

Benoît Roux

Weill Medical College of Cornell University
Departments of Physiology and Biophysics
1300 York Avenue
New York, NY 10021
Tel: (212) 746-6018
Fax: (212) 746-4843
benoit.roux@med.cornell.edu
<http://thallium.med.cornell.edu/RouxLab>

EDUCATION

- Ph.D.** 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.S.** Physics Department, University of Montreal, Quebec, Canada. Advisor: Professor Rémy Sauvé. Dissertation title: *"Analysis of Patch Clamp Signals"*. Degree conferred: September, 1984
- B.S.** Physics Department, University of Montreal, Québec, Canada. Degree conferred: December, 1981

PROFESSIONAL EXPERIENCE

- 2004– Professor in the Department of Physiology and Biophysics, Weill Medical College of Cornell University
- 1999–2004 Professor in the Department of Biochemistry, Weill Medical College of Cornell University
- 1999 Visiting Professor, in the laboratory of Rod MacKinnon at The Rockefeller University (on sabbatical leave from the Université de Montréal)
- 1996–1999 Associate Professor in the Departments of Physics and Chemistry, Université de Montréal, Canada
- 1992–1996 Assistant Professor in the Departments of Physics and Chemistry, Université de Montréal, Canada
- 1991–1992 Visiting Researcher in the laboratory of Dr. Jeremy Smith in the: Laboratoire d'Ingénierie des Protéines at the CEA in Saclay, France
- 1985–1990 Research assistant in the laboratory of Martin Karplus in the Chemistry Department at Harvard University
- 1989 Visiting Researcher in the laboratory of Richard R. Ernst in the Department of Physical Chemistry at the ETH Zentrum, Zürich

HONOR AND AWARDS

1998	Rutherford Medal, The Royal Society of Canada
1998	Noranda Lecture Award, The Chemical Institute of Canada
1996–1999	Research Fellow of the Medical Research Council of Canada
1993–1999	Research Fellow of the Fonds de Recherche Sante Quebec
1990	Medical Research Council of Canada, Post-Doctoral Fellowship
1985–1986	Fonds de Consolidation et Aide à la Recherche, Doctoral Fellowship
1983–1987	Medical Research Council of Canada, Doctoral Fellowship.
1982	Fonds de Consolidation et Aide à la Recherche, Master Scholarship.

PROFESSIONAL ACTIVITIES

- Permanent member of the BBBA study section at NIH (2001–2005)
- Current developer of the biomolecular simulation program CHARMM, Accelrys
- Editorial Board Member of the Biophysical Journal (1995–2000)
- Editorial Board Member of PROTEINS (since 2000)
- Editorial Board Member of Journal of Computational Chemistry (since 2004)
- Editorial Board Member of Journal of Chemical Theory and Computations (since 2004)
- Co-editor with Thomas Simonson of a Special Issue of *Biophysical Chemistry* on “Implicit Solvent for Biomolecular Simulations”, vol 78 (1999)
- Member of the Biophysical Society (since 1985)

BOOKS EDITED

- Biological Membranes: A Molecular Perspective from Computation and Experiments, K. Merz and B. Roux Eds., Birkhauser Cambridge MA, (1996).
- Computational Biochemistry and Biophysics, Oren M. Becker, Alexander D. MacKerell, Benoit Roux, and Masakatsu Watanabe Eds., Marcel Dekker, (2001).

CURRENT RESEARCH FUNDING

- Grant NIH-GM 62342
Title: *Computational studies of ion channels*
Period August 1st 2005 until July 31st 2009
- Grant NSF-0415784
Title: *Free Energy in biomolecular systems: development and application of computational approaches*
Period September 1st 2004 until August 31st, 2008
- Grant NIH-CA 93577
Title: *Conformational flexibility in activation of Src-kinase*
Period April 1st 2002 until March 31st 2006
- Grant NIH-GM 072558
Title: *Polarizable force field for proteins and lipids*
Period February 1st 2005 until January 31st 2009
- Grant NIH-GM070971
Title: *Putting Molecular Dynamics to the Test: Ion Permeation*
Period August 1st 2005 until July 31st 2009

PAST FUNDING

- Grant NSF-0110847
Title: *Free Energy in biomolecular systems: development and application of computational approaches*
Period September 1st 2001 until August 31st, 2004
- Grant Merck Research Laboratory
Title: *Structural models of K-channels/Toxins complexes*
Period 2001
- Grant NIH-GM 62342
Title: *Computational studies of ion channels*
Period January 1st 2001 until December 31st 2004
- Grant Merck Research Laboratory
Title: *Structural models of K-channels/Toxins complexes*
Period 2001

