

I am an enthusiastic scientist and educator with over a decade of experience in the field of peptide chemistry. My projects have focused on the development of structurally diverse, passively permeable macrocyclic peptide therapeutics as well as the molecular recognition of peptides and proteins by synthetic receptors. I have experience in medicinal chemistry, analytical techniques, research project management, and mentorship in both academia and industry. My current role in the dynamic start-up environment of Circle Pharma draws on my technical skills and leadership abilities.

PROFESSIONAL

Circle Pharma, Inc., South San Francisco, CA

Associate Director, Chemistry

March 2023 – Present

- Oversee operation of Peptide Discovery Synthesis Platform Team
- Serve as Project Lead for 3rd Undisclosed Discovery Target

Senior Scientist II, Medicinal Chemistry

June 2020 – February 2023

- Served as lead chemist on team that designed orally bioavailable peptidic macrocycles demonstrating IV and Oral in vivo efficacy in mouse tumor models for Circle's Cyclin A discovery program
- Served as project manager and lead chemist for a 2nd undisclosed target program with an external partner
- Led build of 3rd iteration of Circle's Peptide Synthesis Platform to introduce efficient solid-phase cyclization, and other optimized semi-automated synthetic strategies
- Evaluated, selected, and managed CROs conducting synthetic and DMPK work

Scientist II, Head of Chemistry

October 2018 – May 2020

- Served as lead chemist on Circle's Cyclin A protect team, delivering cell-permeable peptidic macrocycles that demonstrate mechanistic target engagement against Cyclin A/CDK2:E2F and anti-proliferative activity in small cell lung cancer cell lines ($IC_{50} < 50$ nM)
- Managed the day-to-day operations of internal production pipeline as well as the Chemistry research lab (5 FTEs)
- Served as the primary point of contact and advisor for outsourced Chemistry CRO projects
- Partnered with external Facilities Consultant to lead Chemistry lab relocation planning efforts
- Worked closely with the CEO, CSO, and Director of Biology on an on-going basis to contribute to overall company strategy and organizational decision-making

Scientist I, Platform Development, Synthesis

January 2017 – October 2018

- Developed novel cyclative release chemistry for the synthesis of peptidic macrocycles
- Synthesized small-molecules on a multi-gram scale (heterocycles, N-alkylated amino acids, amines)
- Optimized solid-phase peptide synthesis workflows to increase synthetic throughput and compound diversity

EDUCATION

Trinity University, San Antonio, TX

2015 – 2016

Postdoctoral Research Fellow | Advisor: Professor Adam R. Urbach

Molecular Recognition of Peptides and Proteins by Cucurbit[n]uril-based Synthetic Receptors

- Demonstrated the use of a single-component optical sensor to monitor peptide binding
- Demonstrated selective recognition of modified insulin in a complex mixture
- Assisted in the management of an undergraduate research laboratory

University of California, Santa Cruz, CA

2009 – 2015

Ph.D., Chemical Biology/Organic Chemistry | Advisor: Professor R. Scott Lokey

Structure-Permeability Relationships of Natural Product-Inspired Cyclic Peptides

- Designed and synthesized orally bioavailable cyclic peptides with non-proteinogenic amino acids
- Optimized the physicochemical properties of a cyclic peptide natural product
- Determined the solution structure of cyclic peptides using NMR and computational techniques

Skidmore College, Saratoga Springs, NY

2004 – 2008

B.A., Biochemistry, magna cum laude | Advisor: Professor Michelle W. Frey

*Expression, Purification, and Characterization of a Surface-Associated Aminopeptidase from *Vibrio fischeri*.*

