

**Jerome Baudry, Ph.D.**

**Associate Professor**

**University of Tennessee, Knoxville**  
**Department of Biochemistry and Cellular and Molecular Biology**  
**UT/ORNL Center for Molecular Biophysics**  
**jbaudry@utk.edu**

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**Ph.D., Molecular Biophysics.**

December 1997. University Pierre and Marie Curie(Paris-6) Paris, France. Advisor: Jeremy C. Smith.  
*Highest Honors ("Très Honorable avec Félicitations")*.

**Positions:**

*2014 – to date: Associate Professor with Tenure,*  
University of Tennessee, Knoxville. Department of Biochemistry and Cellular and Molecular Biology.  
Group Leader, UT/ORNL Center for Molecular Biophysics  
Adjunct faculty, Genome Science and Technology  
Adjunct faculty, Department of Pharmaceutical Sciences, University of Tennessee 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: Graduate Student*  
University Pierre and Marie Curie (Paris-6) 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. Bruyères-le-Châtel, France.

### Research funding since independent tenure-track position

#### Research Grants since 2008:

Total funded to-date (including all collaborative labs): \$5,151,677; Total directly to Baudry lab: \$1,069,053

National Institutes of Health.

SBIR Phase 1

Small molecule inhibitors of PCSK9

Grant total: \$261,259

Funds to Baudry (consulting): \$18,682

Role: UTK PI (industrial partner: Sarfez Pharmaceuticals, Inc.)

This project targets protein:protein interactions through small molecular effectors to modulate function and activity of PCSK9.

National Institutes of Health.

2R01 GM072285-06. 04/01/2015 – 03/30/2020

*Computational Genomics of Signal Transduction*

Grant total: \$1,284,495

Funds to Baudry Lab: \$147,215

Role: Co-investigator / (Igor Zhulin, lead PI, University of Tennessee, Knoxville)

NIH - National Institute of General Medical Sciences

This project aims at integrating together several molecules of the chemotaxis system responsible for signal transduction in bacteria. The Baudry lab is running the molecular simulations to characterize the role of protein/protein interactions and dynamics in the functioning of the multi-protein complex.

National Institutes of Health.

NIH NIAID 2R01AI052293-11A1

08/01/2014 - 07/31/2019

Effort: 11%

*Transport across two membranes by AcrAB-TolC*

Role: Co-PI / UTK lead PI (Elena Zgurskaya, lead PI, University of Oklahoma)

Grant total: \$1,766,412

Funds to Baudry Lab: \$95,013

- This project targets protein:protein interactions through small molecule effectors to address contemporary issues in drug elimination in bacterial cells. The Baudry lab leads the computational aspect of the project using supercomputing tools and protocols developed in the lab to screen large chemical databases against a large number of protein structures.

National Institutes of Health.

- NIAMS Building Interdisciplinary Research Team (BIRT) 4/17/14 - 8/31/15

Role: Co-Investigator / UTK Principal Investigator. (Leigh Quarles, PD. University of Tennessee Health Science Center, Memphis)

Grant total: \$149,427.

Funds to Baudry Lab: \$85,411

- The goal of this project is to discover small molecules capable of modulating the activation of FGFR/ $\alpha$ -Klotho co-receptor complexes in target tissues and regulate the bone release of fibroblastic growth factor 23 (FGF23). The Baudry lab runs the computational aspect of the project using supercomputing tools and protocols developed in the lab to screen large chemical databases against a large number of protein structures.

Department of Energy

Massive Ensemble Docking for Drug Toxicity Prediction

5/01/13 - 4/30/14

Role: Principal Investigator

Grant total: \$71,755.

Funds to Baudry Lab: \$71,755

-This project develops and applies supercomputing protocols to perform massive database screening against large protein databases to identify cross-reactive ligands.

National Institutes of Health. SBIR 1R43HL114261 07/01/2012 – 06/30/2013

Novel Modulators of Plasminogen Activator Inhibitor Functional Activities

Role: co-Principal Investigator (subcontract with Shifa Biopharmaceutical Principal Investigator, Cynthia Peterson lead-PI at UTK)

Grant total: \$347,218. Subcontract funding: \$99,287. Funds to Baudry Lab: \$46,643

-This project aims at discovering novel small molecules effective in the coagulation cascade without the poor side effects of current pharmaceuticals. The Baudry lab is running the entire computational part, i.e., performing massive screening of chemicals against a large number of protein structures to discover chemicals that bind at a protein/protein interfacial region. Tools and protocols developed in the lab are used for the structure-based discovery approach of the project.

The Alpha One Foundation 07/01/2012 – 06/30/2014

Searching for Small Molecules as Potent Inhibitors of Z-AAT

Role: UTK Principal Investigator (Valerie Berthelie Lead PI, UT-Medical Center)

Grant total: \$200,000. Funds to Baudry Lab: \$29,443.

