BIO:

Professor Jerome Baudry is the Pei-Ling Chan Professor of Biological Sciences, University of Alabama, Huntsville; Department of Biological Sciences. Dr. Baudry obtained his Ph.D. in Molecular Biophysics with the highest Honors from the University of Paris, UPMC/Sorbonne Universities, France. He subsequently joined the group of Klaus Schulten at the University of Illinois at Urbana-Champaign as a post-doc. After his post-doctoral work, Dr. Baudry worked in the pharmaceutical industry as a Research Scientist, and then accepted a Senior Research Scientist position back in Illinois on a non-tenure track research faculty position. Dr. Baudry joined the University of Tennessee, Knoxville and the UT/ORNL Center for Molecular Biophysics as a tenure track Assistant Professor in 2008. In 2014, he was promoted to Associate Professor with tenure. In August 2017, Dr. Baudry joined UAH as Pei-Ling Chan Professor. At UAH, Dr. Baudry's group develops and applies methods and protocols for computational drug discovery, both on small-molecules and biologicals, within academic, national laboratories and industrial collaborations.

Positions:

2014 – 2017: Pei-Ling Chan Professor of Biological Sciences, University of Alabama, Huntsville.

2014 – 2017: Associate Professor with Tenure. University of Tennessee, Knoxville. Department of Biochemistry and Cellular and Molecular Biology (BCMB)
UT/ORNL Center for Molecular Biophysics, Oak Ridge National Laboratory
UT/ORNL Genome Science and Technology
UT Department of Pharmaceutical Sciences, College of Pharmacy.

2008 – 2014: Assistant Professor,
University of Tennessee, Knoxville. Department of Biochemistry and Cellular and Molecular Biology.

2006 –2008: Research Assistant Professor in Chemical Sciences (non tenure-track)
University of Illinois at Urbana-Champaign, School of Chemical Sciences.

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

1994 - 1997: PhD. Student
University of Paris UPMC, Molecular Biophysics graduate school, Paris, France,
and Atomic Energy Commission, Molecular Simulation Laboratory, Saclay, France.
Research Advisor: Jeremy C. Smith

1993 - 1994: Military Service, Research Associate.
Ministry of Defense and Atomic Energy Commission. Direction of Military Applications, Bruyères-le-Châtel, France.

RESEARCH INTERESTS:

- Drug discovery
- Computational biology
- Molecular biophysics
- Pharmaceuticals
- Molecular modeling

EDUCATION:

Ph.D., Molecular Biophysics.
University of Paris UPMC - Sorbonne Universités, Paris, France.
Highest Honors ("Très Honorable avec Félicitations").

PEER-REVIEWED PUBLICATIONS - FROM MOST RECENT.
***An asterisk (*) indicates J. Baudry as Corresponding Author*.**

68. (*) Thermophilic Enzyme or Mesophilic Enzyme with Enhanced Thermostability: Can We Draw a Line?
X Jing, W Evangelista Falcón, J Baudry, EH Serpersu
The Journal of Physical Chemistry B. **DOI:** 10.1021/acs.jpcb.7b04519. 2017

67. Identification and Structure-Activity Relationships of Novel Compounds that Potentiate the Activities of Antibiotics in Escherichia coli
KM Haynes, N Abdali, V Jhawar, HI Zgurskaya, JM Parks, AT Green, Jerome Baudry, Valentin V Rybenkov, Jeremy C Smith, John K Walker
Journal of Medicinal Chemistry. **DOI:** 10.1021/acs.jmedchem.7b00453. 2017

66. Structure-based design of broadly protective group a streptococcal M protein-based vaccines
JB Dale, PR Smeesters, HS Courtney, TA Penfound, CM Hohn, JC Smith, J. Baudry
Vaccine 35 (1), 19-26. 2017

65. Novel small molecule JP-153 targets the Src-FAK-paxillin signaling complex to inhibit VEGF-induced retinal angiogenesis
Jordan J. Toutounchian, Jayaprakash Pagadala, Duane D. Miller, Jerome Baudry, Frank Park, Edward Chaum and Charles R. Yates
Molecular Pharmacology January 1, 2017, 91 (1) 1-13;

64., Structure-based design of broadly protective group a streptococcal M protein-based vaccines
James B. Dale, Pierre R. Smeesters, Harry S. Courtney, Thomas A. Penfound, Claudia M. Hohn, Jeremy C. Smith, Jerome Y. Baudry
Vaccine, Volume 35, Issue 1, 2017, Pages 19-26, ISSN 0264-410X,.

