Jerome Baudry, Ph.D.
Mrs. Pei-Ling Chan Chair and Professor

The University of Alabama in Huntsville
Department of Biological Sciences
jerome.baudry@uah.edu

***Curriculum Vitae*, November 2020**

Ph.D., Molecular Biophysics.
December 1997**.** University of Paris - Sorbonne Universités, Pierre and Marie Curie, Paris, France.
Advisor: Jeremy C. Smith.
Highest Honors ("Très Honorable avec Félicitations").

Positions:
August 2017 – to date: **Mrs. Pei-Ling Chan Chair and Professor**
The University of Alabama in Huntsville
Department of Biological Sciences

2014 – August 2017: Associate Professor with Tenure. University of Tennessee, Knoxville. Department of Biochemistry and Cellular and Molecular Biology (BCMB).

Group Leader, UT/ORNL Center for Molecular Biophysics, Oak Ridge National Laboratory
Core faculty, UT/ORNL Genome Science and Technology, Knoxville
Adjunct faculty, University of Tennessee, Department of Pharmaceutical Sciences, College of Pharmacy, Memphis

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 of Paris Pierre and Marie Curie, 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

Research Grants since 2008:
Total funded to-date (including all collaborative labs): $9,241,749; Total directly to Baudry lab: $1,623,477

RAISBRPUAH-JB Baudry (lead PI) 2018-2020
Reynold American Incorporated
Grant total: $289,841 (Funds to Baudry Lab:): $289,841
2018-2020
Title: Computational modeling of toxicants and protein interactions
The purpose of this project is to characterize the cytochrome P450 substrates and metabolites of harmful chemical contained in tobacco products.
Role: lead PI

National Institutes of Health.
1R01AI132117-01
NIH-R01 Structure-based design of a broadly protective group A streptococcal vaccine
Grant total: $3,603,585 (Funds to Baudry Lab:): $348,225
2017-2022
NIH - NIAID
Lead PI : Jim Dale (UTHSC)
Baudry UAH PI.
Support: One graduate student and one month summer salary for Baudry

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
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/α-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 a 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 Berthelier 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. A*pplication 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:

Fibroblast Growth Factor 23 Antagonists And Related Compositions And Methods
Patent Application, 2019

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. Berthelier and J. Baudry, 2012

Publications - From Most Recent.
***An asterisk (*) indicates a publication with J. Baudry as Corresponding Author*:**

Published since independent position (2008)
(from most recent):

88. Structure based virtual screening identifies small molecule effectors for the sialoglycan binding protein Hsa
R Agarwal, BA Bensing, D Mi, PN Vinson, J Baudry, TM Iverson, JC Smith
Biochemical Journal 477 (19), 3695-3707, 2020

87. Supercomputer-based ensemble docking drug discovery pipeline with application to Covid-19
A Acharya, R Agarwal, M Baker, J Baudry, D Bhowmik, S Boehm, et al.
ChemRxiv 2020

86 Structure-based group A streptococcal vaccine design: Helical wheel homology predicts antibody cross-reactivity among streptococcal M protein–derived peptides
MP Aranha, TA Penfound, JA Spencer, R Agarwal, J Baudry, JB Dale, ...
Journal of Biological Chemistry 295 (12), 3826-3836, 2020

85. Sequential dynamics of Stearoyl-CoA Desaturase-1 (SCD1)/ligand binding and unbinding mechanism: A computational study
A Petroff, RL Weir, CR Yates, JD Ng, J Baudry,
bioRxiv, 2020

84. High Performance Computing Prediction of Potential Natural Product Inhibitors of SARS-CoV-2 Key Targets.
K. Byler, J Landman, J Baudry
ChemRxiv 2020

83. Structure based virtual screening identifies novel competitive inhibitors for the sialoglycan binding protein Hsa
R Agarwal, BA Bensing, D Mi, PN Vinson, J Baudry, TM Iverson, JC Smith
bioRxiv, 2020

