Curriculum Vitae

Dr. Scott E. Feller
Department of Chemistry
Wabash College
301 W. Wabash Ave
Crawfordsville IN 47933
office (765) 361-6175
home (765) 275-2211
fax (765) 361-6149
e-mail fellers@wabash.edu
www.lipid.wabash.edu

EDUCATION

Ph.D., Physical Chemistry, University of California, Davis. Dec 1993. Dissertation: Application of the Hypernetted Chain Approximation to the Electrical Double Layer. Advisor: Dr. Donald A. McQuarrie.

B.A., Major: Chemistry, Minor: Mathematics, Willamette University, May 1989.

ADMINISTRATIVE EXPERIENCE

Chair, Division of Natural Sciences & Mathematics, Wabash College, 2009-present.

Chair, Department of Chemistry, Wabash College, 2006-2009.

TEACHING EXPERIENCE

Professor of Chemistry, Wabash College, 2009-present.

Associate Professor of Chemistry, Wabash College, 2003-2009.

Assistant Professor of Chemistry, Wabash College, 1998-2003, Introductory Chemistry with Laboratory, Quantitative Chemistry with Laboratory, Physical Chemistry with Laboratory, Cultures and Traditions (all College, great books type course), Descriptive Chemistry with Laboratory, Non-majors Chemistry with Laboratory, Student Research Advisor.

Visiting Assistant Professor, Whitman College, 1996-1998, Introductory Chemistry with laboratory, Molecular Modeling, Chaos & Scientific Computing, Intro Chem Lab coordinator, Student Research Advisor.

Teaching Assistant, University of California at Davis, 1989-1993, Introductory Chemistry with Laboratory, Physical Chemistry (graduate & undergraduate levels).

RESEARCH EXPERIENCE

Visiting Scientist, IBM Research – Watson Laboratory, Yorktown Heights NY, 6/04-6/07.

Principal Investigator, Department of Chemistry, Wabash College, 7/98-present.

Principal Investigator, Department of Chemistry, Whitman College, 9/96-7/98.

Staff Fellow, Center for Biologics Evaluation & Research (FDA laboratory at the National Institutes of Health), 2/94-8/96. Supervisor: Dr Richard Pastor, Biophysics Laboratory.

Visiting Researcher, University of Leipzig, May 1996. Supervisor: Dr. Frank Volke, Department of Physics.

Graduate Study, UCDavis, 1/90-12/93. Supervisor: Dr. D.A. McQuarrie, Department of Chemistry.

Visiting Researcher, Universidad Autonoma Metropolitina-Iztapalapa (Mexico City), June-July 1992. Supervisor: Dr. Marcelo Lozada-Cassou, Department of Physics.

Research Assistant, Willamette University, 9/88-5/89. Supervisor: Dr. Arthur Payton, Department of Chemistry.

GRANTS AND FELLOWSHIPS

National Science Foundation. Title: MRI: Acquisition of a Computer Cluster for undergraduate Chemistry Research and Teaching by the Midwest Undergraduate Computational Chemistry Consortium (MU3C). Amount: $299,942. Period: 10/1/2010-9/30/2013. Co-PI with Krueger, Polik, Kuwata, & Kohen.

National Science Foundation. Title: RUI: Exploring Lipid Interactions Using Atomistic Models. Amount: $500,000. Period: 5/2010-5/2015.

National Science Foundation. Title: RUI: Atomistic Simulations of Lipid Bilayer Membranes. Amount: $268,252. Period: 5/2006-5/2010.

National Institutes of Health, Nanomedicine center (one of 10 co-P.I.'s). Title: National Center for the Design of Biomimetic Nanoconductors. Amount $6,500,000 ($188,681 for Wabash). Period 9/2005-9/2009.

Henry Dreyfus Teacher-Scholar Award. Title: Computational studies of lipid-protein interactions. Amount $60,000. Period 9/2003-9/2008.

National Science Foundation, special grants program. Title: Examining student outcomes associated with undergraduate research participation at Wabash College. Amount $36,297. Period: 2001-2003

National Science Foundation, CAREER award. Title: Use of atomic-level models to study lipid bilayer membranes and to enhance undergraduate teaching. Amount: $500,000. Period: 5/2001-5/2006.

National Science Foundation, CCLI program. Title: Molecular Modeling Throughout the Chemistry Curriculum. Amount: $36,874. Period: 2000-2002.

Byron K. Trippet summer research award, Wabash College. Period: summer 1999 & 2000.

National Science Foundation travel award to attend CECAM conference in Lyon, France. July 1999.

National Science Foundation, RUI program. Title: Molecular Dynamics Simulations of Lipid Bilayer Membranes. Amount: $156,418. Period: 5/1998-5/2001.

Food and Drug Administration, Office of Vaccine Research & Review. Title: Computer Modelling of Varicella (chicken pox). Amount: $19,768. Period: 1997.

Bradford Borge Graduate Fellowship, University of California, Davis.

PROFESSIONAL AFFILIATIONS

American Chemical Society
Midwest Association of Chemistry Teachers at Liberal Arts Colleges
Council on Undergraduate Research
Biophysical Society

PROFESSIONAL SERVICE

Reviewer for: *Biophysical Journal*, *Journal of Chemical Physics*, *Journal of Physical Chemistry*, *Journal of the American Chemical Society*, *Physical Chemistry Chemical Physics*, *Journal of Molecular Biology*, *Journal of Computational Physics*, *Langmuir*, *Chemistry and Physics of Lipids*, *European Biophysical Journal*, *Journal of Chemical Theory and Computation*, *Biochimica Biophysica Acta.*, *Journal of Membrane Biology*, *Journal of Computational Chemistry*, *Proceedings of the National Academies of Science*, and *Journal of Chemical Education*.

Review panel member: Molecular Biophysics section National Science Foundation; Course, Curriculum, and Laboratory Improvement section National Science Foundation; Department of Energy; Ohio Supercomputer Center; Membrane Biochemistry & Biophysics section National Institutes of Health.