-The goal of this project is to discover small molecules effective against the polymerization of Z-AAT. The Baudry lab is running the entire computational part of the research, i.e. identifying reactive protein states and small molecules capable of binding in these states to prevent polymerization using the screening tools and strategies developed in the lab.

National Institutes of Health. 2R01 GM072285-06 04/01/2010 – 03/31/2014

NIGMS

Computational Genomics of Signal Transduction

Role: Co-Investigator (Igor Jouline, PI. University of Tennessee, Knoxville)

Grant total: \$1,117,757. Funds to Baudry Lab: \$341,249

- This project aims at integrating together several molecules of the chemotaxis system responsible for signal transduction in bacteria. The Baudry lab is running the molecular simulations to characterize the role of protein/protein interactions and dynamics in the functioning of the multi-protein complex.

National Institutes of Health 1KL2RR031974 07/01/2010 – 03/31/2015

Georgetown-Howard Universities Center for Clinical and Translational Science

Role: Pilot Project Task Leader, (Joseph Verbalis, Georgetown University and Thomas Mellman, Howard University, PIs)

Grant total: \$150,000. Funds to Baudry Lab: \$150,000

- The goal of this project is to develop massive screening tools on supercomputing architectures and developed in the lab, and to apply the tools in the discovery of new small molecules capable of modulating the HDAC4 protein in prostate cancer.

Computational Competitive Awards:

US Department of Energy

INCITE Leadership Computing

Role: Co-PI (J.C. Gumbart, Georgia Tech., Lead PI)

Determining the role of AcrA in the bacterial multidrug efflux pump

38M SU hours on Titan, 2017

Computing time attributed to the Baudry lab: 33%

National Center for Computational Sciences (NCCS)

Director Discretionary Application

Role: Principal Investigator

Drugging the undrugable, 2014  
10M SU hours on Titan  
Computing time attributed to the Baudry lab: 100%

National Center for Computational Sciences (NCCS)  
Director Discretionary Application  
Role: Principal Investigator  
Massive screening for drug discovery and toxicity prediction, 2013  
5M SU hours on Titan  
Computing time attributed to the Baudry lab: 100%

National Institutes for Supercomputing Sciences (NICS)  
Role: Principal Investigator  
High-throughput Docking in Undergraduate Curriculum. Awarded 70,000 CPU hours on Kraken Supercomputer for a BCMB undergraduate class, 2013  
Computing time attributed to the Baudry lab: 100%

National Center for Computational Sciences (NCCS)  
Director Discretionary Application  
Role: Principal Investigator  
Dynamics of the Chemotaxis Receptor, 2012  
5M SU hours on Titan  
Computing time attributed to the Baudry lab: 100%

National Resource for Biomedical Supercomputing (NRBSC)/Pittsburgh Supercomputing Center  
Role: Principal Investigator  
Dynamics of the Chemotaxis Receptor on the Anton Supercomputer. 50,000 Anton node-hours.  
Multi-microseconds molecular dynamics simulations of the signaling domain of the bacterial chemotaxis receptor  
Computing time attributed to the Baudry lab: 100%

Amazon/ AWS in Education research grant  
Role: Principal Investigator  
Amazon Cloud Computing Award: Virtual High-Throughput Docking using Cloud Infrastructure. Allocation: 7500 CPU hours  
The project develops and implements virtual docking on Cloud computational architectures.  
Computing time attributed to the Baudry lab: 100%

National Center for Computational Sciences  
Director Discretionary Application  
Role: Task Leader  
High Performance Computing for Rational Drug Discovery and Design, Supercomputing molecular discovery of prostate cancer molecular effectors  
5.8 million CPU hours on Jaguar  
The projects develops and implements virtual docking on High Performance Computers.  
Computing time attributed to the Baudry lab: 100%

National Science Foundation/Teragrid 2008-2009  
Role: Co- Principal Investigator (J.C. Smith, PI)  
Molecular Dynamics Simulations in Bioenergy, Bioremediation and Protein Dynamics 2.4 million CPU hours

National Science Foundation/Teragrid 2009-2010  
Role: Co- Principal Investigator (J.C. Smith, PI)  
Molecular Dynamics Simulations in Bioenergy, Bioremediation and Protein Dynamics 2 million CPU hours

National Center for Computational Sciences  
Director Discretionary Application  
Drugging the “undruggable”: Ensemble discovery of modulators of oncogenic Ras.  
Role: Principal Investigator  
10 M SUs requested on Titan

**US and International Patent Applications with TransTech Pharma:**

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.*

**Invention Disclosure, University of Tennessee:**

Novel FGF-23 Antagonists Determined by Virtual High-Throughput Screening  
Ongoing disclosure application. 2015

Refinement and IP generation for a New Drug Candidate for Type 2 Diabetes  
Ongoing disclosure application. 2015

Computational technology to screen efficiently on supercomputers potential molecular effectors on several protein structures and their isoforms.  
By S. Ellingson, J. Smith & J. Baudry, 2012 (code released in the public domain).