63. A computationally identified compound antagonizes excess FGF-23 signaling in renal tubules and a mouse model of hypophosphatemia
By Zhousheng Xiao, Demian Riccardi, Hector A. Velazquez, Ai L. Chin, Charles R. Yates, Jesse D. Carrick, Jeremy C. Smith, Jerome Baudry, L. Darryl Quarles.
Sci. Signal.22 Nov 2016 : ra113

62. Reviving Antibiotics: Efflux Pump Inhibitors That Interact with AcrA, a Membrane Fusion Protein of the AcrAB-TolC Multidrug Efflux Pump
Narges Abdali, Jerry M. Parks, Keith M. Haynes, Julie L. Chaney, Adam T. Green, David Wolloscheck, John K. Walker, Valentin V. Rybenkov, Jerome Baudry, Jeremy C. Smith, and Helen I. Zgurskaya
ACS Infectious Diseases 2016
DOI: 10.1021/acsinfecdis.6b00167

61. (*) Highly Dynamic Anion–Quadrupole Networks in Proteins
Karan Kapoor, Michael R. Duff, Amit Upadhyay, Joel C. Bucci, Arnold M. Saxton, Robert J. Hinde, Elizabeth E. Howell, and Jerome Baudry
Biochemistry **2016** 55 (43), 6056-6069
DOI: 10.1021/acs.biochem.6b00624

60. (*) Ensemble-based docking: From hit discovery to metabolism and toxicity predictions
W Evangelista, RL Weir, SR Ellingson, JB Harris, K Kapoor, JC Smith, and J. Baudry
Bioorganic & Medicinal Chemistry (2016) 24 (20), 4928-4935
(Baudry co-corresponding author with Smith)

59. Evidence for Osteocalcin Binding and Activation of GPRC6A in β-Cells
M Pi, K Kapoor, R Ye, SK Nishimoto, JC Smith, J Baudry, LD Quarles
Endocrinology (2016) 157 (5), 1866-1880

58. (*) Discovery of Novel Non-Active Site Inhibitors of the Prothrombinase Enzyme Complex
K. Kapoor, N. McGill, C. Peterson, H. Meyers, M. Blackburn and J. Baudry
J. Chem. Inf. Model. (2016) 56 (3), 535-547
(Baudry co-corresponding author with Blackburn)

57. General Trends of Dihedral Conformational Transitions in a Globular Protein
Y. Miao, J. Baudry, JC. Smith and A. McCammon
PROTEINS: Structure, Function, and Bioinformatics (2016) DOI: 10.1002/prot.24996

56. Structural and Functional Evidence for Testosterone Activation of GPRC6A in Peripheral Tissues
M Pi, K Kapoor, Y Wu, R Ye, SE Senogles, SK Nishimoto, DJ Hwang, DD Miller, R Narayanan, JC Smith, J. Baudry, and LD Quarles
Molecular Endocrinology (2015) 29 (12), 1759-1773

55. (*) Discovery of an Inhibitor of Z-Alpha 1 Antitrypsin Polymerization
V. Berthelier, J.B. Harris, K.N. Estenson, and J. Baudry
PLOS ONE (2015) 10.1371/journal.pone.0126256
(Baudry co-corresponding author with Berthelier)

54. Multi-Conformer Ensemble Docking to Difficult Protein Targets
S Ellingson, Y. Miao, J. Baudry and J.C. Smith
J. Phys. Chem. B. (2014), DOI**:** 10.1021/jp506511p

53. (*) Molecular Interactions Between Photosystem I and Ferredoxin: An Integrated Energy Frustration and Experimental Model
D.J. Cashman; T. Zhu; R.F. Simmerman; C. Scott; B.D. Bruce, and J. Baudry

