

Jerome Baudry, Ph.D.

Research Assistant Professor

School of Chemical Sciences,
University of Illinois at Urbana-Champaign
Urbana, IL 61801, USA
jerome@scs.uiuc.edu

Telephone: (217) 244-3210

Grants and Awards:

- ACTIVE: Senior Collaborator (Mary Schuler, PI),
Catalytic Site Definition in insect P450s.
National Institutes of Health R01 GM071826A 08/01/04 – 07/31/08.
- ACTIVE: Co-Principal Investigator (Mary Schuler, PI; Chad Rienstra and Steven Sligar, co-PIs)
Integrated Theoretical and Experimental Studies of P450 Structure and Function
National Institutes of Health R01 GM079530 06/01/07 – 05/31/11
- ABRA award, TransTech Pharma, Inc., 2001
- Highest Honors for Ph.D. thesis, University Paris-6, 1997.
- Atomic Energy Commission, France. Ph.D. grant, 1994-1997

Peer-Reviewed Publications - From Most Recent. (*): Indicates J. Baudry as Corresponding Author.

Biasing Reaction Pathways with Mechanical Force.
C. R. Hickenboth, J.S. Moore, S.R. White, N. R. Sottos, J. Baudry, and S.R. Wilson
Nature, (2007) 446:423-427

(*) van der Waals Interactions and Decrease of the Rotational Barrier of Methyl-size Rotators: A Theoretical Study.
J. Baudry
J. Am. Chem. Soc. (2006) 128(34):11088-11093

Class-Dependent Sequence Alignment Strategy Improves the Structural and Functional Modeling of P450s.
J. Baudry, S. Rupasinghe, and M. Schuler
Protein Eng. Des. Sel. (2006) 19(8):345-353

(*) Can Proteins and Crystals Self-Catalyze Methyl Rotations?
J. Baudry and J.C. Smith
J. Phys. Chem. B. (2005) 109:20572-20578

(*) Structure-based Design and In-Silico Virtual Screening of combinatorial Libraries. A Combined Chemical/Computational Assignment.
J. Baudry and P. Hergenrother
J. Chem. Edu. (2005) 82(6):890-894

Ile115Leu Mutation in the SRS1 Region of an Insect Cytochrome P450 (CYP6B1) Compromises Substrate Turnover via Changes in a Predicted Product Release Channel.
Z. Wen, J. Baudry, M.R. Berenbaum, and M.A. Schuler
Protein Eng. Des. Sel. (2005) 18(4):191-199

A Retinoic Acid Binding Cytochrome P450: CYP120A1 from *Synechocystis* sp. PCC 6803.
N. Ke, J. Baudry, T. Makris, M. A. Schuler and S. G. Sligar
Arch. Biochem. Biophys. (2005) 436:110-120

(*) Complementarities and Convergence of Results in Bacteriorhodopsin Trimer Simulations.
J. Baudry, E. Tajkhorshid and K. Schulten
Biophys. J. (2004). 87:1394-1395

Classical Force Field Parameters for the Heme Prosthetic Group of Cytochrome C.
F. Autenrieth, E. Tajkhorshid, J. Baudry, and Z. Luthey-Schulten
J. Comp. Chem. (2004) 25(13):1613-1622

Structural and Functional Evolution of Insect CYP6B proteins: from Specialist to Generalist P450.
X. Li., J. Baudry, M.R. Berenbaum and M. A. Schuler
Proc. Natl. Acad. Sci. USA. (2004) 101(9):2939-2944.

Identification of Variable Amino Acids in the SRS1 Region of CYP6B1 Modulating Furanocoumarin Metabolism.
L. Pan, Z. Wen, J. Baudry, M.R. Berenbaum and M.A. Schuler
Arch. Biochem. Biophys. (2004) 422(1):31-41.

Common Active Site Architecture and Binding Strategy of Four Phenylpropanoid P450s from *Arabidopsis thaliana* as Revealed by Molecular Modeling.
S. Rupasinghe, J. Baudry and M. A. Schuler
Protein Engineering (2003) 16:721-731.

Molecular Docking of Substrates and Inhibitors in the Catalytic Site of CYP6B1, an Insect Cytochrome P450 Monooxygenase.
J. Baudry, W. Li, L. Pan, M.R. Berenbaum and M. A. Schuler
Protein Engineering (2003) 16(8):577-587.