Editorial Board Member: *Chemistry and Physics of Lipids*, *Journal of Membrane Biology*, *Biophysical Journal*

Chemistry Council Member, Campus Liason: Council on Undergraduate Research.

Chair, 2008 Membrane Structure and Assembly Subgroup, Biophysical Society

HONORS AND AWARDS

McClain-McTurnan-Arnold Excellence in Teaching Award, Wabash College, 2009.

Henry Dreyfus Teacher Scholar, Dreyfus Foundation, 2003-2008.

Award for Excellence in Undergraduate Chemical Research, given by Indiana University and Eli Lilly, 2001.

Scientific Achievement award for top research group (1 of 3 members), Food & Drug Administration; Center Director's award for Scientific Achievement, Center for Biologics Evaluation & Research/FDA, 1996.
Award for Outstanding Accomplishments in Graduate Program, UCDavis, 1991

Willamette University: American Chemical Society Scholarship, American Institute of Chemists award for Top Graduating Senior in Chemistry, Graduated Cum Laude, 1989

UNDERGRADUATE RESEARCH STUDENTS

Olivia Uitto – PhD, University of Utah
Roger Armen – PhD, University of Washington
Matthew Schneider – computer programmer, Cincinatti OH
Matthew Kriech – PhD, University of Utah
Robert Dirks – PhD, Cal Tech
Chris Brown – MD, University of Cincinatti
Matthew Strader – PhD, University of California at Berkeley
Adam Moser – PhD student, University of Minnesota
Damon Carl – PhD student, University of Utah
Joe Scanlon – PhD, University of Minnesota; Asst Professor Ripon College
John Dustman – M.S. Stanford University
Jesse Ward – PhD student, University of Michigan
Galen Collins – PhD student, University of San Diego
Matt Roark – computer systems administrator, Wabash College
Xincheng Liu – PhD student, University of Texas
Zeyu Lu – current Wabash student
James Gorman – current Wabash student
Bo Wang – current Wabash student
Shengshuang Zhu – current Wabash student

INVITED PRESENTATIONS

"Variational Solutions to Integral Equation Theories of the Electrical Double Layer", 1994 National ACS meeting, Washington DC.

"Surface Tension-Area Isotherms of a DPPC Bilayer and Monolayer from Molecular Dynamics Computer Simulations", 1995 National ACS meeting, Chicago IL.

"Time Scales of Lipid Dynamics", 1996 Gordon Conference on Chemistry at Interfaces, Meriden NH.

"Interpretation of NOESY Cross-Relaxation Rates from Molecular Dynamics Simulation of a Lipid Bilayers", 1999 CECAM Conference on Lipid Bilayer Membranes and Membrane Associated Proteins, Lyon France.

"Building a Supercomputer for Computational Chemistry", 1999 Consortium of Liberal Arts Colleges (CLAC) annual meeting, Reed College.

"Interpretation of NOESY Cross-Relaxation Rates from Molecular Dynamics Simulation of a Lipid Bilayers", 2000 International Bunsen Discussion meeting on interactions of biopolymers with model membranes, Halle Germany.

"Lipid Dynamics from Simulation and Experiment", 2000 FASEB meeting on membrane biophysics, Saxon's River VT.

"New Insights into Biomembrane Structure from Two-Dimensional Overhauser Enhancement Spectroscopy – MD Simulations", 2001 Mesilla Workshop on the Structure and Dynamics of Biomembranes, Las Cruces NM.

"Molecular Dynamics Simulations of Saturated and Polyunsaturated Lipid Bilayer Membranes", 2002 International Society for the Study of Fatty Acids and Lipids, Montreal Canada.

"Polyunsaturated Lipid Bilayer Membranes: Insights from Molecular Dynamics Computer Simulations", 2003 University of Michigan Membrane Biophysics Symposium.

"Insights into Polyunsaturated Lipids from Molecular Dynamics Simulations", 2004 Biophysical Society Annual Meeting.

"Understanding the unique properties of polyunsaturated lipids", Biological Membranes: Emerging Challenges at the Interface between Theory, Computer Simulation, and Experiment, Sun Valley Idaho, 2004.

"Molecular Dynamics Simulations of Saturated and Polyunsaturated Lipid Bilayer Membranes", Molecular Interface Symposium, Osaka, Japan 2004.

"Understanding the unique properties of polyunsaturated lipids", Midwest Computational Structural Biology Workshop, Augusta MI, 2005.

"The unique properties of polyunsaturated lipids", Biological Membranes: Structure and Function, Ohio Center for Technology and Science, Columbus OH, 2005.

"Roles for omega-3 fatty acids in the function of membrane proteins", 2006 Annual Meeting of the American Chemical Society, San Fransisco CA.

"Unique properties of polyunsaturated lipids and their interactions with membrane proteins", Gordon Research Conference on Ion Channels, Tilton NH.

"Validating membrane simulations through comparison with NMR and X-ray scattering experiments", 2007 Annual Meeting of the American Chemical Society, Chicago IL.

"Interactions of omega-3 fatty acids with rhodopsin", 2007 University of Delaware Membrane Protein Symposium, Newark DE

"Properties of lipids containing docosahexaenoic acid and their interactions with the integral membrane protein rhodopsin", 2008 International Society for the Study of Fatty Acids and Lipids, Kansas City MO.

S.E. Feller, "Structure and Dynamics of a Fluid Phase Bilayer on a Solid Support as Observed by a Molecular Dynamics Computer Simulation" 2009 ACS Colloid & Surface Science Symposium, Columbia University.

S.E. Feller "Structure of a Lipidated ras Peptide Bound to a Phospholipid Bilayer" 2009 Telluride Science Center workshop on Membranes and membrane proteins: Challenges for theory and experiment.

S.E. Feller "A Reinterpretation of Neutron Scattering Experiments on a Lipidated Ras Peptide Using Replica Exchange Molecular Dynamics" 2011 ACS Annual meeting, Anaheim CA.