Journal of Molecular Recognition (2014), 27 (10), 597-608.
(Baudry co- corresponding author with Bruce)

52. (*) A Computational Approach Predicting CYP450 Metabolism and Estrogenic activity of an Endocrine Disrupting Compound (PCB-30)
J.B. Harris, M.L. Eldridge, G. Sayler, F. Menn, A.C. Layton, and J. Baudry
Environmental Toxicology and Chemistry (2014), 33 (7), 1615-1623.
(Baudry co- corresponding author with Layton)

51. (*) Polypharmacology and Supercomputer-Based Docking: Opportunities and Challenges
S. Ellingson, J.C. Smith, and J. Baudry
Molecular Simulation, (2014) DOI: 10.1080/08927022.2014.899699
(Baudry corresponding author)

50. **(*)** A Phenylalanine Rotameric Switch for Signal-State Control in Bacterial Chemoreceptors
D. Ortega, C. Yang, P. Ames, J. Baudry, J.S Parkinson, and I. Zhulin
Nature Communications. (2013), 4, DOI:10.1038/ncomms3881
(Baudry co-corresponding author with Zhulin)

49. Conformational Coupling between Receptor and Kinase Binding Sites through a Conserved Salt Bridge in a Signaling Complex Scaffold Protein
D. Ortega, G. Mo., K. Lee, H. Zhou, J. Baudry, D. Dahlquist, and I. Zhulin
PLOS Comp Biol. (2013), DOI: 10.1371/journal.pcbi.1003337

48. **(*)** Homology Modeling of the CheW Coupling Protein of the Chemotaxis Signaling Complex
D. Cashman, D. Ortega., I. Zhulin., and J. Baudry
PLOS One 8(8): e70705. doi:10.1371/journal.pone.0070705
(Baudry corresponding author)

47**. (*)** VinaMPI: Facilitating Multiple Receptor High-Throughput Virtual Docking on High Performance Computers
S. Ellingson, J.C. Smith, and J. Baudry
J. Comput. Chem. (2013) DOI: 10.1002/jcc.23367
(Baudry corresponding author)

46. **(*)** Accelerating Virtual High-Throughput Ligand Docking: Current Technology and Case Study On a Petascale Supercomputer
SR Ellingson, S Dakshanamurthy, M Brown, JC Smith, and J Baudry.
Concurrency and Computation: Practice and Experience. (2013) DOI:10.1002/cpe.3070
(Baudry corresponding author)

45. **(*)** Three Entropic Classes of Side Chains in a Globular Protein
D. C. Glass, M. Krishnan, J. C. Smith, J. Baudry
J. Phys. Chem. B. (2013), 117 (11): 3127-3134
(Baudry corresponding author)

44. **(*)** STAAR: Statistical Analysis of Aromatic Rings
D.D. Jenkins, J.B. Harris, E.E. Howell, R.J. Hinde, J. Baudry
J. Comput. Chem. (2013), 34(6): 518-22
(Baudry corresponding author)

43. Coupled Flexibility Change in Cytochrome P450cam Substrate Binding Determined by Neutron Scattering, NMR, and Molecular Dynamics Simulation
Y. Miao, Z. Yi, C. Cantrell, D.C. Glass, J. Baudry, N. Jain, J.C. Smith
Biophysical journal (2012), 103 (10): 2167-2176

42. Temperature-Dependent Dynamical Transitions of Different Classes of Amino Acid Residue in a Globular Protein
Y. Miao, Z. Yi, D.C. Glass, L. Hong, M. Tyagi, J Baudry, N. Jain, J.C. Smith
J. Am. Chem. Soc. (2012) 134 (48): 19576-19579

41. **(*)** Accelerating Virtual High-Throughput Ligand Docking: Screening One Million Compounds Using a Petascale Supercomputer
S. Ellingson, S. Dakshanamurthy, M. Brown, J.C. Smith, J. Baudry
ECMLS 2012,
(Baudry corresponding author)