Inhibiting Z-Alpha 1 antitrypsin polymerization  
V. Berthelie and J. Baudry, 2012

**Peer-Reviewed Publications - From Most Recent.**

***An asterisk (\*) indicates a publication with J. Baudry as Corresponding Author:***

**Published since independent tenure-track position at Tennessee (from most recent):**

65. Targeting Src/FAK/Paxillin Signalsome in Neovascular Disease  
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  
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  
In Press. Bioorganic & Medicinal Chemistry (2016)  
(Baudry co-corresponding author with Smith)
59. Evidence for Osteocalcin Binding and Activation of GPRC6A in  $\beta$ -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. Berthelie, J.B. Harris, K.N. Estenson, and J. Baudry  
*PLOS ONE* (2015) 10.1371/journal.pone.0126256  
(Baudry co-corresponding author with Berthelie)
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- $\pi$  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

#### **Honors and Awards, chronological order:**

- Atomic Energy Commission, France. CFA Graduate Fellowship, 1994-1997
- Highest Honors for Ph.D. thesis, University Paris-6, 1997
- ABRA award, TransTech Pharma, Inc., 2001
- University of Tennessee “Quest Scholar” recognition, December 2010.
- Press release and recognition by UTK/ORNL for docking on supercomputer publication (December 2010) [http://web.ornl.gov/ornlhome/print/press\\_release\\_print.cfm?ReleaseNumber=mr20101209-00](http://web.ornl.gov/ornlhome/print/press_release_print.cfm?ReleaseNumber=mr20101209-00)
- Recognition by NICS (National Institute for Computational Sciences) and press release for publication with post-doctoral associate Miao of article in *Biophysical Journal* (2011): <http://www.nics.tennessee.edu/audry-miao> Press release has been re-published by many specialized scientific communication outlets
- Recognition by Quest for article published with post-doctoral associate Miao in *Biophysical Journal*, January 2012
- Outstanding Scholarship Award, Junior Faculty, Department of Biochemistry & Cellular and Molecular Biology, University of Tennessee, 2012.
- Recognition by OLCF (Oak Ridge Leadership Computing Facility) for the American Chemical Society award to graduate student Ellingson. 2013 <https://www.olcf.ornl.gov/2013/06/04/titan-user-recognized-by-the-american-chemical-society/>
- Interview featured in the official Titan description video by OLCF (2013): <http://vimeo.com/52243034> and <http://www.olcf.ornl.gov/titan/>

- Interview and description of work in *Bio-IT World*, leading News publication in the computing industry (2013)

**Honors and Awards to Baudry group members for their work in the Baudry lab:**

*Rebecca Weir, undergraduate student:*

- International Conference for Undergraduate Research (ICUR) (2015) *Toward structure-based prediction of drug candidates' toxicity.* University of Tennessee

*Sally Ellingson, graduate student:*

- American Chemical Society CCG Research Excellence Award. (International award from the American Chemical Society to recognize “the quality and significance of the students’ research”, given to no more than ten students yearly from North- Central and South Americas), 2013. Sally Ellingson is the first UT student to receive this award.
- Science Alliance Graduate Student Award, University of Tennessee, 2013
- Co-PI, High-throughput Docking in Undergraduate Curriculum (Awarded 70,000 CPU hours on Kraken Supercomputer)
- Conference participation grant, SC12 Broader Engagement (BE) Program; 2012
- Neustar scholarship; 2012 Grace Hopper Celebration of Women in Computing (GHC 2012)
- Conference sponsored scholarship; National Biomedical Computation Resource Summer Institute 2012.
- EU-US Summer School on HPC Challenges Participation Grant (XSEDE/Prace)
- Advanced track conference grant; SC11 Broader Engagement (BE); 2011
- NSF funded scholarship to attend Grace Hopper Celebration of Women in Computing (GHC 2011)
- Grad Cohort 2011; Committee on the Status of Women in Computing Research (CRA-W)
- Conference participation grant; the SC10 Broader Engagement (BE) Program; 2010
- SCALE-IT (Scalable Computing and Leading Edge Innovative Technologies in Biology) (IGERT/NSF) graduate student training program 2009-2011

*Jason Harris, graduate student:*

- Science Alliance Graduate Student Award, University of Tennessee, 2014
- Research Grant Award. (\$60,000) Internal Research Grant. University of Tennessee (SCALE-IT). 2013-2014.
- Conference Travel Award. Protein Society Symposium. Boston, MA. July 20-24th, 2013.

