

Curriculum Vitae

Allison Walker

Assistant Professor of Chemistry and Biological Sciences
Vanderbilt University

Email: allison.s.walker@vanderbilt.edu

Personal information

Date of birth: July 29, 1990

Place of birth: Summit, New Jersey, USA

Education

2012-2018 **Ph.D.**, Chemistry (Biophysical Chemistry)
Department of Chemistry
Yale University
New Haven, CT, USA

2008-2012 **BS Chemistry**, with Honors, *magna cum laude*
Department of Chemistry
Brown University
Providence, RI, USA

Research Summary:

Present **Assistant Professor of Chemistry and Biological Sciences**, Vanderbilt University

Research Projects:

Applications of machine learning methods to discover novel natural products with antibiotic activity

Optimization of graph neural networks for prediction of natural product properties and activities

Development of machine learning tools for designing biosynthetic gene clusters

2018-2021 **Postdoctoral Fellow**, Harvard Medical School

Research Projects:

Development of a machine learning method to predict natural product bioactivity based on the sequence of its biosynthetic gene cluster

Heterologous expression of RiPPs from the human microbiome (in collaboration with Chris Voigt's lab and Novartis)

NMR spectra predictions with DFT calculations for atropisomers of Tryptorubin A (in collaboration with Phil Baran's lab) and of complex terpenoids

Advisor: Dr. Jon Clardy

2012-2018 **Ph.D. candidate**, Yale University

Research Projects:

Using statistics and experimental methods to determine allosteric relationships in the ribosome

Using molecular dynamics simulations to determine how information is transferred across the membrane in epidermal growth factor receptor (EGFR)

Computational modeling and experiments to determine mechanism of bisarsenical fluorogenicity

Using molecular dynamics simulations to understand tRNA synthetase substrate selectivity

Advisor: Dr. Alanna Schepartz

2010-2012 **Undergraduate Research Assistant**, Brown University

Research Projects:

Bioinformatics analysis of trinucleotide repeats in the human genome

Effect of CAA interruptions on the structure of DNA containing CAG trinucleotide repeats

Advisor: Dr. Sarah Delaney

2009-2010 **Summer Research Intern**, Alcatel-Lucent
Bell Labs, Murray Hill, NJ, USA

Research Projects:

Computational modeling of idea propagation to analyze the structure of research organizations

Development of a computational method for sorting publications by topic based on title and abstract text. The resulting program was used to sort publications in Bell Labs database for an interactive display in the Bell Labs Museum

Advisor: Dr. Christopher White

Publications:

1. **Walker, A.S.**, Clardy, J. *A Machine Learning Bioinformatics Method to Predict Biological Activity from Biosynthetic Gene Clusters*. *J. Chem. Inf. Model.* 2021. **61** (6). 2560-2571.
(Featured as a supplemental cover)
2. **Walker, A.S.**[#], Russ, W.P., Ranganathan, R., Schepartz, A. *RNA sectors and allosteric function within the ribosome*. *Proc. Natl. Acad. Sci. U.S.A.*, 2020. **177** (33). 19879-19887.
3. **Walker, A.S.**, Pishchany, G., Clardy, J. *Parsing Molecules for Drug Discovery*. *Biochemistry*, 2020. **59** (17). 1645-1646.
4. Reisberg, S.H., Gao, Y., **Walker, A.S.**, Helfrich, E.J.N., Clardy, J., Baran, P.S. *Total synthesis reveals atypical atropisomerism in a small molecule Tryptorubin A*. *Science*, 2020. **367** (6476). 458-463.
5. Sinclair, J.K.L.^{*}, **Walker, A.S.**^{*}, Doerner, A.E., Schepartz, A. *Mechanism of information transfer into and through the plasma membrane by EGFR*. *Cell Chem. Biol.*, 2018. **25** (7). 857-870.
6. **Walker, A.S.**, Rablen, P.R., Schepartz, A., *Rotamer-restricted fluorogenicity of the bis-arsenical ReAsH*. *J. Am. Chem. Soc.*, 2016. **138** (22). 7143-7150.
(Featured in spotlights on recent JACS publications and the cover of the June 8, 2016 JACS issue)
7. Melo Czekster, C., Robertson, W.E., **Walker, A.S.**, Söll, D., Schepartz, A. *In vivo biosynthesis of a β -amino acid-containing protein*. *J. Am. Chem. Soc.*, 2016. **138** (16). 5194-5197.