Departmental seminars: Purdue University, Illinois Institute of Technology, Indiana University, Notre Dame University, Michigan State University, Indiana University Purdue University Indianapolis, National Institute of Alcohol Abuse and Alcoholism, Miami University of Ohio, University of Illinois, IBM Yorktown Heights, University of Chicago, University of Leipzig (Germany), University of North Carolina-Greensboro, Yokohama City University (Japan), University of Kentucky, Washington University, University of Arizona, University of California-Davis, SUNY-Buffalo, Oberlin College, Hope College, University of Kansas, University of North Carolina-Wilmington, Florida State University University of Texas, Cornell-Weil Medical School, University of Rochester, University of Delaware.

BOOKS

Computational Modeling of Membrane Bilayers. Edited by S.E. Feller. Elsevier. 2008.

POSTER PRESENTATIONS AND CONTRIBUTED TALKS (*denotes undergraduate co-authors)

D. Huster, S.E. Feller and K. Gawrisch, "NOESY NMR Crosspeaks Between Lipid Headgroups and Hydrocarbon Chains: Spin Diffusion or Molecular Disorder?", 1999 Biophysical Society Annual Meeting, Baltimore MD.

C.A Brown* and S.E. Feller, "Molecular Dynamics Simulations of Ethanol in a Lipid Bilayer", 2000 American Chemical Society – Indianapolis section poster session.

K. Gawrisch, S.E. Feller, N.V. Eldho, and A.M. Safley, "Conformation and Flexibility of the Polyunsaturated Docosahexaenoic Acid Chain", 2001 Biophysical Society Annual Meeting, Boston MA.

D.T. Nizza, Christopher A. Brown*, S.E. Feller, and K. Gawrisch, "NMR Measurements and MD Simulations of Ethanol-membrane Interactions", 2001 Biophysical Society Annual Meeting, Boston MA.

C.A Brown* and S.E. Feller, "Molecular Dynamics Simulations of Ethanol in a Lipid Bilayer", 2001 National Conference on Undergraduate Research, Lexington KY.

S.E. Feller, R.F. Dallinger, and P.C. McKinney, "Integrating Molecular Modeling Into the General Chemistry Course", 2001 National ACS fall meeting, Chicago IL.

D.R. Carl* and S.E. Feller, "Molecular dynamics simulations of liquid/liquid interfaces: An in depth look at water/octane", 2001 American Chemical Society – Indianapolis section poster session.

A. Moser* and S.E. Feller, "Molecular Modeling of Lipid Bilayer Membranes", 2001 American Chemical Society – Indianapolis section poster session.

M.L. Strader* and S.E. Feller, "A Flexible All-atom Model of Dimethylsulfoxide for Molecular Dynamics Simulations", 2001 American Chemical Society – Indianapolis section poster session

A. Beselman, S.E. Feller, and A.D. MacKerell Jr, "Quantum mechanical study of the intrinsic energetics of the glycerol phosphate linker region of phospholipids", 2002 Biophysical Society Annual Meeting, Boston MA.

D.R. Carl* and S.E. Feller, "Calculating Free Energies of Transferring a Single Water Molecule Through Bulk Layers of Sixteen-Carbon Chains: A Study of Increasing Levels of Unsaturation in Hexadecane Molecules", 2002 American Chemical Society – Indianapolis section poster session.

J. Dustman* and S.E. Feller, "Calculating Viscosities and Related Properties of Alkanes and Alcohols from Molecular Dynamics Simulations", 2002 American Chemical Society – Indianapolis section poster session.

J.D. Scanlon* and S.E. Feller, "Molecular Dynamics Simulations of Humna N-RAS Protein in a Dimyristoylphosphatidylcholine (DMPC) bilayer", 2002 American Chemical Society – Indianapolis section poster session.

S.E. Feller and T.B. Woolf, "Polyunsaturation Effects on Protein:Lipid Interactions: Molecular Dynamics Simulations of Rhodopsin in an Explicit DHA Bilayer", 2003 Biophysical Society Annual Meeting, San Antonio TX.

S.E. Feller, K. Gawrisch and A.D. MacKerell, Jr., "Structural and Dynamic Properties of Polyunsaturated Fatty Acids from Simulation and Experiment", 2003 Biophysical Society Annual Meeting, San Antonio TX.

N.V. Eldho, S.E. Feller, S. Tristram-Nagle, I.V. Polozov, K. Gawrisch, "Polyunsaturated Docosahexaenoic vs. Docosapentaenoic Acid – Differences in Lipid Matrix Properties from the Loss of One Double Bond", 2003 Biophysical Society Annual Meeting, San Antonio TX.

D.R. Carl* and S.E. Feller, "Calculating Free Energies of Transferring a Single Water Molecule Through Bulk Layers of Sixteen-Carbon Chains: A Study of Increasing Levels of Unsaturation in Hexadecane Molecules", National Conference for Undergraduate Research, Salt Lake City UT.

J. Dustman* and S.E. Feller, "A Computational Study of Viscosity in the Lipid Bilayer", 2003 American Chemical Society – Indianapolis section poster session.

J. Ward* and S.E. Feller, "The Effects of Trans-Fatty Acids on Lipid Membranes", 2003 American Chemical Society – Indianapolis section poster session.

S.P. Soni, J. Ward*, S.E. Feller, S.R. Wassall, "Molecular Organization in a Trans Unsaturated Membrane", 2004 Biophysical Society Annual Meeting, Baltimore MD.

J. Dustman*, H.C. Gaede, K. Gawrisch, S.E. Feller, "Interaction of a Series of Aromatic Solutes with a Phospholipid Bilayer", 2004 Biophysical Society Annual Meeting, Baltimore MD.

Y. Liu, N. Kucerka, N. Chu, S. Tristram-Nagle, H.I. Petrache, S.E. Feller, J.F. Nagle, "Structure and Interactions of Biomembranes Using Diffuse X-ray Scattering on Fully Hydrated Oriented Systems ", 2004 Biophysical Society Annual Meeting, Baltimore MD.