- Conference Travel Award. Amount. Computational Biophysics to Systems Biology (CBSB13). Norman, Oklahoma. May 19-21, 2013
- Research Grant Award (\$15,000) Internal Research Grant. University of Tennessee (SCALE-IT). August 2012- July, 2013.
- Workshop Scholarship Award. 7th National Biomedical Computation Resource (NBCR) Summer Institute. La Jolla, California, July 30th- August 3rd, 2012.

*Chelsea Knotts, undergraduate researcher:*

- Competitive Research Stipend, UTK Chancellor's Office and Office of Research, 2011.
- Torchbearer Award, the highest student honor conferred by the University of Tennessee, 2012.

*Andrew Sneed, undergraduate researcher:*

BCMB Department, Best Undergraduate Award, Spring 2009.

*William Hembree, undergraduate researcher in the Baudry laboratory:*

University of Tennessee's "*QUEST Scholar*" recognition for his undergraduate research work and publishing as first author a publication with Jerome Baudry in the *Journal of Physical Chemistry, B*. (publication # 34). April 2012

**Invited Presentations since independent tenure-track at Tennessee:**

*Talks by Jerome Baudry:*

Using supercomputers to discover new pharmaceuticals  
2016 Advancing Computational Biology @ Howard University Symposium  
Howard University, Washington DC  
April 2016

The Role of Protein Dynamics in structure-based drug discovery: the case of membrane proteins.  
Frontiers in Structural Biology of Membrane Protein & Pittsburgh Diffraction Conference  
University of Alabama in Huntsville  
March 2016

Supercomputing, virtual screening and molecular discovery: methods, applications and challenges  
University of Tennessee College of Pharmacy, Memphis, TN  
April 2014.

Supercomputing, virtual screening and molecular discovery: methods, applications and challenges  
Georgia Institute of Technology, Atlanta, GA  
April 2014.

Big Data Methods for Developing New Pharmaceuticals  
50th HPC User Forum

Boston, MA, 2013

Supercomputing and drug discovery: what's so "super" about that?  
East Tennessee State University, March 2013

2012 Smoky Mountains Computational Sciences and Engineering Conference  
Drug discovery at the petascale and big data.  
Gatlinburg, TN, September 2012

Insights on the utilization of *in silico* technologies to promote early stage drug discovery.  
3<sup>rd</sup> Annual Drug Discovery Conference, "Easing the Bottleneck".  
Invited session speaker, Boston, MA. October 2011.

Computational Drug Discovery on Supercomputers  
Department of Chemistry, Appalachian State University, NC. September 2011.

What's Up Doc(k)? Development and applications of virtual protein/ligand docking.  
University of California, San Diego, CA. March 2011.

What's Up Doc(k)? Development and applications of virtual protein/ligand docking.  
University of California, Irvine, CA. March 2011

Supercomputing a sustainable environment: coupling biology and the world's top supercomputer to identify environmental pollutants.  
SACNAS conference, Anaheim, CA, October 2010

Methyl rotational dynamics in biomolecules  
University of Heidelberg, Germany, December 2009

Computational structure-based protein/ligand approaches to bioremediation and detoxification.  
Atomic Energy Commission, Saclay, France, 2009

Talks and poster Presented by Baudry group's members:

*Presented by Dr. Derek Casham, post-doctoral associate:*

Cashman, D.J.; Ortega, D.; Zhulin, I.B.; Baudry, J.Y. A Molecular Jigsaw Puzzle: Putting the Pieces of the Bacterial Chemotaxis System Together.  
ReceptorFest XIV, Salt Lake City; 2011.

*Presented by Dr. Yinglong Miao, postdoctoral associate:*

Miao, Y. and J. Baudry.  
Active site hydration and water diffusion in cytochrome P450cam: a highly dynamic process.  
56<sup>th</sup> Annual Biophysical Society Meeting, San Diego, CA, 2012

(poster) Miao, Y., Z. Yi, N. Jain, J. Baudry and J. C. Smith.  
Decomposition of Neutron Scattering Spectra with Molecular Dynamics Simulations on Dynamics of Cytochrome P450cam.  
Computational Physics Conference, Gatlinburg, TN, 2011

(poster) Miao, Y., Z. Yi, N. Jain, J. Baudry and J. C. Smith.  
Dynamics of Cytochrome P450cam Investigated with Molecular Dynamics Simulations and Neutron Scattering Experiments. Neutron dynamics data bank (nDDB) workshop, Institute Laue Langevin (ILL), Grenoble, France, 2011

