

# J A S O N B R E T H A R R I S

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## CAREER OBJECTIVE

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- Obtain postdoctoral position in an interdisciplinary research and mentoring environment.

## QUALIFICATIONS

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- 7 years research experience in **molecular modeling, computer-aided drug design, and molecular biology.**
- **PI for 2 internal funding grants • 2 first-author, 3 co-author, and 3 abstract publications • 26 citations.**
- Able to write successful funding proposals, communicate, manage budget and personnel, and contribute to team research in a multidisciplinary environment.
- Numerous teaching, curriculum development, and mentoring experiences.

## EDUCATION

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- **2009-2014 - Doctorate of Philosophy** - University of Tennessee & Oak Ridge National Laboratory  
- Major: **Life Science** Minor: **Computer Science**  
- Fellow in an NSF Interdisciplinary Graduate Education Training (IGERT) program. Designed and lead team-based research with multidisciplinary graduate, undergraduate, and high school students.
- **2004-2009 - Bachelor of Science** - University of Tennessee  
- Major: **Biochemistry, Cellular, Molecular Biology**  
- Participated in theory-based undergraduate research.

## PEER-REVIEWED PUBLICATIONS

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- **Jason B. Harris** and Melanie L. Eldridge, Gary Sayler, Fu-Min Menn, Alice C. Layton, Jerome Baudry. **A Computational Approach Predicting CYP450 Metabolism and Estrogenic activity of an Endocrine Disrupting Compound (PCB-30).** (*Environmental Toxicology & Chemistry*). **In Press.** DOI: 10.1002/etc.2595
- **Jason B. Harris**, Valerie Berthelie, Kasey Estenson, Jerome Baudry. **Identification of S-(4-nitrobenzyl)-6-thioguanosine as Inhibitor of Z-Alpha1 Antitrypsin Polymerization.** (recently submitted)
- **Jason B. Harris**, Aaron Mishtal, Caroline S. Rempe, Jerome Baudry, Elizabeth E. Howell, R.J. Hinde. **Anion-pi geometries between protein and ligand structures.** (manuscript drafted)
- David D. Jenkins, **Jason B. Harris**, Elizabeth E. Howell, Robert J. Hinde, Jerome Baudry. **STAAR: STatistical Analysis of Aromatic Rings.** *Journal of Comp. Chemistry.* (March 2013); 34(6):518-22
- Michael C. Brothers, Anna E. Nesbitt, Michael J. Hallock, Sanjeeva G. Rupasinghe, Ming Tang, **Jason Harris**, Jerome Baudry, Mary A Schuler, and Chad M Rienstra. **VITAL NMR: Using Chemical Shift Derived Secondary Structure Information for a Limited Set of Amino Acids to Assess Homology Model Accuracy.** *Journal of Biomolecular NMR.* (January 2012); 52(1): 41–56.
- Vivek Philip, **Jason Harris**, Rachel Adams, Don Nguyen, Jeremy Spiers, Jerome Baudry, Elizabeth E. Howell, Robert J. Hinde. **A Survey of Aspartate- Phenylalanine and Glutamate-Phenylalanine Interactions in the Protein Data Bank: Searching for Anion- $\pi$  Pairs.** *Biochemistry* (April 2011): 50(14):2939-50.

## ABSTRACT PUBLICATIONS

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- Rachel M. Adams, **Jason B. Harris**, Jeremy J. Jay, Beth G. Johnson, Miriam L. Land, Lauren J. Hauser. **Developing measures for microbial genome assembly quality control,** *BMC Bioinformatics* 11, no. Suppl. 4 (March 2010): P14.
- **Jason B. Harris**, David D. Jenkins, Jonathan Reyles, Stephanie Rickett, Jordan M. Utley, Elizabeth E. Howell, Jerome Baudry, R.J. Hinde. **Determining Anion-Quadrupole Interactions Among Protein, DNA, & Ligand Molecules.** *BMC Bioinformatics* 12, no. Suppl. A5. 7(March 2011).

- **Jason B. Harris, Valerie Berthelie, Kasey Estenson, Jerome Baudry. Binding of a small molecule prevents polymerization of mutant alpha-1-antitrypsin and reveals a new binding site for drug discovery.** Special Issue: The 27th Annual Symposium of The Protein Society, *Protein Science* 22, Suppl. S1 (July 2013):1–258.