A β , Aging, and Alzheimer's disease: A Tale, Models, and Hypotheses.
M.O. Chaney, J. Baudry, C. Esh, J. Childress, D.C. Luehrs, T.A. Kokjohn and A.E. Roher
Neurol. Res., (2003), 25(6):581-590

Molecular Basis for the Subtype Discrimination of the Estrogen Receptor Beta Selective Ligand, Diarylpropionitrile.
J. Sun, J. Baudry, J.A. Katzenellenbogen, and B.S. Katzenellenbogen
Mol. Endocrinol. (2003) 17(2):247-258

Steered Molecular Dynamics Investigations of Protein Function.
B. Isralewitz, J. Baudry, J. Gullingsrud, D. Kosztin, and K. Schulten
Journal of Molecular Graphics and Modeling, (2001) 19:13-25

Molecular Dynamics Study of Bacteriorhodopsin and the Purple Membrane.
J. Baudry, E. Tajkhorshid, F. Molnar, J. Phillips and K. Schulten
J. Phys. Chem. B. Feature article (2001) 105(5):905-918

Oligomerization and Fibril Assembly of the Amyloid-beta Protein.
A.E. Roher, J. Baudry, M.O. Chaney, Y.M. Kuo and M.R. Emmerling

Biochemica et Biophysica Acta - Molecular Basis of Disease, (2000) 1502 (1):31-43

From Sequence to Structure and Function: Modelling and Simulation of Light-Activated Membrane Proteins.
J. Baudry, S. Crouzy, B. Roux and J.C. Smith

Genomics and Proteomics- functional and computational aspects. S. Suhai (Ed), Kluwer Academic/Plenum Publishers N.Y. 2000,141-147.

Molecular Dynamics Study of the Nature and Origin of the Twisted Structure of the Retinal Chromophore in Bacteriorhodopsin.

E. Tajkhorshid, J. Baudry, K. Schulten and S. Suhai
Biophys. J. (2000) 78:683-693

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.

S. Crouzy, J. Baudry, J.C. Smith and B. Roux
J. Comp. Chem. (1999) 20,15:644-1658

Simulation Analysis of the Retinal Conformational Equilibrium in Dark-Adapted Bacteriorhodopsin.

J. Baudry, S. Crouzy, B. Roux and J.C. Smith
Biophys. J. (1999) 76:1909-1917

Theoretical Study of Hydrogen-Bonded Molecular Systems: From Peptide Dynamics to the Function of Bacteriorhodopsin.

J. Baudry
Ph.D. Thesis (1997), University Pierre and Marie Curie (Paris 6).

Quantum Chemical and Free Energy Simulation Analysis of Retinal Conformational Energetics.

J. Baudry, S. Crouzy, B. Roux and J.C. Smith
J. Chem. Info. Comput. Sci., (1997) 37:1018-1024

Collective Vibrations in the Crystalline Alanine Dipeptide at Very Low Temperatures.

J. Baudry, R.L. Hayward, H.D. Middendorf and J.C. Smith
J. Mol. Struct. Dyn. (Biological Macromolecular Dynamics). (1997) 49-54

Harmonic and Anharmonic Dynamics in Protein and Molecular Crystals.

J.C. Smith, J. Baudry, S. Hery, A. Lamy, A. Micu and M. Souaille
In *Nonlinear Physics: Theory and Experiment*, Eds. M. Alfani, M. Boiti, L. Martina and F. Pempinelli. World Scientific. (1996) 575-581

Molecular Mechanics Analysis of Peptide Group Bonding Cooperativity and Influence on phi and psi Barriers.

J. Baudry and J.C. Smith
Journal of Molecular Structure. (Theochem), (1994) 308:103-113

Education :

- 1997: *Ph.D., Molecular Biophysics*.
University Pierre and Marie Curie (Paris-6), Paris, and Atomic Energy Commission, Saclay, France.
Advisor: Jeremy C. Smith, (Oak Ridge National Laboratory)
Summa cum laude / Très Honorable avec Félicitations.
- 1992 : *Maîtrise (B.S), Cell Biology and Molecular Biophysics*.

University Pierre and Marie Curie (Paris 6), Paris, France.

Professional Experience:

- *August 2006 – present: Research Assistant Professor in Chemical Sciences*
University of Illinois at Urbana-Champaign, School of Chemical Sciences.
Computational chemistry and molecular modeling applied to molecular discovery, chemistry, biochemistry and material sciences/nanosciences.
- *2002 –2006: Senior Research Scientist*
University of Illinois at Urbana-Champaign, School of Chemical Sciences.
- *2000 –2002: Research Scientist*
TransTech Pharma, Inc., North Carolina.
- *1998 - 2000: Postdoctoral Research Associate*
University of Illinois at Urbana-Champaign, Beckman Institute for Advanced Science and Technology.
Research Advisor: Klaus J. Schulten (University of Illinois at Urbana-Champaign)
- *1994 - 1997: Ph.D. Research Associate*
Atomic Energy Commission, Molecular Simulation Laboratory, Saclay, France.
Research Advisor: Jeremy C. Smith (Oak Ridge National Laboratory)
- *1993 - 1994: Research Assistant*
Ministry of Defense and Atomic Energy Commission, Division of Military Applications. Bruyeres-le-Chatel, France.