(poster) Miao, Y., Z. Yi, N. Jain, J. C. Smith and J. Baudry: Dynamics of Cytochrome P450cam Investigated with Molecular Dynamics Simulations and Neutron Scattering Experiments. Summer School in Biophysics at UT/ORNL, Knoxville, TN, 2010

(poster) Miao, Y., Z. Yi, N. Jain, J. C. Smith and J. Baudry: Dynamics of Substrate Access Channel and Active Site in Cytochrome P450cam Investigated with Molecular Dynamics Simulations and Neutron Scattering Experiments.  
54<sup>th</sup> Annual Biophysical Society Meeting, San Francisco, CA, 2010

*Presented by Dr. Barbara Collignon, postdoctoral associate:*

(poster) B. Collignon, R. Schulz, J.C. Smith, J. Baudry  
Task-Parallel MPI Implementation of Autodock4 for Docking of Very Large Databases of Compounds using High Performance Super-Computers.  
SC10 Supercomputing Conference, New Orleans, LA, 2010

*Presented by Sally Ellingson, GST/SCALE-IT graduate student:*

(poster) S.R. Ellingson, J Smith, and J. Baudry.  
Acceleration of High-Throughput Molecular Docking for Novel Drug Discovery on Supercomputers  
ACS National Meeting , New Orleans, LA, 2013  
(American Chemical Society CCG Research Excellence Award, 2013)

(poster) S.R. Ellingson and J. Baudry  
Acceleration of High-Throughput Molecular Docking for Novel Drug Discovery on Supercomputers  
Smoky Mtn. Computational Sciences and Engineering Meeting, Gatlinburg, TN, 2013

S.R. Ellingson, J.C. Smith and J. Baudry.  
Accelerating Virtual High-Throughput Ligand Docking: Screening One Million Compounds Using a Petascale Supercomputer.  
HPDC12 workshop on Emerging Computational Methods in the Life Sciences, 2012

S.R. Ellingson and J. Baudry.  
Virtual high-throughput molecular docking.  
JICS/GRS Joint Workshop on Large Scale Computer Simulation, 2012

(poster) S.R. Ellingson, J Smith, and J. Baudry.  
Towards High-Throughput Virtual Docking with Multiple Receptor Conformations on High-Performance Computers.  
Smoky Mtn. Computational Sciences and Engineering Gatlinburg, TN, 2012

(poster) S.R. Ellingson, J Smith, and J. Baudry. Towards High-Throughput Virtual Docking with Multiple Receptor Conformations on High-Performance Computers  
Communities Resource Fair SC12 Salt Lake City, UT, 2012

(poster) S.R. Ellingson and J. Baudry.

High-throughput Virtual Molecular Docking on High-Performance Computers (CBSB12 Knoxville, TN and NBCR-SI 2012 La Jolla, CA); 2012

S.R. Ellingson and J. Baudry.

High-Throughput Virtual Molecular Docking: Hadoop Implementation of AutoDock4 on a Private Cloud HPDC11 workshop on Emerging Computational Methods in the Life Sciences, 2011

(poster) S.R. Ellingson and J. Baudry.

High-Throughput Virtual Molecular Docking within the MapReduce Framework of Hadoop ACM-SRC session at GHC11 Portland, OR, 2011

(poster) S.R. Ellingson and J. Baudry.

High-Throughput Virtual Molecular Docking within the MapReduce Framework of Hadoop Communities Resource Fair SC11 Seattle, WA, 2011

(poster) S.R. Ellingson and J. Baudry.

Screening for potential novel drugs with the power of cloud computing CRA-W Grad Cohort Boston, MA 2011

(poster) S.R. Ellingson and J. Baudry.

Screening for potential novel drugs with the power of cloud computing Tennessee Celebration of Women in Computing, 2011

(poster) S.R. Ellingson and J. Baudry. Drug Discovery in a Cloud

Supercomputing EC10, New Orleans, LA, 2010

*Presented by Jason Harris, GST/SCALE-IT graduate student:*

(poster) J.B. Harris, D.D. Jenkins, J. Reyles, S.Rickett, J.M. Utley, E.E. Howell, J.Baudry, R.J. Hinde.

Determining Anion- Quadrupole Interactions Among Protein, DNA, and Ligand Molecules.

Annual UT-ORNL-KBRIN Bioinformatics Summit. Cadiz, KY; April 2011

(Poster and oral) J. B. Harris. Using High-Performance Supercomputing to Find Endocrine Disruptors: A Fast Track to Discovering New Medicines and Protecting the Environment.