PUBLICATIONS and PATENTS

* indicates undergraduate coauthor

1. Anderson, H. R.*, Reeves, W. L., **Bockus, A. T.**, Suating, P., Grice, A. G.*, Gallagher, M.*, Urbach, A. R. Semi-Synthesis of Aminomethyl-Insulin: An Atom-Economic Strategy to Increase the Affinity of a Protein N-Terminus for Recognition by a Synthetic Receptor. *Bioconjugate Chemistry*, 2023, 34, 1, 212-217
2. **Bockus, A. T.** et. al.; 2022. Cyclin Inhibitors. U.S. Patent Application UNDISCLOSED
3. Ramaseshan, M., **Bockus, A. T.** 2022. Cyclative Release of Peptidic Compounds. U.S. Patent 11,299,513, filed July 27, 2018, issued April 12, 2022
4. Hirani, Z.*, Taylor, H. F.*, Babcock, E. F.*, **Bockus, A. T.**, Vardano, C. D., Bielawski, C. W., Urbach, A. R. Molecular Recognition of Methionine-Terminated Peptides by Cucurbit[8]uril. *J. Am. Chem. Soc.*, 2018, 140, (38), 12263-12269
5. **Bockus, A. T.**, Lokey, R. S. Chapter 5: Bioactive and Membrane-Permeable Cyclic Peptide Natural Products. In *Practical Medicinal Chemistry with Macrocycles: Design, Synthesis, and Case Studies*, John Wiley & Sons, Inc, 2017
6. Naylor, M.R., **Bockus A. T.**, Blanco, M-J., Lokey, R. S. Cyclic Peptide Natural Products Chart the Frontier of Oral Bioavailability in the Pursuit of Undruggable Targets. *Curr. Opin. Chem. Biol.*, 2017, 38, 141-147.
7. **Bockus, A. T.**, Smith, L. C.*, Grice, A. G.*, Ali, O. A.*, Young, C. C.*, Mobley W.*, Leek, A., Vinciguerra, B., Roberts, J., Isaacs, L. D., Urbach, A. R. Cucurbit[7]uril-Tetramethylrhodamine Conjugate for Direct Sensing and Cellular Imaging. *J. Am. Chem. Soc.*, 2016, 138 (50), 16549–16552
8. **Bockus A. T.**, Urbach, A. R. Chapter 6: Molecular Recognition of Aromatic Peptides and Proteins in Nature and by Design. In *Aromatic Interactions: Frontiers in Knowledge and Applications (Monographs in Supramolecular Chemistry)*; Royal Society of Chemistry, 2016, 172-213
9. Wei L., **Bockus, A. T.**, Vinciguerra, B., Isaacs, L. D., Urbach, A. R. Predictive Recognition of Native Proteins by Cucurbit[7]uril in a Complex Mixture. *Chem. Commun.*, 2016, 52, 8537-8540
10. **Bockus, A. T.**, Schwochert, J. A., Pye, C. R., Townsend, C. E., Sok, V.*, Bednarek, M., Lokey, R. S. Going Out on a Limb: Delineating the Effects of β -branching, *N*-Methylation, and Sidechain Size on the Permeability, Solubility, and Flexibility of Sanguinamide A Analogs. *J. Med. Chem.*, 2015, 58 (18), 7409-18
11. **Bockus, A. T.**, Lexa, K. W., Pye, C. R., Kalgutkar, A. S., Gardner, J. W.*, Hund, K. C. R.*, Hewitt, W. M., Schwochert, J. A., Glassey, E.*, Price, D. A., Mathiowetz, A. M., Liras, S., Jacobson, M. P., Lokey, R. S. Probing the Physicochemical Boundaries of Cell Permeability and Oral Bioavailability in Lipophilic Macrocycles Inspired by Natural Products. *J. Med. Chem.*, 2015, 58 (11), 4581-4589
12. Ahlbach, C. L.*, Lexa, K. W., **Bockus, A. T.**, Chen, V.*, Crews P., Jacobson M. P., Lokey R. S. Beyond Cyclosporine A: Conformation-Dependent Passive Membrane Permeabilities of Cyclic Peptide Natural Products. *Future Med. Chem.*, 2015, 7 (16), 2121-30
13. **Bockus, A. T.**, McEwen, C. M., Lokey, R. S. Form and Function of Cyclic Peptide Natural Products: A Pharmacokinetic Perspective. *Curr. Top. Med. Chem.*, 2013, 13 (24), 1-16