Teaching, University of Illinois at Urbana-Champaign:

Invited lecturer and/or designed lab projects:

- Chem391: Computational Chemical Biology
- Chem578: Combinatorial Chemistry
- Chem590: Introduction to Chemical Biology
- Chem536: Introduction to Organic Chemistry Research

Workshops designed and organized at the U of I:

- In-silico Ligand Docking (2002 and 2003)
- Nucleic Acids/Ligands Simulations (2002)
- Construction and Volume Calculations in Molecular Crystals (2002)
- Combinatorial Library Design and Screening (2002 and 2003)
- Transition State Analysis and Reaction Modeling (2006)

Professional Service:

Reviewer:

- Biophysical Journal (*Biophys. J.*)
- Journal of the American Chemical Society (*J. Am. Chem. Soc.*)
- Journal of Chemical Education (*J. Chem. Edu.*)
- Journal of Computational Chemistry (*J. Comp. Chem.*)
- Journal of Molecular Modeling (*J. Mol. Model.*)
- Journal of Physical Chemistry-B (*J. Phys. Chem. B*)

- Journal of Physics: Condensed Matter (*J. Phys.: Condens. Matter*)
- Nanotechnology

Grant Application Reviewer:

- The Petroleum Research Fund / American Chemical Society

Membership:

- American Chemical Society

US and International Patents:

- Probes, Systems and Methods for Drug Discovery
A.M.M. Mjalli, C.Y. Wysong, J. Baudry, T.S. Yokum, R. Andrews and W.K. Banner.
Assignee: TransTech Pharma, Inc. Application number: 2003012531
- Systems and Methods for Computer-Aided Molecular Discovery
R.I. Sawafta, J. Baudry M.E. Kutz and G. Subramanian.
Assignee: TransTech Pharma, Inc. Application number: 20040019432.

Oral Presentations:

Molecular Polka: Complex rotations of small molecular rotors in material and biological systems.
University of Wisconsin-Milwaukee. Department of Chemistry and Biochemistry. Invited by Prof. Feinberg. 2007.

From protein function to methyl group rotations and back. Computer simulations of the structure, function and dynamics of protein/ligands interactions and molecular rotors.
University Laval, Quebec-city, Canada. Invited by Prof. Lagüe. 2007.

Molecular Polka: Complex rotations of small molecular rotors in material and biological systems.
7th Understanding Complex Systems Symposium, Urbana, IL, 2007.

From protein function to methyl group rotations and back. Computer simulations of the structure, function and dynamics of protein/ligands interactions and molecular rotors.
University of Tennessee, Knoxville, 2007

Integrated Structural and Functional modeling of P450s: from sequence to structure to ligand discovery.
Atomic Energy Commission, Saclay, France; Invited by Dr F. André, 2006

Molecular Polka: Catalysis of rotation of small molecular rotors through van der Waals interactions.
Beckman Institute for Advanced Science and Technology, Urbana, IL; Invited by Prof. K. Schulten, 2006.

MOE in Material Sciences Simulations: Dynamics of Molecular Rotors in Solid State and Nanosurfaces.
Third Chemical Computing Group User Group Meeting. Montreal, Canada, 2006

Nanobearing at work: Can proteins and crystals self-catalyze methyl rotations?
Beckman Institute for Advanced Science and Technology, Urbana, IL; Invited by Prof. E. Tajkhorsid, 2005.

Low-frequency vibrations in crystals and proteins: Can proteins and crystals self-catalyze methyl rotations?
34th meeting of the Southeast Theoretical Chemistry Association, Knoxville, TN; 2005

Molecular modeling of heme proteins' structure/function.

University of Wisconsin-Milwaukee. Department of Chemistry and Biochemistry. Invited by Prof. B. Feinberg. 2005

Specialization and Specificity of P450s/Substrate Recognition

First Chemical Computing Group User Group Meeting. Montreal, Canada, 2004

The Visualization Laboratory (VizLab): A combined Teaching/Research Platform.