NSF-IGERT 2011 Poster Competition. 2011

(poster) J. B. Harris. Modeling the Specific P450 Metabolism and Induced Estrogenic Activity of PCB-30<sub>2</sub>

National Biomedical Computation Resource Summer Institute,

NBCR-SI; La Jolla, CA; August 2012

(poster) J. B. Harris, V. Berthelier, K. Estenson, J. Baudry. Binding of a small molecule prevents polymerization of mutant alpha-1-antitrypsin and reveals a new binding site for drug discovery.

Protein Society Symposium. Boston, MA.; July 2013

*Presented by Jonathan Reyles, GST/SCALE-IT rotation graduate student:*

(poster) J.Reyles, Y.Miao, J.Baudry, J.C. Smith. Dynamics investigation of the cytochrome p450cam Active site mutant Thr252Ala.

Biophysical Society Meeting, Baltimore, Maryland, 2011.

<b>Teaching since independent tenure-track position</b>				
<b>Classes taught at UTK since 2008</b>	<b>Course #</b>	<b>Course name</b>	<b>Credit Hrs.</b>	<b>% Responsibility for Shared Instruction</b>
Spring 2008	420/610/560	Computational Biology & bioinformatics	3	25%
Fall2008	695	Introduction to Molecular Biophysics	1	33%
Fall2008	615	Advances in Molecular Biophysics	1	33%
Fall2008	140	Introduction to Cell Biology	4	33%
Spring 2009	615	Advances in Molecular Biophysics	1	33%
Spring 2009	420/610/560	Computational Biology & bioinformatics	3	25%
Spring 2009	420	Computational Biology & bioinformatics	3	33%
Fall 2009	615	Advances in Molecular Biophysics	1	33%
Fall 2009	695	Introduction to Molecular Biophysics	1	33%
Spring 2010	420 – sect 1	Computational Biology & bioinformatics	3	33%
Spring 2010	420 – sect2	Computational Biology & bioinformatics	3	33%
Fall 2010	140	Introduction to Cell Biology	4	50%
Fall 2010	615	Advances in Molecular Biophysics	1	33%
Fall 2010	695	Introduction to Molecular Biophysics	1	33%
Spring 2011	140	Introduction to Cell Biology	4	50%

Spring 2011	422-S1	Computational Biology & Bioinformatics	3	33%
Spring 2011	422-S2	Computational Biology & bioinformatics	3	33%
Fall 2011	420	The Structural Basis of Disease	3	100%
Fall 2011	615	Advances in Molecular Biophysics	1	33%
Fall 2011	695	Advances in Molecular Biophysics	1	33%
Fall 2012	420	The Structural Basis of Disease	3	100%
Spring 2013	422	Computational Biology & Bioinformatics	3	100%
Fall 2013	140	Introduction to Cell Biology	4	50%
Fall 2013	420	Computational Biology & Bioinformatics	3	100%
Fall 2013	615	Advances in Molecular Biophysics	1	25%
Fall 2013	615	Advances in Molecular Biophysics	1	33%
Spring 2014	422	Computational Biology & Bioinformatics	3	100%
Fall 2014	420	The Structural Basis of Disease	3	100%
Spring 2015	422	Computational Biology & Bioinformatics	3	50%
Fall 2015	420	The Structural Basis of Disease	3	100%
Spring 2016	422	Computational Biology & Bioinformatics	3	100%
Fall 2015	615	Advances in Molecular Biophysics	1	25%

Fall 2015	615	Advances in Molecular Biophysics	1	33%
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**Supervised Personnel and Students, University of Tennessee:**

*Post-doctorate associates:*

Hector Adam Velasquez. June 2014 – to date, co-supervised with Prof. Smith.

Derek Cashman, December 2010 – July 2013.  
(2 publications)  
(now faculty at Tennessee Tech, Tennessee).

Yinglong Miao, Ph.D., September 2009 – August 2012, co-supervised with Prof. Smith and Prof. Jain  
(4 publications)  
(now postdoctoral associate in the McCammon group, UCSD).

Barbara Collignon, Ph.D., October 2008-May 2011  
(1 publication)  
(now working at IBM Canada).

*Graduate students:*

Jason Harris, GST/Scale-IT; 2010-2014 (now postdoctoral associate, EPA & UNC-Chapel Hill)

Sally Ellingson, GST/Scale-IT; 2010-2014 (now Research Assistant Professor, University of Kentucky, Lexington).

Karan Kapoor, GST; 2011-2015 (now postdoctoral associate, Georgetown University)

Willy Evangelista, BCMB Department; since 2013

*Undergraduate students researchers in the Baudry laboratory:*

William Hembree, Chemistry. Sophomore. Summer 2008 & 2010. (1 publication)

Jeremy Spiers, BCMB. Spring 2009 (1 publication).

Andrew Sneed, (BCMB Best Undergraduate Award, Spring 2009), BCMB. Summer 2008 & 2009.