SELECTED PRESENTATIONS AND POSTERS

Presentations:

1. An Integrated Platform for the Structure-Based Design of Orally Bioavailable Macrocycle Therapeutics, CHI Drug Discovery Chemistry bRo5: Macrocycles, Degradable & More session, San Diego April 2023
2. Polypeptides in Drug Discovery: Targeting Intracellular Protein-Protein Interfaces, Santa Barbara City College, March 2019
3. The Design of Passively Permeable Natural Product-Inspired Cyclic Peptides and The Recognition of Peptides and Proteins by Cucurbit[7]uril, Circle Pharma, Inc., September 2016
4. Structure-Permeability Relationships in Cyclic Peptides Inspired by Natural Products. UCSC, Dissertation Defense, August 2015
5. How to Make Passively Permeable Cyclic Peptides for Drug Discovery, Trinity University, May 2015
6. Going Out on a Limb: Delineating the Effects of β -branching, *N*-Methylation, and Side Chain Size on the Permeability, Solubility, and Flexibility of Sanguinamide A Analogs. Cambridge Healthtech Institute's Drug Discovery Chemistry, San Diego, April 2015
7. Passively Permeable Natural Product-Inspired Peptide Macrocycles. Chemical Biology in the Bay Area Day, UCSF June 2013

8. Synthesis of Rhodamine-Functionalized Cyclic Peptides for Cell Structure Targeting. UCSC Rotation Talk, 2010
9. Synthesis and Preliminary Assays of Water-Soluble Cell Membrane-Permeable Boronic Acid Saccharide Detector. UCSC Rotation Talk, 2009
10. Drugs that Shaped America. China University of Petroleum's Foreign Teacher Lecture Series, 2009
11. Water and Disease. China University of Petroleum's Foreign Teacher Lecture Series, 2008
12. Kinetic Characterization and GFP Localization of a Novel Aminopeptidase from *Vibrio fischeri*. Research presented at the Skidmore College Chemistry Capstone Research Seminar, 2007

Posters:

13. Garcia, P. G., Gleason, C. E., Membreno, M., Hamkins-Indik, F., Situ, G., Levin, B., Wang, E. G., Liu, L., Leung, S., Fraga, B., **Bockus, A. T.**, Aggen, J., Spellmeyer, D., Earp, D. J., Singh, R. Macrocycles inhibiting RxL-mediated binding of substrates to Cyclin A are synthetic lethal in Rb mutated small cell lung carcinoma (SCLC), AACR 2022.
14. (I) Going Out on a Limb: Delineating the Effects of β -branching, *N*-Methylation, and Side Chain Size on the Permeability, Solubility, and Flexibility of Sanguinamide A Analogs. (II) Drug-like Cell Permeability and Oral Bioavailability in Lipophilic Macrocycles Inspired by Natural Products. Cambridge Healthtech Institute's Drug Discovery Chemistry, San Diego, April 2015
15. ISEE PDP Focus Areas Employed to Enhance an Undergraduate Student-Skills Course. Presented at the ISEE PDP Alumni Event, Monterey, March 2014
16. Natural Product Motif-Inspired Amino Acids for the Construction and Permeability Analysis of Modular Linear and Macrocyclic Libraries. Presented at Science and Technology on Maui, March 2012
17. Synthesis and Modeling of a Combinatorial Macrocyclic Polyketide-Inspired Library for Permeability Studies. American Peptide Symposium, San Diego, June 2011
18. Purification and Kinetic Characterization of a Novel Surface-Associated PepN Enzyme Analog from *Vibrio fischeri*. Skidmore College Academic Festival, 2008