S.E. Feller, M.C. Pitman, "A Molecular Dynamics Study of the Interaction of Cholesterol with Saturated and Polyunsaturated Fatty Acids in a Phosphatidylcholine Lipid Bilayer", 2004 Biophysical Society Annual Meeting, Baltimore MD.

M.C. Pitman, S.E. Feller, "Structure and dynamics of 1-stearoyl-2-oleoyl-phosphatidyethanolamine (SOPE) by molecular simulation reveals notable differences compared to 1-palmitoyl-2-oleoyl-phosphatidylcholine (POPC) due to head group hydrogen bonding in SOPE", 2004 Biophysical Society Annual Meeting, Baltimore MD.

N. Kucerka, J.F. Nagle, S.E. Feller, P. Balgavy, "Advanced Models to Obtain Structural Information from Neutron Scattering on LUVs", 2004 Biophysical Society Annual Meeting, Baltimore MD.

J. Ward* and S.E. Feller, "The Effects of Trans-Fatty Acids on Lipid Membranes", 2004 National Conference on Undergraduate Research, Indianapolis IN.

S.P. Soni, J. Ward*, S.E. Feller, S.R. Wassall, "Molecular Organization in a Trans Unsaturated Membrane", 2004 Central Regional Meeting of the American Chemical Society.

S.E. Feller, M.C. Pitman, "A Molecular Dynamics Study of the Interaction of Cholesterol with Saturated and Polyunsaturated Fatty Acids in a Phosphatidylcholine Lipid Bilayer", 2004 Biophysical Discussions meeting, Asilomar, CA.

S.E. Feller, M.C. Pitman, F. Suits, "A Molecular Dynamics Study of the Interaction of Cholesterol with Saturated and Polyunsaturated Fatty Acids in a Phosphatidylcholine Lipid Bilayer", 2005 Biophysical Society Annual Meeting, Long Beach CA.

M.C. Pitman, F. Suits, A. Grossfield, S.E. Feller, "Molecular Dynamics Investigation of Dark-Adapted Rhodopsin in an explicit 2:2:1 SDPE/SDPC/Cholesterol Environment: Membrane Structure and Dynamics", 2005 Biophysical Society Annual Meeting, Long Beach CA.

A. Grossfield, M.C. Pitman, F. Suits, S.E. Feller, "Molecular Dynamics Investigation of Dark-Adapted Rhodopsin in an explicit 2:2:1 SDPE/SDPC/Cholesterol Environment: Protein Structure and Dynamics", 2005 Biophysical Society Annual Meeting, Long Beach CA.

M. Carrillo-Tripp, S.E. Feller, "Lateral Pressure Distribution of Mono and Polyunsaturated Acid Containing Lipid Membranes", 2005 Biophysical Society Annual Meeting, Long Beach CA.

S.E. Feller, A. Vogel, H. Waldmann, K. Arnold, D. Huster, "Molecular Dynamics Simulation of a Lipidated Ras Peptide in Membranes", 2005 Biophysical Society Annual Meeting, Long Beach CA.

A. Vogel, C.P. Katzka, H. Waldmann, K. Arnold, S.E. Feller, M.F. Brown, D. Huster, "Dynamics of a Lipid-Modified Ras Peptide in Membranes Investigated by ^{2}H Solid-State NMR Relaxation and Molecular Dynamics Simulation", 2006 Biophysical Society Annual Meeting, Salt Lake City UT.

S.E. Feller, M.A. McCabe, R. Adlof, S.R. Wassall, "Double Bond Location Determines Molecular Area and Lateral Tension: Solid State ^{2}H NMR and MD Simulations of Positional Isomers of a Monounsaturated Phospholipid Membrane", 2006 Biophysical Society Annual Meeting, Salt Lake City UT.

A. Grossfield, S.E. Feller, M.C. Pitman, "A role for direct interactions in the modulation of rhodopsin by omega-3 polyunsaturated lipids", 2006 Biophysical Society Annual Meeting, Salt Lake City UT.

M.C. Pitman, A. Grossfield, S.E. Feller, "Exploring Activation of Rhodopsin with Large Scale Molecular Dynamics", 2006 Biophysical Society Annual Meeting, Salt Lake City UT.

K. Martinez-Mayorga, P.W. Lau, M.C. Pitman, S.E. Feller, M.F. Brown, "Molecular Dynamics Simulation of Light Activation of Rhodopsin", 2006 Biophysical Society Annual Meeting, Salt Lake City UT.

P.W. Lau, M.C. Pitman, S.E. Feller, M.F. Brown, "Conformational Sensitivity of Retinylidene Cofactor in Rhodopsin Studied by Molecular Dynamics", 2006 Biophysical Society Annual Meeting, Salt Lake City UT.

K. Gawrisch, O. Soubias, N.V. Eldho, W.E. Teague, and S.E. Feller, "Structure and dynamics of polyunsaturated hydrocarbon chains in lipid bilayers and their interaction with G-protein coupled membrane receptors", 2006 American Chemical Society Annual Meeting, San Fransisco CA.

S.E. Feller, "Validating membrane simulations through comparison with NMR and X-ray scattering experiments", 2007 American Chemical Society Annual Meeting, Chicago IL.

A. Grossfield, M.C. Pitman, S.E. Feller, O. Soubias, K. Gawrisch, "The role of water in rhodopsin activation: Insights from two microsecond-scale molecular dynamics simulations" 2007 Biophysical Society Annual Meeting, Baltimore MD.

A. Grossfield, S.E. Feller, M.C. Pitman, "Convergence of molecular dynamics simulations of membrane proteins" 2007 Biophysical Society Annual Meeting, Baltimore MD.