## GRANTS

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- **Author/PI. Internal Research Grant. Award \$60,000.** University of Tennessee (SCALE-IT). "STAAR: Characterizing Anion-Quadrupole Interactions in Biological Systems". Aug 2013-July 2014.
- **Author/PI. Internal Research Grant. Award \$15,000.** "University of Tennessee (SCALE-IT). "Anion-Quadrupole Interactions between Protein-Ligand Molecules". Aug 2012-July 2014.
- **Assisted. NSF Grant (R01).** Unfunded. "Anion-pi Interactions in Proteins, Protein/Protein and Protein/Ligand Complexes". Submitted Jan, 2014.
- **Assisted. NIH Grant (R21).** Unfunded. "Discovery of Environmental Endocrine Disruptors: An Integrated Experimental and Computational Approach". Feb 22, 2012.

## HONORS & AWARDS

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- **Graduate Fellowship Award \$80,000.** Tuition, stipend, & healthcare. **NSF-IGERT Traineeship.** University of Tennessee-Knoxville. Aug 2009- Aug 2011.
- **Science Alliance Award. Award \$3,000.** Recognition of graduate research and teaching. **Science Alliance.** University of Tennessee and Oak Ridge Natl. Lab. April 2014.
- **Workshop Scholarship Award** Registration, food, & lodging. **7th National Biomedical Computation Resource (NBCR) Summer Institute.** La Jolla, California, Jul 30th- Aug 3rd, 2012.
- **Conference Travel Award. Award \$100.00.** Conference poster. **Computational Biophysics to Systems Biology (CBSB13).** Norman, Oklahoma. May 19-21, 2013.
- **Conference Travel Award. Award \$400.00.** Conference poster. **Protein Society Symposium.** Boston, MA. July 20-24th, 2013.

## RESEARCH EXPERIENCES

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### Research Overview

My research interests are to study the environmental and health effects of molecular interactions between biological molecules. I apply computational modeling techniques to predict structural and functional changes to proteins as they interact with small molecules. I also collect experimental measurements to validate these models. I have worked with the estrogen hormone receptor, alpha-1-antitrypsin serine protease, and cytochrome P450 enzymes. I also do fundamental research on an emerging non-covalent interaction called "anion-pi" which is gaining recognition for its structural roles in biological molecules. My research has applications in **environmental toxicology screening, metabolite prediction, data mining, and structure-based drug discovery.** Techniques such as **virtual docking, homology modeling, molecular dynamics, scripting, and molecular biology** are used to carry out my research in these areas.

My advisor is Jerome Baudry at the UT-ORNL Center for Molecular Biophysics. I work in collaboration with Gary Saylor at the UT Center for Environmental Biotechnology, Valerie Berthelie at the UT Graduate School of Medicine, Elizabeth Howell and Robert Hinde at the UT BCMB and Chemistry Graduate Schools.

My research included leading projects for 4 undergraduates, 2 high school students, and 11 other graduate students.

**PhD and IGERT Training Project**  
*Dec 2010- July 2014*

**ANION-PI INTERACTIONS**  
Genome Science and Technology

Knoxville, TN

**Role:** Secured funding to lead research efforts for 11 graduates, 1 undergraduate and 1 high school student.

**Objective:** Study an emerging non-covalent interaction called “anion-pi” within the context of protein and ligand systems, and provide an interdisciplinary research project for graduate student training.

**Results:** Demonstrated geometries at which anion-pi interactions are energetically favorable and showed that these geometries are prevalent within protein structures. Publications for this work are in *Biochemistry (ACS)*, *J. of Computational Chemistry*, and *BMC Bioinformatics*. A searchable database of proteins with this interaction and the search code (STAAR) is available online (<http://staar.bio.utk.edu>).

**Personnel:** Faculty Mentors: 1 biochemist, 1 biophysicist, 1 Chemist  
Graduate Students: 3 computer scientists, 4 biologists, and 5 biophysicists  
Undergraduate Students: 1 senior (microbiology)  
High School Students: 1 senior

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**PhD Project**                      **IDENTIFYING ENDOCRINE DISRUPTORS OF CYP450 METABOLITES**  
*Dec 2010- July 2014*                      Genome Science and Technology                      Knoxville, TN

**Role:** Designed a predictive multi-protein activity model and carried out experimental validations.

**Objective:** Build a model that integrates metabolite prediction, virtual docking, and experimental assays in order to identify compounds and their CYP450 metabolites that behave as endocrine disruptors.

**Results:** Demonstrated that 2-D reactivity information can be paired with 3-D docking simulations to better predict CYP450 metabolism and that a multi-protein docking approach can be used to both predict CYP450 metabolism and the subsequent bioactivity of suspected endocrine disruptors. Publication for this work is accepted to *J. Environ. Toxicol. and Chem.*

**Personnel:** Faculty Mentors: 3 microbiologist, 1 biophysicist, 1 Analytical Chemist  
Graduate Students: 1 biophysicists  
Undergraduate Students: 2 seniors (BCMB)  
High School Students: 1 senior

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**PhD Project**                      **IDENTIFYING ALPHA-1-ANTITRYPSIN DEFICIENCY INHIBITOR**  
*April 2013- July 2014*                      Genome Science and Technology                      Knoxville, TN

**Role:** Designed a computational model to screen for inhibitors to treat alpha-1-antitrypsin deficiency.

**Objective:** Build a virtual docking model to assist in the screening of a 30,000 compound database for inhibitors of alpha-1-antitrypsin polymerization.