Jason Harris, BCMB. Fall 2008, Summer 2009.

Cody Bogema, BCMB. Fall 2008, Summer 2009.

John Anderson, BCMB. Fall 2008, Summer 2009.

Chelsea Knotts, BCMB (Tochbearer Award – the highest student award at the University of Tennessee), Spring 2010 – June 2012

Lindsey Vallee, Pellissippi State Community College: Summer 2010

Vanessa Freeman, BCMB: Summer 2010, Spring 2011.

Jason Williams, Virginia Tech: Summer 2011.

Joseph Summers, BCMB, Fall 2013-Spring 2014

Tyler McBride, BCMB, Fall 2013

Jessica Voiles (in collaboration with Dr. Berthelier), Fall 2013-to date

Richard Law, BMCB, Spring 2014

Rebecca Weir (Summer 2015 to Spring 2016). Funded competitively by the Department of Energy. (2 publications)  
Gus White (UT's Scholars), since Summer 2015  
Shannon Smith, 2016,

*High school students researchers in the Baudry laboratory:*

Marek Twarzynski, Knoxville Catholic High School, Summer 2010 (currently undergraduate at Stanford)  
Journey Stimes, Hardin Valley Academy High School, Fall 2013- Spring 2014

*Rotation students:*

Biochemistry and Cell and Molecular Biology Graduate School:

2008: Kristen Holbrook  
2009: Yuzhuo Chu  
2010: Nicholas Lopes  
2011: Meng Li  
2011: Ran An  
2012: Purva Bhojane  
2013: Wilfredo Evangelista  
2014: Adam Green  
2015: Rupesh garwal

Genome Science and Technology Graduate School:

2009: Dennis Glass (rotation led to publication #45)  
2009: Ritin Sharma and Tian Li  
2009: Jason Harris, Scale-IT  
2010: Sally Ellingson, SCALE-IT  
2010: Tian Li (rotation led to publication # 35)  
2010: Xiaohu Hu (rotation led to publication # 38)  
2010: Aaron Fleetwood  
2011: Jonathan Reyles  
2011: Karan Kapoor  
2012: Kasey Estenson  
2014: Khushboo Bafna  
2016: Jyortimoy

## Service since independent tenure-track position

### a) Institutional Service

#### i) Committee Work Departmental, College and University Levels

##### 1) List of committee work in BCMB Department:

Fall 2009 – Spring 2010 Undergraduate Curriculum committee

Fall 2009 – Spring 2010 Graduate Student Affairs committee

Fall 2009 – Spring 2010 Ad-hoc working group on General Biology Curriculum

Fall 2010 – Spring 2013 Graduate Student Admission Committee

Fall 2011 – to date Development, Publicity and Awards Committee

Fall 2013 – to date Undergraduate Curriculum Committee

2016 – Head, Search Committee, Faculty Search in Computational / Mathematical Biology, BCMB Department and National Institute for Mathematical Biology (NIMBioS)

##### List of committee work in Genome Science and Technology Program:

2009-to date: Curriculum Committee

2011-to date: First year Student Committee

2013-to date: Steering Committee

##### 2) College level committees (Engineering)

iBME, Institute of Biomedical Engineering (New UT-wide institute founded in 2013) 2013-to date: Curriculum Committee

2013-2015: Research Committee and Program Manager, “System Biology and Molecular Medicine” program.

##### 3) University level committees

2009 UT/ORNL Summer School in Biophysics:

Member of the Organization Committee. Chairperson for two conference sessions

2010 UT/ORNL Summer School in Biophysics:

Member of the Organization Committee. Chairperson of Travel Fellowship Committee. Chairperson in two conference sessions.

2012-2013 Search Committee, Governor’s Chair in Bioinformatics.

#### ii) Contributions to the University’s programs

Co-designed a SACNAS event at the 2010 National Meeting. Presented an oral communication “Supercomputing a sustainable environment: coupling biology and the world’s top supercomputer to identify environmental pollutants.

SACNAS conference”, and judge of undergraduate research poster in Biophysics. Anaheim, CA, October 2010

HOSA (Health Occupations Students of America) UTK Chapter:

Academic adviser since the foundation of the UTK chapter (2011). The UTK chapter has grown to 74 members.