A. Vogel, G. Reuther, K.T. Tan, H. Waldmann, J. Kuhlmann, K. Arnold, S.E. Feller, M.F. Brown, D. Huster, "Dynamics of the Lipid-Modified Membrane Anchor of Human N-Ras Investigated by 2H Solid-State NMR Relaxation and Molecular Dynamics Simulations" 2007 Biophysical Society Annual Meeting, Baltimore MD.

S.P. Soni, J. Runyan, J.A. Ward*, S.E. Sen, S.E. Feller, S.R. Wassall, "*Trans* vs. *Cis* Unsaturation: The Effects on Molecular Organization in a Phospholipid Membrane Studied by Solid State ^{2}H NMR Spectroscopy and MD Simulations" 2007 Biophysical Society Annual Meeting, Baltimore MD.

S. Tristram-Nagle, J.N. Sachs, N. Kucerka, S.E. Feller, J.F. Nagle, "Strategy for Structure Determination of Lipid/Cholesterol Bilayers" 2007 Biophysical Society Annual Meeting, Baltimore MD.

P.W. Lau, A. Grossfield, S.E. Feller, M.C. Pitman, M.F. Brown, "Retinal Flexibility of Rhodopsin Illuminated Through Large-Scale Molecular Dynamics Simulations" 2007 Biophysical Society Annual Meeting, Baltimore MD.

K. Martínez-Mayorga, M.C. Pitman, A. Grossfield, S.E. Feller, M.F. Brown, "Visual Receptor Activation Evaluated by Molecular Dynamics Simulations and Solid State ^{2}H NMR Spectroscopy" 2007 Biophysical Society Annual Meeting, Baltimore MD.

A. Vogel, D. Huster, A.V. Struts, S.E. Feller, and M.F. Brown, "Lipid Bilayer Dynamics Investigated by Combined Solid-State NMR Relaxation and Molecular Dynamics Simulations" 2008 Biophysical Society Annual Meeting, Long Beach CA.

A. Grossfield, S.E. Feller, and M.C. Pitman, "Specificity Of Antimicrobial Lipopeptides For Bacterial Membranes: Insights From Molecular Dynamics Simulations" 2008 Biophysical Society Annual Meeting, Long Beach CA.

A. Vogel, T. Schröder, K.T. Tan, C. Lange, H. Waldmann, S.E. Feller, M.F. Brown, and D. Huster, "Structure and Dynamics of the Acyl Chain of Lipid Modified Membrane Proteins Studied by ^{2}H Solid-State NMR and MD Simulation" 2008 Biophysical Society Annual Meeting, Long Beach CA.

K. Martínez-Mayorga, A. Grossfield, J.L. Medina-Franco, M.C. Pitman, S.E. Feller, and M.F. Brown, "Retinal Relaxation in Rhodopsin Activation Viewed by Large-Scale Molecular Dynamics Simulations" 2008 Biophysical Society Annual Meeting, Long Beach CA.

P.W. Lau, A. Grossfield, S.E. Feller, K. Martínez-Mayorga, A.V. Struts, M.C. Pitman, and M.F. Brown, "Molecular Dynamics Simulations Unveil Dynamic Flexibility of Retinal within Binding Pocket of Rhodopsin" 2008 Biophysical Society Annual Meeting, Long Beach CA.

S.P. Soni, J. Runyan, G. Birch, J.A. Ward*, S.E. Sen, S.E. Feller, and S.R. Wassall, "Molecular Organization In A Phospholipid Membrane Containing *Trans* Unsaturation" 2008 Biophysical Society Annual Meeting, Long Beach CA.

S. Feller, M. Roark, P. Tumanen, and H.L. Scott, "Simulation Studies Of The Properties Of Hydrated POPC Lipid Bilayers Interacting With A Nanoporous Solid Silica Substrate" 2008 Biophysical Society Annual Meeting, Long Beach CA.

N. Kucerka, J.F. Nagle, J. Sachs, S.E. Feller, J. Pencer, A. Jackson, and J. Katsaras, "Lipid Area Refinement Based On A Simultaneous Analysis Of Neutron And X-ray Scattering Data And All-atom Molecular Dynamics Simulations" 2008 Biophysical Society Annual Meeting, Long Beach CA.

A. Vogel, G. Reuther, K.T. Tan, H. Waldmann, S.E. Feller, and D. Huster, "Backbone Conformation and Dynamics of the Lipid-Modified Membrane Anchor of Human N-Ras Investigated by Solid-State NMR and Molecular Dynamics Simulations" 2008 Biophysical Society Annual Meeting, Long Beach CA.

P.H. Reggio, A. Grossfield, D. Hurst, K. Gawrisch, S.E. Feller, and M.C. Pitman, "Microsecond Time Scale Molecular Dynamics Simulations : Endocannabinoid Entry Into The Cannabinoid CB2 Receptor Via The Lipid Bilayer" 2008 Biophysical Society Annual Meeting, Long Beach CA.

A. Vogel, M.F. Brown, S.E. Feller, "Headgroup Conformations of Phospholipids from Molecular Dynamics Simulation: Sampling Challenges and Comparison to Experiment" 2009 Biophysical Society Annual Meeting, Boston MA.

A. Vogel, A. Grossfield, M.C. Pitman, S.E. Feller, M.F. Brown, "Lipid-Protein Interactions of Rhodopsin Investigated by Molecular Dynamics Simulations" 2009 Biophysical Society Annual Meeting, Boston MA.

A. Vogel, G. Reuther, K.T. Tan, H. Waldmann, S.E. Feller, M.F. Brown, and D. Huster, "Backbone Conformation and Dynamics of the Lipid-Modified Membrane Anchor of Human N-Ras Investigated by Solid-State NMR and Molecular Dynamics Simulations**"** 2009 Biophysical Society Annual Meeting, Boston MA.

G. Khelashvili, A. Grossfield, S.E. Feller, M.C. Pitman, H. Weinstein, "Structural and dynamic effects of cholesterol at preferred sites of interaction with rhodopsin identified from microsecond length molecular dynamics simulations" 2009 Biophysical Society Annual Meeting, Boston MA.

