

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

jason.b.harris@gmail.com

JasonBretHarris.com ScrubChem.org VirtualDocking.com

CAREER OBJECTIVE

- Lead & enhance the state of art for data-driven biomedical research and informatics.

QUALIFICATIONS

- 10 years combined research experience in **molecular modeling, molecular biology, & informatics**.
- **4 grants • 5 first-author, 4 co-author, & 3 abstract papers • 4 research websites • 96 citations • 4 h-index**.
- Developer of the largest & most annotated source of public biochemical data (ScrubChem.org).
- Able to write successful funding proposals, communicate, manage budget and diverse personnel, and contribute to team research in a multidisciplinary environment.
- Numerous outreach, teaching, curriculum development, and mentoring experiences.
- Academic, Industry, National Laboratory, and Government Agency networks.

EDUCATIONAL EXPERIENCES

- **Visiting Research Scholar & Postdoc Fellow (2014-2017)** - University of North Carolina at Chapel Hill & U.S. Environmental Protection Agency (ORISE program).
-Developing ScrubChem.org in a collaboration with UNC & U.S. EPA.
- **Doctorate of Philosophy (2009-2014)** - University of Tennessee & Oak Ridge National Laboratory
- Major: **Life Science (Biomolecular Modeling)** Minor: **Computer Science**
- Fellow in an NSF Interdisciplinary Graduate Education Training (IGERT) program. Designed and lead team-based computational & experimental research with multidisciplinary graduate, undergraduate, and high school students.
- **Bachelor of Science (2004-2009)** - University of Tennessee
- Major: **Biochemistry, Cellular, Molecular Biology**
- Participated in clinical & theory-based research.

TECHNICAL & PROFESSIONAL SKILLS

Molecular Modeling	NAMD	Workshop and Curriculum Development
Cheminformatics	CADD	Teaching
Computational Chemistry	Programming	Project Management
Data Science	Perl	Scientific Writing
Drug Discovery	Python	Grant Writing
Molecular Biology	C++	Experimental Biology
Databases (mysql, SQL)	C#, ASP.Net	<i>In Vitro</i> & <i>In Vivo</i> Assays
Data Mining & Integration	Visual Studio	RNA & DNA Isolation
Homology Modeling	ETL (SSIS)	PCR
Molecular Dynamics	Web Design	Cell Plating & Culturing
Virtual Docking	HTML, CSS, JS	Plasmid Cloning
MOE	OpenBabel	Electrophoresis
AutoDock	GAMESS	Thin-layer Chromatography
Schrodinger (Maestro)	VMD	Computing Hardware
NCBI Databases	Ontologies	High Performance Computing (HPC)

PEER-REVIEWED PUBLICATIONS

- Currently submitting 2 first-author manuscripts: **ScrubChem: Cleaning of PubChem Bioassay Data** (full article), **ScrubChem: Building Example Bioactivity Datasets from Public Bioassay Data** (data descriptor), and preparing 1 first-author manuscript: **ScrubChem.org: An Online Bioactivity Database** (application).
- Wilfredo Evangelista, Rebecca L. Weir, Sally R. Ellingson, **Jason B. Harris**, Karan Kapoor, Jeremy C. Smith, Jerome Baudry. **Ensemble-based docking: From hit discovery to metabolism and toxicity predictions**. *Bioorganic & Medicinal Chemistry*. (July 2016); 24(20):4928–4935
- **Jason B. Harris and Valerie Berthelie**r, Kasey Estenson, Jerome Baudry. **Discovery of an Inhibitor of Z-Alpha1 Antitrypsin Polymerization**. *PLoS ONE*. (May 2015); doi:10.1371/journal.pone.0126256.
- **Jason B. Harris and Melanie L. Eldridge**, Gary Saylor, 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*). (May 2014); doi: 10.1002/etc.2595.
- **Jason B. Harris**, Aaron Mishtal, Caroline S. Rempe, Jerome Baudry, Elizabeth E. Howell, R.J. Hinde. **Anion- π geometries between protein and ligand structures**. (Doctoral Dissertation Chapter, Univeristy of Tennessee).
- 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, Sanjeewa 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- π Pairs**. *Biochemistry* .(April 2011); 50(14):2939-50.

ABSTRACT PUBLICATIONS

- **Jason B. Harris**, Valerie Berthelie'r, 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, Suppli. S1 (July 2013):1–258.
- **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. Suppli. A5. 7 (March 2011).
- 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. Suppli. 4 (March 2010): P14.