8. Melicher, M.S., **Walker, A. S.**, Shen, J. Miller, S.J., Schepartz, A. *Improved carbohydrate recognition in water with an electrostatically enhanced β -peptide bundle*. Org. Lett., 2015. **17** (19). 4718-4721.
9. Melicher, M.S., Chu, J., **Walker, A.S.**, Miller, S.J., Baxter, R.H., Schepartz, A. *A β -boronopeptide bundle of known structure as a vehicle for polyol recognition*. Org. Lett., 2013. **15** (19). 5048-5051.
10. Hobert, E.M., Doerner, A.E., **Walker A.S.**, Schepartz, A. *Effective molarity redux: proximity as a guiding force in chemistry and biology*. Isr. J. Chem. 2013. **53** (8). 567-576.

* denotes that authors contributed equally to the publication

denotes that I am listed as a corresponding author on the publication

Fellowship Awards:

2018	NIH F32 Postdoctoral Fellow
2012	NSF Graduate Research Fellow

Achievements and Awards:

2019	Poster award, American Society of Pharmacognosy Annual Meeting
2016	Featured on the statistics blog FiveThirtyEight for developing a machine learning algorithm that predicts Oscar-winning films based on movie review text. Algorithm had the best performance of all algorithms featured on the blog in 2016. Also featured by WTNH News 8 and Yale News.
2011	Undergraduate Teaching and Research Award from Brown University to pursue summer research
2008	Girl Scout Gold Award Developed and taught a week-long class to expose middle school girls to the basics of computer programming

Teaching Experience:

2017	Teaching Assistant for Yale University's Mathematical Tools for Computer Science (CPSC 202)
2015-2016	Teaching Assistant for Yale University's General Chemistry (CHEM 161 and 167)
2014-2016	Mentored first year graduate students and undergraduates in the Schepartz lab
2009-2012	Teaching Assistant for Brown University's General Chemistry (CHEM 33)
2010-2012	Chemistry and Physics Tutor, Brown Science Center
2009-2010	Mentor for Brown Science Prep Wrote lesson plans covering variety of science and math topics Assisted Providence, RI high school students with college application process

Presentations

2021	Invited to present at workshop on Artificial Intelligence for Natural Product Drug Discovery at the Lorentz Center in Leiden, NL, September 2021.
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- 2020 Presented poster at the Gordon Research Conference on Marine Natural Products:
Walker, A.S., Clardy, J., *A machine learning tool for predicting natural product antimicrobial activity.*
- 2019 Presented poster at the American Society of Pharmacognosy Annual Meeting:
Walker, A.S., Clardy, J., *A machine learning tool for predicting natural product antimicrobial activity.*
- 2019 Presented poster at the Boston Bacterial Meeting:
Walker, A.S., Clardy, J., *A machine learning tool for predicting natural product antimicrobial activity.*
- 2017 Presented poster at the Annual Biophysical Society Meeting:
Walker, A.S., Schepartz, A. *Applying computational and biophysical methods to elucidate bis-arsenical fluorogenicity and binding to tetracycline motifs.*
- 2017 Presented poster at the NYAS Structural Biology Group 12th Winter Meeting:
Sinclair, J.K.L., **Walker A.S.**, Schepartz, A. *Growth factor specific dynamics of the EGFR transmembrane domain.*
- 2015 Presented talk at the Yale Chemistry Symposium:
Applying statistical coupling analysis to ribosomal RNA

Skills

Experimental Science: PCR and cloning, protein expression and purification, biochemical assays, flow cytometry, continuous culture of bacteria in a turbidostat, preparation of samples for deep sequencing and deep sequencing data processing, extraction and purification of bacterial secondary metabolites, LC-MS/MS.

Programming and Computational Biology/Chemistry: Programming in Python, MATLAB, Java, C, C++, and Scala, knowledge of machine learning and bioinformatics algorithms, MD simulations in Gromacs and Rosetta, QM and NMR DFT calculations in Gaussian.