S.P. Soni, J. Runyan, G. Birch, J.A. Ward, S.E. Sen, S.E. Feller, S.R. Wassall, "The Effect of *Trans* Unsaturation on Molecular Organization in a Phospholipid Membrane" 2009 Biophysical Society Annual Meeting, Boston MA.

B. Mertz, S.E. Feller, M.F. Brown, "Computational Insights into Retinal Dynamics in Rhodopsin" 2010 Biophysical Society Annual Meeting, San Fransisco CA.

S.E. Feller "Unique lipid-protein interactions observered in molecular dynamics simulations of rhodopsin in a polyunsaturated membrane" 2010 American Society for Biochemistry and Molecular Biology Annual Meeting, Anaheim CA.

PUBLICATIONS (* denotes student co-authors)

1. A.D. Payton and S.E. Feller, "The Absolute Value of the Standard Partial Molar Entropy of the Hydrogen Ion in Aqueous Solution at 25°C", *J. Electro. Chem. Soc.* **137**, 183 (1990).

2. A.D. Payton, T.R. Eubanks, S.E. Feller and T.G. O'Donnell, "A Further Comparison of Theoretical and Experimental Limiting Slopes for the Concentration Dependence of Thermoelectric Powers in Aqueous Hydrochloric Acid at 25 and 15°C", *J. Electro. Chem. Soc.* **137**, 1028 (1990).

3. J.E. Curry, S.E. Feller and D.A. McQuarrie, "A Variational Solution of the Nonlinear Poisson-Boltzmann Equation Inside a Spherical Cavity", *J. Colloid Interface Sci.* **143**, 527 (1991).

4. S.E. Feller and D.A. McQuarrie, "A Variational Solution to the Hypernetted Chain Equation Applied to the Electrical Double Layer", *J. Phys. Chem.* **96**, 3454 (1992).

5. L. Yeomans, S.E. Feller, E. Sanchez and M. Lozada-Cassou, "The Structure of Electrolytes in Cylindrical Pores", *J. Chem. Phys.* **98**, 1436 (1993).

6. S.E. Feller and D.A. McQuarrie, "Calculation of the Force Between Planar Electrical Double Layers Containing Counterion Mixtures", *Mol. Phys.* **80**, 721 (1993).

7. S.E. Feller and D.A. McQuarrie, "Ion Distribution and Force Between Two Charged Plates: A Variational Solution of the Three Point Extension Hypernetted Chain Equations", *J. Colloid Interface Sci.* **162**, 208 (1994).

8. S.E. Feller and D.A. McQuarrie, "Ionic Size Effects on the Force Between Planar Electrical Double Layers", *J. Phys. Chem.* **97**, 12083 (1993).

9. J.A. Greathouse, S.E. Feller and D.A. McQuarrie, "The Modified Gouy-Chapman Theory: Comparison Between Electrical Double Layer Models of Clay Swelling", *Langmuir*, **10**, 2125 (1994).

10. S.E. Feller, Y. Zhang, R.W. Pastor and B.R. Brooks, "Molecular Dynamics Simulation at Constant Pressure: The Langevin Piston Method", *J. Chem. Phys.*, **103**, 4613 (1995).

11. R.W. Pastor and S.E. Feller, "Time Scales of Lipid Dynamics and Molecular Dynamics", in *Membrane Structure and Dynamics*, K.M. Merz and B. Roux (Eds.), Birkhauser, Boston, (1996).

12. Y. Zhang, S.E. Feller, B.R. Brooks and R.W. Pastor, "Computer Simulation of Liquid Interfaces I: Theory and Application to Octane/Water", *J. Chem. Phys.*, **103**, 10252 (1995).

13. S.E. Feller, Y. Zhang and R.W. Pastor, "Computer Simulation of Liquid Interfaces II: Surface Tension-Area Dependence of a Bilayer and Monolayer", *J. Chem. Phys.*, **103**, 10267 (1995).

14. N. Tjandra, S.E. Feller, R.W. Pastor and A. Bax, "Rotational Diffusion Anisotropy of Human Ubiquitin from ^{15}N NMR Relaxation", *J. Amer. Chem. Soc.*, **117**, 12562 (1995).

15. S.E. Feller and R.W. Pastor, "On Simulating Lipid Bilayers with an Applied Surface Tension: Periodic Boundary Conditions and Undulations", *Biophys. J.*, **71**, 1350 (1996).

16. S.E. Feller, R.W. Pastor, A. Rojnuckarin, S. Bogusz and B.R. Brooks, "The Effect of Force Truncation on MD Simulations of Bulk Water Transport Properties and Interfacial Water Structural Properties", *J. Phys. Chem.*, **100**, 17011 (1996).

17. S.E. Feller and R.W. Pastor, "Length Scales of Lipid Dynamics and Molecular Dynamics", in *Proceedings of the Pacific Symposium on Biocomputing*. R.B. Altman, A.K. Dunker, L. Hunter, T.E. Klein, Eds. World Scientific, Singapore, pp. 142-150 (1997).

18. S.E. Feller, D. Yin, R.W. Pastor and A. MacKerrell, Jr., "Molecular Dynamics Simulation of Unsaturated Lipids at How Hydration: Paramterization and Comparison with Diffraction Studies", *Biophysical J.*, **73**, 2269-2279 (1997).

19. S.E. Feller, R.M. Venable and R.W. Pastor, "Computer Simulation of a DPPC Phospholipid Bilayer: Structural Changes as a Function of Molecular Surface Area", *Langmuir*, **13**, 6555-6561 (1997).

20. H.I Petrache, S.E. Feller and J.F. Nagle, "Partial Volumes from MD Simulations", *Biophysical J.*, **72**, 2237-2241 (1997).

21. R.S. Armen*, O.D. Uitto* and S.E. Feller, "Phospholipid Component Volumes. I. Determination and Application to Diffraction Refinement Methods", *Biophysical J.*, **75**, 734-744 (1998).