LIST OF PUBLICATIONS

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 ROUX B., "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. Am. 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, J.C. SMITH, "Computer Simulations of the Flexibility of a Series of Synthetic Peptide Analogues", *Biopol.* **33**, 1249-1270 (1993).
13. M. FERRAND, G. ZACCAI, M. NINA, J.C. SMITH, C. ETCHEBEST and ROUX, B., "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. Am. 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", *Biopol.* **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 ¹⁵N 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.* **91**, 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 Born radii for continuum electrostatic calculations based on molecular dynamics free energy simulations", *J. Phys. Chem. B* **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. B* **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. B* **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 retinal conformational energetics", *J. Chem. Inf. Comp. Sci.* **37**, 1018-1024 (1997).
49. R.R. KETCHUM, 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. BERNÈCHE, 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. Struc. Funct. 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. M. NINA, W. IM and B. ROUX, "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**, 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: thermodynamic 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", *Eur. Biophys. J.* **29**, 439-454 (2000).
72. B. ROUX, S. BERNÈCHE and W. IM, "Ion channel, permeation and electrostatics: Insight into the function of KcsA", *Biochemistry* **39**, 13295-13306 (2000).
73. P. LAGUE, M.J. ZUCKERMANN and B. ROUX, "Lipid-mediated interactions between 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. SOUAILLE 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**, 115-126 (2001).
79. W. IM, S. BERNÈCHE and B. ROUX, "Generalized Solvent Boundary Potential for Computer Simulations", *J. Chem. Phys.* **114**, 2924-2937 (2001).
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).
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87. R. POMES and B. ROUX, "Molecular Mechanism of H⁺ Conduction in the Single-File Water Chain of the Gramicidin Channel", *Biophys. J.* **82**, 2304-2316 (2002).
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90. M. SIMOES, L. GARNEAU, H. KLEIN, U. BANDERALI, F. HOBEILA, B. ROUX, L. PARENT and R. SAUVÉ. "Cysteine Mutagenesis and Computer Modeling of the S6 Region of an Intermediate Conductance IKCa Channel", *J. Gen. Physiol.* **120**, 99-116 (2002).
91. W. IM and B. ROUX, "Ion Permeation and Selectivity of OmpF Porin: A Theoretical Study Based on Molecular Dynamics, Brownian Dynamics, and Continuum Electrodiffusion Theory.", *J. Mol. Biol.***322**, 851-869 (2002).
92. N. K. BANAVALI, W. IM and B. ROUX, "Electrostatic free energy calculations using the generalized boundary potential", *J. Chem. Phys.* **117**, 7381-7388 (2002).
93. L. PARENT, R. SAUVÉ, S. BERNÈCHE and B. ROUX "A bas les barrières d'énergie dans les canaux potassiques!", *Med. Sci.* **18**, 604-609 (2002).
94. N. K. BANAVALI and B. ROUX, "Atomic radii for continuum electrostatics calculations on nucleic acids", *J. Phys. Chem. B* **106**, 11026-11035 (2002).
95. M.A.L. ERIKSSON and B. ROUX, "Modeling the structure of Agitoxin in complex with the Shaker K⁺ channel. A computational approach based on experimental distance restraints extracted from thermodynamic mutant cycles", *Biophys. J.* **83**, 2595-2609 (2002).
96. L. YANG, W. BEARD, S. WILSON, B. ROUX, S. BROYDE, T. SCHLICK. "Local deformations revealed by dynamics simulations of DNA polymerase Beta with DNA mismatches at the primer terminus", *J. Mol. Biol.* **321**, 459-478 (2002).
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99. G. LAMOUREUX and B. ROUX, "Modeling Induced Polarization with Classical Drude Oscillators: Theory and Molecular Dynamics Simulation Algorithm", *J. Chem. Phys.* **119**, 3025-3039 (2003).
100. T.W. ALLEN, O.S. ANDERSEN and B. ROUX, "The structure of gramicidin A in a lipid bilayer environment determined using molecular dynamics simulations and solid-state NMR data", *J. Am. Chem. Soc.* **125**, 9868-9877 (2003).
101. M. LAINE, M.C.A. LIN, J.A. BANNISTER, W.R. SILVERMAN, B. ROUX and D.M. PAPA ZIAN, "Atomic proximity between S4 segment and pore domain in Shaker potassium channels", *Neuron* **39**, 467-481 (2003).
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104. N. CHAKRABARTI, E. TAJKHORSHID, B. ROUX and R. POMES. "Molecular Basis of Proton Blockage in Aquaporins", *Structure* **12**, 65-74 (2004).
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