

Jeremy Ryan Ash

PHD STUDENT · BIOINFORMATICS

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Education

North Carolina State University

BIOINFORMATICS, PH.D. | STATISTICS, M.S.

- GPA: 3.74

Raleigh, NC, USA

Aug. 2014 - PRESENT

The University of Texas at Austin

BIOLOGY, B.S.

- Concentration: Neurobiology

Raleigh, NC, USA

August 2013

Skills

Programming R, Python, Java, Bash, SAS, REX

Other Chem/Bioinformatics, Data Analysis, Statistics, High Performance Computing, Linux, Network Analysis, Simulation

Experience

Graduate Research Assistant

NCSU

ADVISORS: DENIS FOURCHES AND JACQUELINE HUGHES OLIVER

August 2015 - PRESENT

- Statistical methods development for QSAR models – models predicting the bioactivity of small molecules given their chemical structure.
- Developing **chemmodlab** (<https://github.com/jrash/chemmodlab>), an R package for building cheminformatics machine learning models.
- Developing confidence interval estimation methods for hit enrichment curves.

Graduate Research Assistant

NCSU

ADVISOR: JEFF THORNE

Aug. 2014 – July 2015

- Group project with the labs of Scott Schmidler (Duke), and Jotun Hein (Oxford) hosted by The Statistical and Applied Mathematical Sciences Institute.
- Improved the biological realism of insertion and deletion in a Bayesian model for the joint estimation of phylogeny and protein structure alignment. Implemented in the software **Statalign** (<http://statalign.github.io/>).

Research Associate

LSU

ADVISOR: JEREMY BROWN

Feb. 2014 – Aug. 2015

- Collaborated with the lab of Kyle Gallivan (Florida State University) developing **TreeScaper** (<https://github.com/whuang08/TreeScaper>), software for analysis of phylogenetic networks.

Research Assistant

UT Austin

ADVISORS: HAROLD ZAKON AND DAVID HILLIS

Dec. 2012 – Dec. 2013

- Used genetics, an array of phylogenetics software, programming, statistics, and high performance computing to predict functional divergences of sodium channels during their evolutionary history.

Research Assistant

UT Austin

ADVISOR: DANIEL JOHNSTON

Oct. 2012 – Oct. 2013

- Studied the involvement of the prefrontal cortex in trace eyelid conditioning in mice using behavioral training, genetic engineering, and histology.

Courses

STATISTICS PH. D.

- Statistical Theory I&II (Casella Berger)
- Linear Models and Var. Comp. (Monahan)
- Computing for Statistical Research
- Exp. Statistics For Biological Sciences
- Real Analysis

STATISTICS MASTERS

- Introduction to Statistical Learning
- Applied Bayesian Analysis
- Linear Models and Regression

BIOINFORMATICS PH. D.

- Bioinformatics I&II
- Comp. Met. for Molecular Biology
- Bioinformatics Consulting

Teaching

Society of Systematics Biologists Conference

Baton Rouge, LA.

WORKSHOP INSTRUCTOR

Jan. 2017

- Lead and prepared all materials for a workshop on **TreeScaper**, software that I helped develop.
- Materials can be found here: <https://github.com/ssb2017/treescapers>.

Awards

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|-----------|---|-------------------|
| 2014-2018 | Ruth L. Kirschstein (NIH) Research Fellowship in Bioinformatics | \$23,000 per year |
| Fall 2018 | Triangle Center of Evolutionary Medicine Fellowship | \$15,000 |
| 2014 | NCSU Graduate School Fellowship | \$4,000 |

Publications

Ash JR, Kuenemann MA, Rotroff D, Motsinger-Reif A, and Fourches D. *Structure-Based Approach to Exploring and Modeling Trait-Associated Metabolite Profiles*. Bioinformatics (In Review).

Ash JR and Hughes-Oliver J. *chemmodlab: A Cheminformatics Modeling Laboratory for Fitting and Assessing Machine Learning Models*. R Journal (In Review).

Menden MP, Wang D, Guan Y, Mason M, BenceSzalai, Bulusu KC, Yu T, Kang J, Jeon M, Wolfinger R, Nguyen T, Zaslavskiy M, **AstraZeneca-Sanger Drug Combination DREAM Consorti**, Jang IS, Ghazoui Z, Ahsen ME, Vogel R, Neto EC, Norman T, Tang EKY, Garnett MJ, Di Veroli G, Fawell S, Stolovitzky G, Guinney J, Dry JR, and Saez-Rodriguez J. *Community Assessment of Cancer Drug Combination Screens Identifies Strategies for Synergy Prediction*. Nat. Commun. (In Review). bioRxiv 200451.