22. S.E. Feller and R.W. Pastor, "Constant Surface Tension Simulations of Lipid Bilayers: the Sensitivity of Surface Areas and Compressibilities", *J. Chem. Phys.*, **111**,1281-1287 (1999).

23. S.E. Feller, D. Huster and K. Gawrisch, "Interpretation of NOESY Cross-relaxation Rates from Molecular Dynamics Simulation of a Lipid Bilayer", *J. Amer. Chem. Soc.*, **121**, 8963-8964 (1999).

24. S.E. Feller and A.D. MacKerell, Jr., "An Improved Empirical Potential Energy Function for Molecular Simulations of Phospholipids", *J. Phys. Chem. B*, **104**, 7510-7515 (2000).

25. S.E. Feller, "Molecular Dynamics Simulations of Lipid Bilayers", *J. Curr Opin. Coll. Int. Sci.*, **5**, 217-223 (2000).

26. S.E. Feller and C.F. Blaich, "Error Estimates for Fitted Parameters: Application to HCl/DCl Vibrational-Rotational Spectroscopy", *J. Chem. Ed.*, **77**, 409-412 (2001).

27. S.E. Feller, "Molecular Dynamics Simulation of Phospholipid Bilayers" *in* Lipid Bilayers, John Katsaras and Thomas Gutberlet (Eds.), Springer, 2000:89-107.

28. M.J. Schneider* and S.E. Feller, "Molecular Dynamics Simulations of a Phospholipid Detergent Mixture", *J. Phys. Chem.*, **105**, 1331-1337 (2001).

29. S.E. Feller, K. Gawrisch and A.D. MacKerell, Jr., "Polyunsaturated Fatty Acids in Lipid Bilayers: Intrinsic and Environmental Contributions to Their Unique Physical Properties", *J. Amer. Chem. Soc.*, **124**, 318-326 (2002).

30. S.E. Feller, C.A. Brown*, D.T. Nizza and K. Gawrisch, "NOESY cross-relaxation rates and ethanol distribution across membranes", *Biophys. J.*, **82**, 1396-1404 (2002).

31. M.L. Strader* and S.E. Feller, "A Flexible All-atom Model of Dimethylsulfoxide for Molecular Dynamics Simulations", *J. Phys. Chem. A*, **106**, 1074-1080 (2002).

32. A.T.S. Taylor and S.E. Feller, "Structural Studies of Phycobiliproteins from *Spirulina*: Combining Spectroscopy, Thermodynamics, and Molecular Modeling in an Undergraduate Biochemistry Experiment", *J. Chem. Ed*., **79**, 1467 (2002).

33. R.W. Pastor, R.M. Venable and S.E. Feller, "Lipid Bilayers, NMR Relaxation, and Computer Simulations", *Acc. Chem. Res*., **35**, 438-446 (2002).

34. H.A. Stern and S.E. Feller, "Calculation of the Dielectric Permitivitty Profile for a Nonuniform System: Application to a Lipid Bilayer Simulation", *J. Chem. Phys.*, **118**, 3401-3413 (2003).

35. S.E. Feller, K. Gawrisch, and T.B. Woolf, "Rhodopsin Exhbits a Preference for Solvation by Polyunsaturated Docosohexaenoic Acid", *J. Amer. Chem. Soc*., **125**, 4434-4435 (2003).

36. N.V. Eldho, S.E. Feller, S. Tristram-Nagle, I.V. Polozov, K. Gawrisch, "Polyunsaturated Docosahexaenoic vs. Docosapentaenoic Acid – Differences in Lipid Matrix Properties from the Loss of One Double Bond", *J. Amer. Chem. Soc.*, **125**, 6409-6421 (2003).

37. D.R. Carl* and S.E. Feller, "Free Energy of Water Transfer into a Hydrophobic Medium: The Effect of Polyunsaturation", *Langmuir*, **19**, 8560-8564 (2003).

38. S.E. Feller, R.F. Dallinger, and P.C. McKinney, **"**A Program of Computational Chemistry Exercises for the First-Semester General Chemistry Course", *J. Chem. Ed.*, **81**, 283-287 (2004).

39. N. Kurcerka, J.F Nagle, S.E. Feller and P. Balgavy, "Models to analyze small angle neutron scattering from unilamellar lipid vesicles", *Phys Rev E*. **69**, 051903 (2004).

40. C. Roach, S.E. Feller, J.A. Ward*, S.R. Shaikh, M. Zerouga, and W. Stillwell, "Comparison of *Cis* and *Trans* Fatty Acid Containing Phosphatidylcholines on Membrane Properties", *Biochemistry* **43**, 6344-6351 (2004).

41. Pitman, M. C.; Suits, F.; MacKerell, A. D., Jr.; Feller, S. E., "Molecular-Level Organization of Saturated and Polyunsaturated Fatty Acids in a Phosphatidylcholine Bilayer Containing Cholesterol", *Biochemistry* **43**, 15318-15328 (2004).

42. Pitman, M. C.; Grossfield, A.; Suits, F.; Feller, S. E., "Role of cholesterol and polyunsaturated chains in lipid-protein interactions: Molecular dynamics simulation of rhodopsin in a realistic membrane environment", *J. Am. Chem. Soc* **127**:4576-4577 (2005).

43. Suits, F.; Pitman, M. C.; Feller, S. E., "Molecular Dynamics Investigation of the Structural Properties of Phosphatidylethanolamine Lipid Bilayers", *J. Chem. Phys.* 122:244714 (2005).

44. Pitman, M. C.; Suits, F.; Gawrisch, K.; Feller, S. E., "Molecular Dynamics Investigation of the Dynamical Properties of Phosphatidylethanolamine Lipid Bilayers", *J. Chem. Phys.* 122:244715 (2005).

45. Feller, S.E.; Gawrisch, K., "Properties of docosahexaenoic acid-containing lipids and their influence on the function of the GPCR rhodopsin", *Curr. Opin. Struct. Bio*. **15**:416-422 (2005).