University of Illinois' Classroom Technologies User Group. 2003

Computational chemistry: how modeling is assisting and transforming Chemistry and Biochemistry.

American Chemical Society- SC meeting, Urbana, 2003

Molecular Simulation of a Functional Biomembrane.

Olga G. Nalbandov Symposium, Conference on Membrane Proteins: Experimental and Computational Approaches to Understanding Cellular Function. Invited by Prof. Z. Luthey-Schulten. Urbana, 2002.

Retinal's photoisomerization in bacteriorhodopsin.

218th American Chemical Society meeting, New Orleans, 1999.

Structure-function relationships in bacteriorhodopsin.

Department of Cell and Structural Biology, University of Illinois at Urbana-Champaign, Invited by Prof. T. Ebrey. 1999.

Thermodynamic stability of water in bR's active site.

243th Biophysical Society meeting, Baltimore, 1999

Free energy calculations in molecular modeling.

Paris Molecular Modeling meeting, Saclay, France, 1997

Hydrogen bonds and intermolecular interactions in peptide models.

National Institute of Agronomic Research (I.N.R.A), Jouy-en-Josas, France, 1993

Poster Presentations:

(*): presented in person.

Cyclic transition states in the catalysis of proton transfer in glutamate racemase: implications for antibacterial drug design.

D. Dodd, J. Baudry, K. Pankow, J.G Reese, S.R. Blanke and M.A. Spies.

UIUC Biochemistry Fall Conference, Urbana, 2007

Modeling the interactions of a silica surface embedded with a dipeptide imprint.

L.A. Kinsinger, P.C Lauterbur, and J. Baudry

ACS National Meeting, Atlanta, GA, 2006

(*) Coupling of structural and functional P450 molecular modeling.

J. Baudry and M.A. Schuler.

14th International Conference on Cytochromes P450. Dallas, TX, 2005

(*) MOE as a central platform in computational chemistry classes.

J. Baudry

1st Chemical Computing Group User Group Meeting. Montreal, Canada, 2004

Molecular modeling and site-directed mutagenesis defining catalytic sites in insect P450s metabolizing allelochemicals and insecticides

J. Baudry, X. Li, Z. Wen, L. Pan, M.R. Berenbaum and M.A. Schuler

13th International Conference on Cytochrome P450s, Prague, Czech Republic. 2003

Molecular modeling and site-directed mutagenesis defining catalytic sites in insect P450s metabolizing allelochemicals and insecticides.

J. Baudry, L. Pan, M.R. Berenbaum and M.A. Schuler,

Cell & Molecular Biology / Molecular Biophysics Research Symposium. Beckman Institute for Advanced Science and Technology. Urbana, IL, 2002.

Active site architecture of four phenylpropanoid P450s from *Arabidopsis thaliana* as revealed by molecular modeling.

S. Rupasinghe, J. Baudry, Mary A. Schuler

Cell & Molecular Biology / Molecular Biophysics Research Symposium. Beckman Institute for Advanced Science and Technology. Urbana, IL, 2002

Active site architecture of four phenylpropanoid P450s from *Arabidopsis thaliana* as revealed by molecular modeling.

S. Rupasinghe, J. Baudry, Mary A. Schuler

6th International Symposium on P450 Biodiversity: Functional Biochemistry & Molecular Biology of P450 Cytochromes in Microorganisms, Plants and Insects, Los Angeles, CA, 2002.

Molecular modeling and site-directed mutageneses defining the catalytic site in an insect P450 metabolizing furanocoumarins.

J. Baudry, L. Pan, M.R. Berenbaum and M.A. Schuler

6th International Symposium on P450 Biodiversity: Functional Biochemistry & Molecular Biology of P450 Cytochromes in Microorganisms, Plants and Insects, Los Angeles, CA, 2002.

Molecular dynamics study of the nature and the origin of the twisted structure of the retinal chromophore in bacteriorhodopsin.

E. Tajkhorshid, J. Baudry, K. Schulten and S. Suhai

Workshop on Electronic and structural dynamics of light-induced processes in bacteriorhodopsin, Lausanne, Switzerland.

(*) Theoretical study of the dark-adapted state of bacteriorhodopsin.

J. Baudry, S. Crouzy, B. Roux and J.C. Smith

2nd European Biophysical Societies Association meeting, Orleans, France, 1997

(*) Rotations around the C13=C14 and C15=N16 double bonds in retinal: free energy calculations using an improved force field.

J. Baudry, S. Crouzy, B. Roux and J.C. Smith

7th International conference on Retinal Proteins, Zichron Yaacov, Israel, 1996