GRANTS

- **Assisted. DOE Grant (DTRA JSTO-CBD)**. Award: \$500,000/yr. Sandia National Laboratory. "Development of blood brain barrier penetrating antibody therapeutics for encephalitic alphaviruses". Oct. 2017 – Sept. 2020.
- **Assisted. NIH Grant (U01)**. Award: \$437,810/yr. University of North Carolina Chapel Hill. "Drug Repurposing for Cancer Therapy: from Man to Molecules to Man". Sept. 2016 – Aug 2017.
- **Author/PI*. Internal Research Grant**. Award \$60,000. University of Tennessee (SCALE-II). "STAAR: Characterizing Anion-Quadrupole Interactions in Biological Systems". Aug 2013-July 2014. *educational PI
- **Author/PI*. Internal Research Grant**. Award \$15,000. "University of Tennessee (SCALE-II). "Anion-Quadrupole Interactions between Protein-Ligand Molecules". Aug 2012-July 2014. *educational PI
- **Assisted. NSF Grant (R01)**. Unfunded. "Anion- π 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

- **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.

INVITED TALKS

- **American Chemical Society.** Washington, D.C. Cleaning PubChem Bioassay Data. (**August 2017**).
- **Big Data to Knowledge(BD2K)/LINCS Symposia.** Cincinnati, OH. ScrubChem: Cleaning PubChem Bioassay Data. (**May 2017**).
- **Computational Biology to Systems Biology Symposia.** Cincinnati, OH. ScrubChem: Cleaning PubChem Bioassay Data. (**May 2017**).
- **Oak Ridge National Laboratory, Center for Molecular Biophysics Seminar.** Oak Ridge, TN. ScrubChem: Cleaning PubChem Bioassay Data. (**May 2017**).
- **Broad Institute (Harvard/MIT).** Cambridge, MA. ScrubChem: Cleaning PubChem Bioassay Data. (**April 2017**).
- **NIH Specialized Information Services.** Washington D.C. ScrubChem: Cleaning PubChem Bioassay Data. (**July 2016**).

RESEARCH EXPERIENCES

Research Overview

My research involves **both experimental & computational methods**. I study the environmental and health effects caused from interactions between biological and inorganic molecules. I mostly connect data with computational modeling techniques to predict structural and functional changes to biological systems as they interact with small molecules. I also collect, integrate, and redistribute large amounts of public bioassay information in an effort to enhance data-driven research for other scientists and move forward the state of art for biomedical research. I have prior experiences in experimental *in vitro* and *in vivo* studies which has been useful in the gathering, interpretation, and re-use of aggregated bioactivity data. I have done focused projects on nuclear hormone receptors, alpha-1-antitrypsin serine protease, and cytochrome P450 enzymes. I have contributed to the study of an emerging non-covalent interaction called "anion- π " which is gaining recognition for its fundamental structural role in several biological molecules. A highlight from this project included leading and securing funding (PI training during my PhD) to train 4 undergraduates, 2 high school students, and 11 graduate interdisciplinary students.

Techniques such as **virtual docking, homology modeling, molecular dynamics, data-mining, programming, databases, web-design, and molecular biology** are some of the tools I have used to carry out my research in these areas.

My Postdoc mentor is Alex Tropsha at the University of North Carolina Chapel Hill's Eshelman School of Pharmacy. My PhD advisor was Jerome Baudry at the University of Tennessee and Oak Ridge National Laboratory's Center for Molecular Biophysics. My close collaborations include: Gary Saylor at the UT Center for Environmental Biotechnology, Valerie Berthelier at the UT Graduate School of Medicine, Elizabeth Howell and Robert Hinde at the UT BCMB and Chemistry Graduate Schools, and several researchers at the U.S. EPA.

Postdoc Project **SCRUBCHEM**
Aug 2014-present U.S. EPA & University of North Carolina Chapel Hill Research Triangle Park, NC

Role: Designer & Lead.

Objective: Collect large amounts of public bioassay data for re-use in predictive modeling, assay development, and regulatory decision-making.

Results: Digitally curated millions of public bioassay records from PubChem and other sources into a database. The database is accessible online at ScrubChem.org and provides data to EPA's Comptox.epa.gov as well as ILINCS.org. ScrubChem is the largest and most detailed aggregation of public information available for referencing and generating biochemical datasets.