## **b) Disciplinary Service**

### Evaluation of peer research / scholarship / creative activity

#### Reviewer for:

Biophysical Journal  
Chemical Biology and Drug Design  
Current Medicinal Chemistry  
Environmental Science & Technology  
Journal of the American Chemical Society  
Journal of Chemical Education  
Journal of Computational Chemistry  
Journal of Molecular Modeling  
Journal of Physical Chemistry-B  
Journal of Physics: Condensed Matter  
Journal of Chemical Information and Modeling;  
Journal of Enzyme Inhibition and Medicinal Chemistry  
Nanotechnology  
Nature Chemical Biology  
PLOS One.  
Scientific Reports (Nature Publishing Group)

#### Ad-hoc reviewer for the National Science Foundation:

Program: Chemical Structure, Dynamics and Mechanisms (CSDM), Division of Chemistry, Fall 2009.  
Program: Algebra, Number Theory and Combinatorics (ANTC), Division of Mathematical Sciences, Spring 2010  
Division of Undergraduate Education, Summer 2014  
Division of Molecular and Cellular Biosciences, Summer 2014  
Division of Molecular and Cellular Biosciences, Spring 2015

#### Panel Member for the National Science Foundation:

Division of Molecular and Cellular Biosciences, Structural Molecular Biophysics review panel, 2016- to date

#### NIH Center Advisory Board:

Member, Advisory Board for NIH Center for Macromolecular Modeling and Bioinformatics, November 2015

#### Advisory Board Member:

RCMI External Advisory Committee member, Howard University, 2015-to date

Department of Energy: Ad hoc reviewer of supercomputing grant applications for the Oak Ridge Leadership Computing Facilities, Director Discretion Project Applications

## **c) Professional Service**

### i) Service to public and private organizations

2010 Tennessee Junior Science and Humanities Symposium,

Laboratory host: demonstration of lab and computational biophysics to high school students.  
2010-to date: Tennessee Science Olympiads, Event coordinator, and State Judge for the High School “Protein Modeling Event”  
2010- to date: The Governor’s Schools of Tennessee, High School level lectures on protein modeling,  
2011: Talk on Biology and Computational research; Bearden Middle School, Knoxville, TN,  
2011: Talk on Biology and computational Research; Hardin Valley Academy High School, Knoxville, TN  
2012: Program committee & Session chair: 2012 Joint JICS/GRS Workshop on Large-Scale Computer Simulation. Oak Ridge.  
2012- to date: NSF-IGERT poster competition judge, national poster competition presented by NSF-IGERT funded graduate students.  
2014-present Elected member, Board, Association of doctorate Students of Paris University Paris-6.

ii) Service to industry, e.g., training, workshops, consulting

Member of the UTK / UT-Battelle - ORNL / Georgetown University “Comprehensive Drug Discovery & Development Institute”.

Scientific collaboration with Shifa Biopharmaceuticals, NIH-SBIR.

Scientific collaboration with Sarfez USA, Inc, NIH-SBIR

Co-founder of Minerva Discovery, Inc.

**Membership on graduate committees outside of the Baudry group:**

<b>Student</b>	<b>Program</b>	<b>Degree</b>	<b>Project Title</b>	<b>Date completed</b>
Craig Helstowski	GST	Ph.D.	Mode of ubiquitin binding to deubiquitinating enzymes	Left program
Monique LeMieux	GST	M.S.	Antitrypsin serpins	2012
Jun Wang	Microbiol.	Ph.D.	Microbial Modulation of Endocrine Disruptors	2015
Yuzhuo Chu	BCMB	Ph.D.	QM/MM Studies on Product Specificity of Protein Lysine Methyltransferases	2013
Tian Li	GST	Ph.D.	Function of Aquaporin	2014
Yao Jianzhuang	BCMB	Ph.D.	Molecular Modeling	2014
Li Meng	BCMB	Ph.D.	Bioenergy	2014
Xiaohu Hu	GST	Ph.D.	Molecular Modeling	In progress
Ayla Norris	GST	M.S.	Plant Biology	2013
Davi Ortega	Physics	Ph.D.	Molecular Modeling and Bioinformatics of chemotaxis	2013
Non (Prakitchai) Chotewutmontri,	GST	Ph.D.	Characterization of transit peptide recognitions	2013
Bhojane, Purva	BCMB	Ph.D.	Osmolyte effects on enzyme that show DHFR activity	In progress
Estenson, Kasey	GST	Ph.D.	AAT characterization	In progress
Dennis Glass	GST	Ph.D.	Molecular modeling of biomolecules	2012
Benjamin Lindner	GST	Ph.D.	Molecular modeling of biomolecules	2012
Jing Zhou	GST	Ph.D.	Molecular modeling of biomolecules	In progress
Jun Wang	GST	Ph.D.	Environmental toxicity of nuclear receptors' ligands	In Progress
Jordan Toutouchian	Pharma. Sciences	Ph.D.	Drug Discovery	In Progress
Yufei Yue	BCMB	Ph.D.	Molecular modeling of methyl transferase	In Progress
Zachary Beamer	BCMB	Ph.D.	Plant transmembrane structure/function	In Progress