46. Carrillo-Tripp, M., Feller, S.E., "Evidence for a Mechanism by Which ω-3 Polyunsaturated Lipids May Affect Membrane Protein Function", *Biochemistry* **44**:10164-10169 (2005).

47. Fitch, B.G.; Rayshubskiy, A.; Eleftheriou, M.; Ward. C.J.T.; Giampapa, M.; Zhestkov, Y.; Pitman, M.C.; Suits, F.; Grossfield, A.; Pitera, J.; Swope, W.; Zhou, R.; Germain, R.S., Feller, S.E., "Blue Matter: Strong Scaling of Molecular Dynamics on Blue Gene/L", IBM Research Technical Report RC3688 (2005).

48. Grossfield, A.; Feller, S. E.; Pitman, M. C., "A role for direct interactions in the modulation of rhodopsin by ω-3 polyunsaturated lipids", *Proc. Nat. Acad. Sci* **103**: 4888-4893 (2006).

49. Grossfield, A.; Feller, S. E.; Pitman, M. C., "Contribution of Omega-3 Fatty Acids to the Thermodynamics of Membrane Protein Solvation", *J. Phys. Chem. B* **110**: 8907-8909 (2006).

50. Martínez-Mayorga, K.; Pitman, M.C.; Grossfield, A.; Feller, S.E.; Brown, M.F., "Retinal Counterion Switch Mechanism in Vision Evaluated by Molecular Simulations", *J. Am. Chem. Soc*. **128**: 16502-16503 (2006).

51. Grossfield, A.; Feller, S. E.; Pitman, M. C., "Convergence of Molecular Dynamics Simulations of Membrane Proteins", *Proteins: Struc Func Gen* **67**: 31-40 (2007)

52. Alexander Vogel, A.; Tan, K.T.; Waldmann, H.; Feller, S.E.; Brown, M.F.; Huster, D. "Flexibility of Ras Lipid Modifications Studied by ^{2}H Solid-State NMR and Molecular Dynamics Simulations", *Biophys. J*. **93**: 2697-2712 (2007).

53. P.W. Lau, A. Grossfield, S.E. Feller, M.C. Pitman, M.F. Brown, "Dynamic Structure of Retinylidene Ligand of Rhodopsin Probed by Molecular Simulations", *J. Mol. Bio*. **372**: 906-917 (2007).

54. S.E. Feller, "Acyl Chain Conformations in Phospholipid Bilayers: A Comparative Study of Docosahexaenoic Acid and Saturated Fatty Acids", *Chem. Phys. Lipids* **153**: 76-80 (2008).

55. N. Kucerka, J.F. Nagle, J.N. Sachs, S.E. Feller, J. Pencer, A.J. Jackson, and J. Katsaras, "Lipid bilayer structure determined by the simultaneous analysis of neutron and x-ray scattering data", *Biophys. J*. **95**: 2356-2367 (2008).

56. A. Grossfield, M.C. Pitman, S.E. Feller, O. Soubias, K. Gawrisch, "Internal hydration increases during activation of the G-protein-coupled receptor rhodopsin", *J. Mol. Bio*. **381**: 478-486 (2008).

57. M. Roark, S.E. Feller, "Structure and Dynamics of a Fluid Phase Bilayer on a Solid Support as Observed by a Molecular Dynamics Computer Simulation", *Langmuir*, **24**: 12469–12473 (2008).

58. G.F. Salgado, R. Marquant R, A. Vogel, I.D. Alves, S.E. Feller, N. Morellet, S. Bouaziz, "Structural Studies of HIV-1 Gag p6ct and Its Interaction with Vpr Determined by Solution Nuclear Magnetic Resonance", *Biochemistry*, **48**: 2355-2367 (2009).

59. G. Khelashvili, A. Grossfield, S.E. Feller, M.C. Pitman, H. Weinstein, "Structural and dynamic effects of cholesterol at preferred sites of interaction with rhodopsin identified from microsecond length molecular dynamics simulations", *Proteins*, **76**:403-417 (2009).

60. M. Roark, SE Feller, "Molecular Dynamics Simulation Study of Correlated Motions in Phospholipid Bilayer Membranes", *J. Phys. Chem. B*, **113**: 13229-13234 (2009).

61. S.P. Soni, J.A. Ward*, S.E. Sen, S.E. Feller, S.R. Wassall, "Effect of Trans Unsaturation on Molecular Organization in a Phospholipid Membrane", *Biochemistry*, **48**: 11097-11107 (2009).

62. G.F. Salgado, A. Vogel, R. Marquant, S.E. Feller, S. Bouaziz, I.D. Alves, "The Role of Membranes in the Organization of HIV-1 Gag p6 and Vpr: p6 Shows High Affinity for Membrane Bilayers Which Substantially Increases the Interaction between p6 and Vpr", *J. Med. Chem.*, **52**: 7157-7162 (2009).

63. A. Vogel, G. Reuther, M.B. Roark, K.T. Tan, H. Waldmann, S.E. Feller, D. Huster, "Backbone conformational flexibility of the lipid modified membrane anchor of the human N-Ras protein investigated by solid-state NMR and molecular dynamics simulation", *BBA-Biomembranes*, **1798**: 275-285 (2010).

64. S.R. Wassall, M.A. McCabe, C.D. Wassall, R.O. Adlof, S.E. Feller, "Solid-State H-2 NMR and MD Simulations of Positional Isomers of a Monounsaturated Phospholipid Membrane: Structural Implications of Double Bond Location", *J. Phys. Chem. B*, **114**: 11474-11483 (2010)

65. D.P. Hurst, A. Grossfield, D.L. Lynch, S. Feller, T.D. Romo, K. Gawrisch, M.C. Pitman, P.H. Reggio, "A Lipid Pathway for Ligand Binding Is Necessary for a Cannabinoid G Protein-coupled Receptor", *J. Biol. Chem.*, **285**:17954-17964 (2010)