Personnel: Mentors: 1 Toxicologist, 1 Pharmacologist, 1 Computer Scientist

Designer: 1 Chemical Data Scientist

PhD and IGERT Training Project **ANION-PI INTERACTIONS**
Dec 2010- July 2014 Genome Science and Technology Knoxville, TN

Role: Project Lead: 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 (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

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 biophysicist

Undergraduate Students: 2 seniors (BCMB)

High School Students: 1 senior

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. Paper accepted to *PLOS1* and abstract published in *Protein Science*.
Personnel: Faculty Mentors: 1 biochemist, 1 biophysicist
Graduate Students: 1 biophysicists, 1 biochemist

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

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 made 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

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)

Undergraduate Research
August 2008-May 2009

HOMOLOGY MODEL ASSESSMENT

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 assessing 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)

HHMI Research Scholar
May 2004– Aug 2004

REGULATION OF DIAPAUSE

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

CONFERENCE POSTERS

- POSTER **Jason B. Harris**, Joshua C. Harris, Olexandr Isayev, Alex Tropsha, Richard Judson. (2017 May) **ScrubChem: Cleaning of PubChem Bioassay Data**. Big Data to Knowledge (BD2K)/LINCS 2017. Cincinnati, OH.
- POSTER **Jason B. Harris**, Joshua C. Harris, Olexandr Isayev, Alex Tropsha, Richard Judson. (2017 May) **ScrubChem: Cleaning of PubChem Bioassay Data**. Computational Biology to Systems Biology (CBSB) 2017. Cincinnati, OH.
- POSTER **Jason B. Harris**, Joshua C. Harris, Olexandr Isayev, Alex Tropsha, Richard Judson. (2017 March) **ScrubChem: Cleaning of PubChem Bioassay Data to Create Diverse and Massive Bioactivity Datasets for Use in Modeling Applications**. Society of Toxicology 2017. Baltimore, MD.
- POSTER **Jason B. Harris**, Richard Judson. (2016 March) **ScrubChem: Building Bioactivity Datasets from PubChem Bioassay Data**. Society of Toxicology 2016. New Orleans, LA.
- 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.
- 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**. (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.** (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,** 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 **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 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.

TEACHING EXPERIENCES

- **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 wet-lab section)
 - Fall 2013 (Lecture TA)
 - Fall 2013 (Guest Lecturer on replication, transcription, and translation)
 - Fall 2012 (TA for 2 wet-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 on drug discovery using computers & wet-lab)
 - Summer 2013 (Designed and taught curriculum on drug discovery using computers & wet-lab)
- **University of Tennessee - UTK/Knox County Pre-Collegiate Research Scholars Program**
 - Fall 2013-Spring 2014 (research mentor for a high school student)

OUTREACH & VOLUNTEER EXPERIENCES

- **Networking and Leadership Training Organization** - Training group leader at U.S. EPA (2014-2017)
- **Science Fair Judge** - Tate's Regional Elementary Science Fair (April 7, 2014)

JOURNAL PEER-REVIEWER

- *Chemical Research in Toxicology* (ACS Journal)
- *Environmental Science & Technology* (ACS Journal)
- *SAR and QSAR in Environmental Research* (T&F)

PROFESSIONAL MEMBERSHIPS

- American Society for Biochemistry and Molecular Biology (ASBMB)
- American Chemical Society (ACS)
- Protein Society
- Society of Toxicology (SOT)

HOBBIES/INTERESTS

- Social dancing (Lindy/Swing, Blues, Tango, Bachata, Salsa, etc.)
- DIY Home Projects & Tools (top to bottom, ins & outs)
- Computing (hardware/software)
- Strategy Board and Card Games
- News& Politics (current events)
- Coin Collecting
- Nature & Outdoors & Travel

REFERENCES

- | | | |
|---|---------------------------------------|----------------|
| ▪ Jerome Baudry (jbaudry@utk.edu) | Assoc. Professor, UTK BCMB | (865) 576 0930 |
| ▪ Alex Tropsha (alex_tropsha@unc.edu) | Assoc. Dean of Pharmacy, UNC Pharm. | (919) 966-2155 |
| ▪ Harry Richards (harry@utk.edu) | Research Assist. Professor, UTK Eng. | (865) 599-4553 |
| ▪ Oles Alexander (olexandr@email.unc.edu) | Research Assoc. Professor, UNC Pharm. | (601) 212-3658 |
| ▪ Elizabeth Howell (lzh@utk.edu) | Professor, UTK BCMB | (865) 974 4507 |
| ▪ Robert Hinde (rhinde@utk.edu) | Assoc. Dean & Professor, UTK Chem. | (865) 974 9053 |

Request for letters of recommendation can be sent directly to me (jason.b.harris@gmail.com) or to my references.