**Results:** Predicted and validated a new inhibitor for alpha-1-antitrypsin polymerization using a screening assay and theoretical homology model of alpha-1-antitrypsin in an intermediate state. Virtual docking found a novel binding site for the location of inhibition. Submitted to *Biochemistry (ACS)* and abstract published in *Protein Science*.

**Personnel:** Faculty Mentors: 1 biochemist, 1 biophysicist  
Graduate Students: 1 biophysicists, 1 biochemist

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**IGERT Training Project**                      **KUDZU GROWTH MODEL**  
*Aug 2010-Dec 2010*                      Genome Science and Technology                      Knoxville, TN

**Role:** Participated as a team member for part of my IGERT training.

**Objective:** Assess control methods for an invasive plant species, kudzu, in the city of Knoxville, TN.

**Results:** Demonstrated early and late season treatment using combination of herbicides, controlled burns, and grazing animals were best practices for efficient kudzu control measures.

**Personnel:** Faculty Mentors: 1 ecologist  
Graduate Students: 1 ecologist, 1 mathematician, 1 biophysicist

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**IGERT Training Project****GENOME ASSEMBLY CONTROL***Jan 2010-May 2010*

Genome Science and Technology

Knoxville, TN

**Role:** Participated as a team member for part of my IGERT training.**Objective:** Statistically identify mistakes during automated gene annotation.**Results:** Presented poster “Developing Measures for Microbial Genome Assembly Control”, at the 2010 UT-ORNL-KBRIN Bioinformatics Summit and published abstract in *BMC Bioinformatics*.**Personnel:** Faculty Mentors: 1 bioinformatician  
Graduate Students: 1 computer Scientist, 1 mathematician, 1 biophysicist, 1 biologist

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**Graduate Research Assistant****MODELING CYP450 XplA GENE***Jan 2010-May 2010*

Oak Ridge National Laboratory

Oak Ridge, TN

**Role:** Managed the work of 1 summer undergraduate student.**Objective:** Create a theoretical model of a CYP450 enzyme involved in the degradation of pollutants.**Results:** Created homology model for CYP450 XplA gene that explained binding of 3 explosive pollutant molecules. Presented poster entitled, “Engineering the Bioremediation of Explosive Pollutants”, and data used in grant submission.**Personnel:** Faculty Mentors: 1 biophysicist  
Graduate Students: 1 biophysicists  
Undergraduate Students: 1 senior (BCMB)

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**Undergraduate Research****HOMOLOGY MODEL ASSESSMENT***August 2008-May 2009*

University of Tennessee

Knoxville, TN

**Role:** Created CYP450 homology models and blind-fold scored them using a developmental approach.**Objective:** Qualitatively assess scoring of homology models using a new method involving NMR chemical shift data.**Results:** Showed that NMR chemical shift data could assist in assess quality of homology models. A publication is available in the *Journal of Biomolecular NMR*.**Personnel:** Faculty Mentors: 1 biophysicist (UT), 1 chemist (Illinois, Urbana-Champaign).  
Graduate Students: 1 chemist (Illinois, Urbana-Champaign)  
Undergraduate Students: 1 senior (BCMB)

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**HHMI Research Scholar****REGULATION OF DIAPAUSE***May 2004– Aug 2004*

ETSU Biology Dept.

Johnson City, TN

**Role:** Received position as a graduating high school student to learn molecular biology techniques.**Objective:** Identify genes related to regulation of the diapause state in *Sarcophagidae* flies which is associated with an increased lifespan (‘Methuselah gene’ research).**Results:** I learned insect growth, dissection, Primer design, RT-PCR, gel electrophoresis, and plasmid cloning.**Personnel:** Faculty Mentors: 1 geneticist, 1 biochemist  
Graduate Students: 2 biologist  
Undergraduate Students: 1 graduating senior