82. Novel K-Means Clustering-based Undersampling and Feature Selection for Drug Discovery Applications
VS Akondi, V Menon, J Baudry, J Whittle
2019 IEEE International Conference on Bioinformatics and Biomedicine, 2019

81. Ligand-Dependent Sodium Ion Dynamics within the A_{2A} Adenosine Receptor: A Molecular Dynamics Study
X Hu, MD Smith, BM Humphreys, AT Green, JM Parks, JY Baudry, et al.
The Journal of Physical Chemistry B 123 (38), 7947-7954, 2019

80. Interdimer zipping in the chemoreceptor signaling domain revealed by molecular dynamics simulations
MG Petukh, DR Ortega, J Baudry, IB Zhulin

bioRxiv, 2019

79. Ensemble Docking in Drug Discovery: How Many Protein Configurations from Molecular Dynamics Simulations Are Needed to Reproduce Known Ligand Binding?
W Evangelista, SR Ellingson, JC Smith, JY Baudry
The Journal of Physical Chemistry B

78. Small molecule condensin inhibitors
H Zhao, ZM Petrushenko, JK Walker, J Baudry, HI Zgurskaya, ...
ACS infectious diseases 4 (12), 1737-1745

77. Ensemble Docking in Drug Discovery
R E Amaro, J Baudry, J Chodera, Ö Demir, J A McCammon, Y Miao, J C Smith
Volume 114, Issue 10, 22 May 2018, Pages 2271-2278

76. Computationally identified novel agonists for GPRC6A
M Pi, K Kapoor, R Ye, DJ Hwang, DD Miller, JC Smith, J Baudry, LD Quarles
PloS one 13 (4), e0195980 2018

75. GPCR6A is a Molecular Target for the Natural Products Gallate and EGCG in Green Tea
M Pi, K Kapoor, R Ye, JC Smith, J Baudry, LD Quarles
Molecular nutrition & food research 2018
https://doi.org/10.1002/mnfr.201700770

74. Ensemble docking to difficult targets in early-stage drug discovery: Methodology and application to fibroblast growth factor 23
HA Velazquez, D Riccardi, Z Xiao, LD Quarles, CR Yates, J Baudry, JC Smith
Chemical biology & drug design 91 (2), 2018, 491-504

73. Polycystin-1 interacts with TAZ to stimulate osteoblastogenesis and inhibit adipogenesis
Z Xiao, J Baudry, L Cao, J Huang, H Chen, CR Yates, W Li, B Dong, CM Waters, JC Smith, LD Quarles
The Journal of clinical investigation 128 (1), 2018, 157-174

72. Binding Mechanisms of Electron Transport Proteins with Cyanobacterial Photosystem I: An Integrated Computational and Experimental Model
K Kapoor, DJ Cashman, L Nientimp, BD Bruce, J Baudry
J. Phys. Chem. B, 2018, 122 (3), 2017, 1026–1036,

71. Novel Small Molecule JP-153 Targets the Src-FAK-Paxillin Signaling Complex to Inhibit VEGF-Induced Retinal Angiogenesis (vol 91, pg 1, 2017)
JJ Toutounchian, J Pagadala, DD Miller, J Baudry, F Park, E Chaum, V Morales-Tirado, CR Yates
MOLECULAR PHARMACOLOGY 92 (6), 2017, 627-627

70. The quinic acid derivative KZ-41 prevents glucose-induced caspase-3 activation in retinal endothelial cells through an IGF-1 receptor dependent mechanism
H He, RL Weir, JJ Toutounchian, J Pagadala, JJ Steinle, J Baudry, DD Miller, CR Yates
PloS one 12 (8), 2017, e0180808

69. Thermophilic Enzyme or Mesophilic Enzyme with Enhanced Thermostability: Can We Draw a Line?
X Jing, W Evangelista Falcon, J Baudry, EH Serpersu
The Journal of Physical Chemistry B 121 (29), 2017, 7086-7094