HONORS AND AWARDS

- ISEE/AWI Professional Development Program Travel Grant 2011 – 2013
- American Peptide Symposium Travel Grant 2011
- California Regents Fellowship 2009
- Outstanding Foreign Teacher Award, China University of Petroleum 2008
- Charlotte W. Fehey Prize: Outstanding Chemistry Student, Skidmore College 2008
- Chemistry Departmental Honors, Skidmore College 2008
- Honors Forum, Skidmore College 2004 – 2008
- Highest Honors, Skidmore College 2004 – 2007
- Periclean Honors Society, Skidmore College 2006
- Eagle Scout, Project: Tully Lake Disc Golf Course, Troop 8 Athol 2004

PROFESSIONAL DEVELOPMENT

- Manager Essentials Lab Course with Enspira 2021
- Drew University's 34th Annual Residential Medicinal Chemistry Course 2021
- Introduction to Molecular Modeling in Drug Discovery, Schrodinger virtual course 2020
- American Chemical Society Postdoc to PUI Workshop, Furman University, Greenville, SC 2016
- UCSC Institute for Scientist and Engineer Educators Professional Development Program 2011 – 2013

CONSULTING

- DiCE Molecules, Redwood City, CA 2016
- Circle Pharma, Inc., South San Francisco, CA 2016

TEACHING

Lecture Courses

- Guest Lecturer, CHEM3432 (Analytical Chemistry), 1 lecture, Trinity University 2016
- Guest Lecturer, CHEM2319 (Organic Chemistry I), 4 lectures, Trinity University 2016
- Guest Lecturer, CHEM2320 (Organic Chemistry II), 5 lectures, Trinity University 2015
- Guest Lecturer, CHEM4346 (Drug Design), 2 lectures, Trinity University 2015
- Instructor, COWL10 (Becoming a Successful Student), 2 full courses, UCSC 2014, 2015
- Guest Lecturer, CHEM110 (Intermediate Organic Chemistry), 2 lectures, UCSC 2015
- Teaching Assistant, CHEM110 (Intermediate Organic Chemistry), 1 quarter, UCSC 2013
- Teaching Assistant, Discussion, CHEM108A/B (Organic Chemistry), 5 quarters, UCSC 2011 – 2015
- Instructor, Oral English, 2 semesters, China University of Petroleum 2008 – 2009
- Instructor, American & British Cultures, 2 semesters, China University of Petroleum 2008 – 2009
- Instructor, English Extensive Reading, 1 semester, China University of Petroleum 2008 – 2009
- Co-Instructor, Fast-Paced Chemistry, Johns Hopkins Center for Talented Youth 2008

Laboratory Courses

- Instructor, CHEM2119 (Methods in Organic Chemistry), Trinity University 2016
- Instructor, CHEM2130 (Advanced Chemical Principles Lab), Trinity University 2016
- Guest Instructor, CHEM2220 (Organic Synthesis Laboratory), Trinity University 2015
- Teaching Assistant, CHEM1A/B (General Chemistry Lab), 2 quarters, UCSC 2010
- Teaching Assistant, Organic Chemistry, 3 semesters, Skidmore College 2006 – 2008

Mentoring

- Co-supervised 5 Undergraduate Research Students, Trinity University 2015 – 2016
- Supervised 7 Undergraduate Research Students (3 Theses), UCSC 2010 – 2015
- Supervised 2 High School Students, Science Internship Program, UCSC 2013

Outreach

- STEM Careers Podcast Guest 2019
- Volunteer, SBCC Science Discovery Day 2019
- Co-Instructor, Baccalaureate Bridge to the Biomedical Sciences Mini Research Camp, UCSC 2015
- Design Team Leader and Co-Instructor, Institute for Scientist and Engineer Educators
 - Drug Design, UC Santa Barbara 2013
 - Physicochemical Properties and Intermolecular Forces, UCSC 2012
 - Stem Cells Short Course, UCSC 2011
- Co-Instructor, Expanding Your Horizons Conference, Monterey CA 2012

REFERENCES

Available upon request