40. **(*)** High-Throughput Virtual Molecular Docking with AutoDockCloud
S.R. Ellingson and J. Baudry
Concurrency and Computation: Practice and Experience.2012 doi: 10.1002/cpe.2926
(Baudry corresponding author)

39. Derivation of Mean-Square Displacements for Protein Dynamics from Elastic Incoherent Neutron Scattering
Z. Yi, Y. Miao, J. Baudry, N. Jain, and J. C. Smith
J. Phys. Chem. B. (2012),116 (16): 5028–5036

38. **(*)** Coenzyme-A Binding to the Aminoglycoside Acetyltransferase (3)-IIIb Increases Conformational Sampling of Antibiotic Binding Site.
X. Hu, A.L. Norris, J. Baudry, and E.H. Serpersu.
Biochemistry (2011) 50(48): 10559-10565
(Baudry co-corresponding author)

37. VITAL NMR: Using Chemical Shift Derived Secondary Structure Information for a Limited Set of Amino Acids to Assess Homology Model Accuracy
M.C. Brothers , A.E. Nesbitt, M.J. Hallock, S.G. Rupasinghe, M. Tang, J. Harris, J. Baudry, M.A. Schuler, and C.M. Rienstra
J. Biomolecular NMR. (2011) EPub ahead of print. PMID:22183804

36. **(*)** Active site hydration and water diffusion in cytochrome P450cam: a highly dynamic process.
Y. Miao and J. Baudry
Biophysical Journal, (2011), 101 (6): 1493-1503
(Baudry corresponding author)

35. Arabidopsis NIP7;1: An anther-specific boric acid transporter of the aquaporin superfamily regulated by an unusual tyrosine in helix 2 of the transport pore.
T. Li, C. Won-Gyu, I. Wallace, J. Baudry, and D. Roberts
Biochemistry, (2011), 50(31): 6633–6641

34. **(*)** Three-dimensional mapping of micro-environmental control of methyl rotational barriers.
W.I. Hembree and J. Baudry
J. Phys. Chem. B. (2011**)**, *115* (26): 8575–8580
(Baudry corresponding author)

33. **(*)** High-Throughput Virtual Molecular Docking: Hadoop Implementation of AutoDock4 on a Private Cloud.
S.R. Ellingson and J. Baudry
ECMLS 2011
(Baudry corresponding author)

32. A survey of aspartate-phenylalanine and glutamate-phenylalanine interactions in the protein data bank: searching for anion-π pairs.
V. Phillips, J. Harris, R, Adams, D. Nguyen, J. Spiers, J. Baudry, E.E. Howell and R.J. Hinde
Biochemistry, (2011) 50 (14):2939-2950

31. (*)Task-parallel message passing interface implementation of Autodock4 for docking of very large databases of compounds using high-performance super-computers.
B. Collignon, R. Schulz, J.C. Smith and J. Baudry
J. Comput. Chem. (2011) 32 (6): 1202–1209
(Baudry corresponding author)

Published based on work done before independent position: 30 publications, 14 with Baudry first author, 4 with Baudry corresponding author.

30 other publications

Selected pre-independent papers:

Biasing reaction pathways with mechanical force
CR Hickenboth, JS Moore, SR White, NR Sottos, J Baudry, SR Wilson
Nature 446 (7134), 423-427 (2007)

(*) Van der Waals interactions and decrease of the rotational barrier of methyl-sized rotators: a theoretical study
J Baudry
Journal of the American Chemical Society 128 (34), 11088-11093 (2006)

Determinants of catalytic power and ligand binding in glutamate racemase
MA Spies, JG Reese, D Dodd, KL Pankow, SR Blanke, J Baudry
Journal of the American Chemical Society 131 (14), 5274-5284 (2008)

(*) Can proteins and crystals self-catalyze methyl rotations?
J Baudry, JC Smith
The Journal of Physical Chemistry B 109 (43), 20572-20578 (2005)

(*)Structure-Based Design and In Silico Virtual Screening of Combinatorial Libraries. A Combined Chemical-

Computational Project
J Baudry, PJ Hergenrother
J. Chem. Educ 82 (6), 890 (2005)