68. 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, J Baudry, VV Rybenkov, JC Smith, JK Walker
Journal of Medicinal Chemistry 60 (14), 2017, 6205-6219

67. 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), 2017, 19-26

66. Novel small molecule JP-153 targets the Src-FAK-paxillin signaling complex to inhibit VEGF-induced retinal angiogenesis
JJ Toutounchian, J Pagadala, DD Miller, J Baudry, F Park, E Chaum, CR Yates
Molecular pharmacology 91 (1), 2017, 1-13

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 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 publications amongst the 30 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)

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

-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/baudry-miao

-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 Ellignson. 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)

-Outstanding Scholarship Award, Senior Faculty, Department of Biochemistry & Cellular and Molecular Biology, University of Tennessee, 2017.
-
UAH NEWS, August 29, 2017 https://www.uah.edu/news/people/jerome-baudry-named-pei-ling-chan-eminent-scholar-in-biological-sciences

- Article in UAH Magazine, Fall 2017 issue

- Article in UAH Annual Report 2017

- Hyperion HPC Innovation Excellent Award at SC20,

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

At the University of Tennessee, Knoxville, 2008-2017:

Rebecca Weir, undergraduate student:

- Research Alliance in Math and Science (RAMS) Scholarship, Department of Energy, Summer 2015.

Willy Evangelista,graduate student:

- NSF travel support Award, International Conference Travel to European Center for Advanced Atomic and Molecular Calculations. Julich, Gemrany, Summer 2015.

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 position:

Talks by Jerome Baudry:

Supercomputer-based Drug Discovery against SARS-CoV-2
American Association of Pharmaceutical Scientists. October 2020

Structure-based design of broadly protective group A streptococcal M protein-based vaccines.
UGM Meeting, Chemical Computing Group, Montreal, Canada, June 2018

Pharmaceceutcal discovery in the pre-exascale era.
TERATEC Forum, June 2018
Ecole Polytechnique, Palaiseau, France

Protein Dynamics and drug discovery: from hits to toxicity prediction
Bluegrass Molecular Biophysics Symposium
University of Kentucky, Lexington, 2018

Computational drug discovery: from proteome to drugs
University of Texas Health, San Antonio, Department of Biochemistry and Structural Biology, Lozano Long School of Medicine. October 2017

Computational Drug Discovery: From Proteome to Drug
University of Illinois at Urbana Champaign, Beckman Institute, December 2017

The physics of drug discovery
University of Alabama, Huntsville, Department of Physics, February 2018

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.
3rd 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:

At UAH

Presented by Mrs. Anna Petroff, graduate student:

Homology modeling of a human membrane desaturase
A. Petroff, J. Ng, R. Yates, J. Baudry
UGM Meeting, Chemical Computing Group, Montreal, Canada, June 2018

Presented by Mr. Jay Spencer, graduate student:

Computational selection of vaccine peptides with moe
Jay Alan Spencer, James B. Dale, Jeremy Smith, Michelle Aranha, Rupesh Agarawal, and Jerome Y. Baudry
UGM Meeting, Chemical Computing Group, Montreal, Canada, June 2018

At UTK/ORNL

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.
56th 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.
54th 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 theSpecific P450 Metabolism and Induced Estrogenic Activity of PCB-30. 7th 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.