- POSTER Adams, Rachel M., **Harris, Jason B.**, Jay, Jeremy J., Johnson, Beth, Land, Miriam L., Hauser, Loren J. (2010 March). **Developing measures for microbial genome quality control.** UT-ORNL-KBRIN Bioinformatics Summit. Cadiz, KY.
- POSTER **Harris J. B.**, Philip V., Adams, R. M., Nguyen, D., Spiers, J., Baudry, J., Howell E. E., Hinde R. J. (July 2010). **A PDB search for the anion-quadrupole interaction.** UT-ORNL Summer School in Biophysics. Knoxville, TN.
- POSTER **Jason B. Harris**, David D. Jenkins, Jonathan Reyles, Stephanie Rickett, Jordan M. Utley, Elizabeth E. Howell, Jerome Baudry, Robert J. Hinde. (2011 April) **Determining Anion- Quadrupole Interactions Among Protein, DNA, and Ligand Molecules.** UT-ORNL-KBRIN Bioinformatics Summit. Cadiz, KY.
- POSTER **Jason B. Harris.** (2011 May) **Using High-Performance Supercomputing to Find Endocrine Disruptors: A Fast Track to Discovering New Medicines and Protecting the Environment.** NSF-IGERT 2011 Poster Competition. Online ([Link](#)).
- ORAL
- POSTER **Jason B. Harris.** (2012 June) **Using High-Performance Supercomputing to Find Endocrine Disruptors: A Fast Track to Discovering New Medicines and Protecting the Environment.** Computational Biophysics to Systems Biology (CBSB12) Workshop. Knoxville, TN.
- POSTER **Jason B. Harris.** (2012 August) **Modeling the Specific P450 Metabolism and Induced Estrogenic Activity of PCB-30.** 7th National Biomedical Computation Resource Summer Institute (NBCR 2012). La Jolla, CA.
- POSTER **Jason B. Harris**, Valerie Berthelie, Kasey Estenson, Jerome Baudry. (2013 July) **Binding of a small molecule prevents polymerization of mutant alpha-1-antitrypsin and reveals a new binding site for drug discovery.** Protein Society 2013 Symposium. Boston, MA.

#### TEACHING EXPERIENCES

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- **University of Tennessee - BCMB 517 (Physical Biochemistry)**
  - Spring 2014 (Guest Lecturer on Molecular Dynamics)
  - Spring 2014 (Guest Lecturer on Virtual Docking)
- **University of Tennessee - LIFE SCIENCE 541 (GST Colloquium)**
  - Spring 2014 (Designed and taught workshop on molecular dynamics)
  - Spring 2014 (Designed and taught workshop on remote cluster computing)
- **University of Tennessee - BCMB 420 (Structural Aspects of Disease)**
  - Fall 2013 (Guest Lecturer on alpha-1-antitrypsi deficiency)
- **University of Tennessee - Biology 140 (Organization and Function of the Cell)**
  - Fall 2013 (TA for 1 lab section)
  - Fall 2013 (Lecture TA)
  - Fall 2013 (Guest Lecturer on replication, transcription, and translation)
  - Fall 2012 (TA for 2 lab sections)
- **University of Tennessee - KIDSU Summer Camp for rising 9th-12th graders (Virtual Biology: Using Computers to Discover New Medicines)**

- Summer 2014 (Designed and taught curriculum)
- Summer 2013 (Designed and taught curriculum)
- **University of Tennessee - UTK/Knox County Pre-Collegiate Research Scholars Program**
  - Fall 2013-Spring 2014 (research mentor for a high school student)

#### OUTREACH EXPERIENCES

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- **Science Fair Judge** - Tate's Regional Elementary Science Fair (April 7, 2014)

#### JOURNAL PEER-REVIEWER

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- *Environmental Science & Technology* (ACS Journal)

#### PROFESSIONAL MEMBERSHIPS

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- **American Society for Biochemistry and Molecular Biology (ASBMB)**
- **American Chemical Society (ACS)**
- **Protein Society**

#### TECHNICAL & PROFESSIONAL SKILLS

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Molecular Modeling	NAMD	Workshop and Curriculum Development
Computational Chemistry	AutoDock	Project Management
Cheminformatics	Perl	Scientific Writing
Drug Discovery	Python	Grant Writing
Molecular Biology	C++	Teaching
CADD	HTML	Pipetting
Virtual Docking	OpenBabel	Cell Culturing
Homology Modeling	GAMESS	Plasmid Cloning
Molecular Dynamics	PCR	Agarose Gel Electrophoresis
MOE	DNA Extraction	Thin-layer Chromatography
VMD	RNA Extraction	

#### REFERENCES

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|-----------------------------------|--|----------------|
| ▪ Jerome Baudry (jbaudry@utk.edu) | Assist. Professor, UTK Dept. BCMB        | (865) 576 0930 |
| ▪ Elizabeth Howell (lzh@utk.edu)  | Professor, UTK Dept. BCMB                | (865) 974 4507 |
| ▪ Robert Hinde (rhinde@utk.edu)   | Assoc. Dean & Professor, UTK Dept. Chem. | (865) 974 9053 |

*Request for letters of recommendation can be sent directly to me ([jhari43@utk.edu](mailto:jhari43@utk.edu)) or to my references.*