Ash JR and Fourches D. *Characterizing the Chemical Space of ERK2 Kinase Inhibitors Using Descriptors Computed from Molecular Dynamics Trajectories*. Journal of Chemical Information and Modeling. 2017, 57 (6), 1286-1299.

- Awarded ACS Editor's Choice, May 19, 2017.

Huang W, Zhou G, Marchand M, **Ash JR**, Morris D, Van Dooren P, Brown JM, Gallivan KA, and Wilgenbusch JC. *TreeScaper: Visualizing and Extracting Phylogenetic Signal from Sets of Trees*. Mol. Biol. Evol. 2016, 33 (12), 3314-3316.

Selected Presentations

American Chemical Society Conference

Washington, DC

PRESENTATION

Aug. 2017

Ash JR and Fourches D. *Characterizing the Chemical Space of Kinase Inhibitors Using Molecular Descriptors Computed from MD Trajectories*.

American Chemical Society Conference

Washington, DC

POSTER

Aug. 2017

Ash JR, Kuenemann MA, and Fourches D. *Cheminformatics Approach to Exploring and Modeling Trait-Associated Metabolic Profiles*.

- 2017 ACS Division of Chemical Information Scholarship of Excellence (\$1000).

American Chemical Society Conference

Philadelphia, PA

POSTER

Aug. 2016

Ash JR and Fourches D. *Leveraging GPU-Accelerated Molecular Dynamics Simulations to Compute and Analyze the 4D Chemical Descriptor Space of ERK2 Kinase Inhibitors*.

- Also presented at German Conference on Cheminformatics. Fulda, Germany. November 2016.

Evolution Conference

Philadelphia, PA

PRESENTATION

Aug. 2016

Guifang Zhou, **Jeremy Ash**, Wen Huang, Melissa Marchand, David Morris, Paul Van Dooren, James C. Wilgenbusch, Jeremy M. Brown, Kyle A. Gallivan. *A network framework to explore phylogenetic structure in genomic data.* (presented by Guifang Zhou).

American Chemical Society Conference

Philadelphia, PA

POSTER

Aug. 2016

Ash JR and Fourches D. *Leveraging GPU-Accelerated Molecular Dynamics Simulations to Compute and Analyze the 4D Chemical Descriptor Space of ERK2 Kinase Inhibitors.*

- Also presented at German Conference on Cheminformatics. Fulda, Germany. November 2016.

American Chemical Society Conference

Boston, MA

POSTER

Aug. 2015

Fourches D. and **Ash JR** *Next-Generation Approaches In Cheminformatics.* (presented by Denis Fourches).

- Also presented at Triangle Statistical Genetics Conference. Research Triangle Park, NC. November 2015.

SAMSI Bioinformatics Transition Workshop

RTP, NC

PRESENTATION

May 2015

Gary Larson, **Jeremy Ash**, Jeffrey Thorne, Scott Schmidler. *Improving the Biological Realism of Insertions and Deletions in a Bayesian Model for Simultaneous Estimation of Alignment and Phylogeny.* (Presented by Scott Schmidler).

Evolution Conference

Raleigh, NC

POSTER

July 2014

Ash JR, Huang W, Zhou G, Wilgenbusch J, Gallivan K, Marchand M, and Brown J. *Community Detection on Networks of Topologies and Bipartitions Identifies Conflicting Phylogenetic Signal.*

Evolution Conference

Raleigh, NC

PRESENTATION

July 2014

Jeremy Brown, Guifang Zhou, Wen Huang, **Jeremy Ash**, Melissa Marchand, Kyle Gallivan, James Wilgenbusch. *Using networks to explore quantify, and summarize phylogenetic tree space.* (presented by Jeremy Brown).

The Center of Learning and Memory Conference

Austin, TX

POSTER

April 2013

Jeremy Ash*, William Taylor*, Jennifer Siegel, Richard Gray, Daniel Johnston, Raymond Chitwood, *Advances in Trace Eyelid Conditioning in Mice.* *Contributed equally.

- Also presented at the Society of Neuroscience Conference in San Diego, CA, November 2013.

Student Organizations

2017-2018 **President**, Genomic Sciences Graduate Student Association

Raleigh, NC, USA

References

Contact any of my former advisors for references.