Presented by Rebecca Weir, Undergraduate student:

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

Teaching since independent tenure-track position				
Classes taught at UAH since 2018	**Course #**	**Course name**	**Credit Hrs.**	**% Responsibility for Shared Instruction**
Fall 2018	BYS601	Bioinformatics/ Computational drug discovery	3	100%
Spring 2019	BYS119	Principles of Biology	4	100%
Classes taught at UTK since 2008	**Course #**	**Course name**	**Credit Hrs.**	**% Responsibility for Shared Instruction**
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%
Fall 2015	615	Advances in Molecular Biophysics	1	25%
Fall 2015	615	Advances in Molecular Biophysics	1	33%
Spring 2016	422	Computational Biology & Bioinformatics	3	100%
Fall 2016	420	The Structural Basis of Disease	3	100%
Spring 2017	530	Experimental Design and Analysis	3	50%

Supervised Personnel and Students,

Post-doctorate associates:
University of Alabama in Huntsville:

Dr. Noriko Inoguchi, January 2018 – to date

Dr. Kendall Byler, July 2018-to date

University of Tennessee:

Hector Adam Velasquez. June 2014 – 2016, co-supervised with Prof. Smith.
(2 publications)
now Research Scientist, Atlanta, GA

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 (4 publications)
(now faculty at Kansas University).

Barbara Collignon, Ph.D., October 2008-May 2011
(1 publication)
now Analayst at Bank of Canada.

Graduate students:

University of Alabama in Huntsville:

Mrs. Anna Petroff, August 2017 – to date
Mr. Jay Spencer, January 2018 – to date
Mrs. Amy Ridings, August 2018 – to date
Mrs. Jana Whittle, August 2018 – to date

University of Tennessee:

Jason Harris, GST/Scale-IT; 2010-2014 (now Scientist at CDD Vault, Burlingame, CA)

Sally Ellingson, GST/Scale-IT; 2010-2014 (now faculty, University of Kentucky, Lexington.

Karan Kapoor, GST; 2011-2015 (now postdoctoral associate, University of Illinois at Urbana Champaign)

Willy Evangelista, BCMB Department; 2013-2017 (now faculty, University of Lima, Peru)

Undergraduate students researchers in the Baudry laboratory:

University of Alabama in Huntsville:

Shannon Howes: "The Vaginal Microbiota and Gut Microbiota: How Our Bacterial Populations Underlie Susceptibility to Inflammatory Diseases"
Bethany Kregger: "The Interrelationships between the Human Microbiome, Inflammation, and Diabetes"
Kyrie Chandler: "How Genetics Influence Susceptibility to Chronic Inflammatory Disease"
Olivia de la Paz: "Diet-based Protective Compounds for the Prevention of Neurodegenerative Disease"
Samantha Martin: "Nutraceutical Interventions in Psychiatric Disease"

University of Tennessee:

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,
Jay Spencer, Spring 2017- to date

Postgraduate researchers in the Baudry laboratory:

Rebecca Weir since 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 Agarwal

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
2016: Sarah Cooper

Service since independent tenure-track position

a) Institutional Service

University of Alabama in Huntsville:

Evolution faculty recruiting committee, Department of Biological Sciences
Chan Chair recruiting committee, Department of Physics
Faculty Senate
Research Council

University of Tennessee:

i) Committee Work Departmental, College and University Levels

2009 –Search Committee, Faculty Search in Biophysics, 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)

2017 –Search Committee, Faculty Search in Biophysics, BCMB Department

2017 –Search Committee, Faculty Search in Biophysics, Physics Department

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

2015-2016 Admission Commitee

2) College level committees (Engineering)

iBME, Institute of Biomedical Engineering 2013-2015: 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, 2015 – to date

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

National Academy of Sciences
DE Shawn/Anton proposal review panel, 2018-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, LLC.

Co-founder and Chief Scientific Officer of Seattle Discovery, LLC

Membership on graduate committees outside of the Baudry group:

University of Tennessee:

Student	Program	Degree	Project Title	Date completed
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	2016
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	2016
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	2016
Jordan Toutounchian	Pharma. Sciences	Ph.D	Drug Discovery	2016
Yufei Yue	BCMB	Ph.D.	Molecular modeling of methyl transferase	In Progress
Zachary Beamer	BCMB	Ph.D.	Plant transmembrane structure/function	In Progress