NINA and B. ROUX, "Supramolecular Interactions and Atomic Dynamics in Proteins and Peptide Crystals. Jumps, Lattice Waves and Liquid-Like Diffusion", *NATO ASI Advanced Research Workshop on Supramolecular Chemistry*, G. Wippf, Ed., Kluwer, 457-475 (1994).
- B6. T.B. WOOLF, J. DESHARNAIS and B. ROUX, "Structure and Dynamics of the Sidechains of the Gramicidin Channel in a DMPC Bilayer", *NATO ASI Advanced Research Workshop on Supramolecular Chemistry*, G. Wippf, Ed., Kluwer, 519-531 (1994).
- B7. B. ROUX, "Theory of Transport in Ion Channels: From Molecular Dynamics Simulations to Experiments", in *Computer Simulation in Molecular Biology*, J. Goodefellow, Ed., VCH Weinheim, Chap. 6, 133-169 (1995).
- B8. B. ROUX and T.B. WOOLF, "Molecular Dynamics Simulation of Pfl Coat Protein in a Phospholipid Bilayer", in *Biological Membranes A Molecular Perspective from Computation and Experiments*, K. Merz and B. Roux, Eds., Birkhauser, Cambridge, MA, 555-587 (1996).
- B9. R.R. KETCHEM, B. ROUX and T.A. CROSS, "Computational Refinement Through Solid State NMR and Energy Constraints of a Membrane Bound Polypeptide", in *Biological Membranes A Molecular Perspective from Computation and Experiments*, K. Merz and B. Roux, Eds., Birkhauser, Cambridge, MA, 299-322 (1996).

- B10. B. ROUX and T.B. WOOLF, "Influence of Small Perturbations on the Conductance of an Ion Channel", in *Progress in Cell Research*, Vol. 6, M. Sokabe, A. Auerbach and F. Sigworth, Eds., Elsevier Science BV, 261-268 (1997).
- B11. B. ROUX and T.B. WOOLF, "Molecular Dynamics Simulation of Gramicidin A in a Phospholipid Membrane: Comparison with Solid State NMR Data", in *Human to Proteins, Advances in Computational Life Sciences Vol. 2*, M.T. Michalewicz, Ed., CSIRO Publishing, 183-200 (1998).
- B12. B. ROUX, "Environment of a Membrane Protein", in *The Encyclopedia of Computational Chemistry*, Schleyer, P. v. R.; Allinger, N.L.; Clark, T.; Gasteiger, J.; Kollman, P.A.; Schaefer III, H.F.; Schreiner, P.R., Eds.; John Wiley & Sons, Chichester (1998).
- B13. A.D. MACKERELL JR. B. BROOKS, C.L. BROOKS III, L. NILSSON, Y. WON, B. ROUX AND M. KARPLUS, "CHARMM: The Energy Function and the Program", in *The Encyclopedia of Computational Chemistry*, Schleyer, P. v. R.; Allinger, N.L.; Clark, T.; Gasteiger, J.; Kollman, P.A.; Schaefer III, H.F.; Schreiner, P.R., Eds., John Wiley & Sons, Chichester (1998).
- B14. B. ROUX AND S. CROUZY, "Theoretical Studies of Activated Processes in Biological Ion Channels", in *Classical and Quantum Dynamics in Condensed Phase Simulations*, B.J. Berne, G. Ciccotti and D.F. Coker, Eds., World Scientific Ltd., 445-462 (1998).
- B15. R. ELBER, B. ROUX AND R. OLENDER, "Applications of a Stochastic Path Integral Approach to the Computations of an Optimal Path and Ensembles of Trajectories", in *Lecture Notes in Computational Science and Engineering*, Vol. 4, "Computational Molecular Dynamics: Challenges, Methods, Ideas", P. Deuffhard, J. Hermans, B. Leimkuhler, A.E. Mark, S. Reich, and R.D. Skeel, Eds., 263-280, Springer-Verlag, Berlin Heidelberg (1999).
- B16. J. BAUDRY, S. CROUZY, B. ROUX and J.C. SMITH, "Modeling and Simulation of Light-Activated Membrane Proteins", *Genomics and Proteomics: Proceedings*, S. Suhai, Ed., Plenum, New York (1999).
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