EDUCATION

Ph.D. in Chemistry, University of Illinois at Urbana-Champaign (UIUC), U.S.A.

08/2014-12/2019

Dissertation title: The biosynthesis and discovery of lanthipeptides

Committee: Wilfred A. van der Donk (Chair), Paul J. Hergenrother, Satish K. Nair, Douglas A. Mitchell

B.S. in Chemistry, University of Science and Technology of China (USTC), China

09/2010-05/2014

RESEARCH EXPERIENCE

Postdoctoral Scholar for Prof. David Baker, University of Washington

01/2020-present

- Project completed: Hallucination of closed repeat proteins containing central pockets
- Project completed: De novo protein design for binding and sensing small molecules
- Project in progress: Protein design for enzyme specificity engineering

Graduate Research Assistant for Prof. Wilfred A. van der Donk, UIUC

08/2014-12/2019

- Project completed: Target-guided discovery of new lanthipeptide with novel mode of action
- Project completed: Substrate-assisted enzymatic formation of lysinoalanine in duramycin
- Project completed: The mode of action of lipid II targeting two-component lantibiotics

Visiting Scholar with Prof. N. I. Martin, Utrecht University, the Netherlands

10/2015-12/2015

• Achieved isothermal calorimetry titration on lipid II-lantibiotic systems in collaboration with Dr. P. 't Hart, Dr. N. I. Martin, and Dr. E. J. Breukink.

Research Assistant for Prof. Gaolin Liang, USTC

11/2011-06/2014

- Independent Project: A new facile method for the fabrication of a 3D gold nanoparticle array with excellent surface-enhanced Raman scattering (SERS) performance
- Compound preparations and manuscript preparations for multiple molecular imaging projects

Team Member of team USTC_China, MIT iGEM 2011

10/2010-11/2011

- Project: Self-organizing Bacteria
- Individual contribution: Participated in designing and constructing a system that is able to drive one bacterial colony into two groups based on chemotaxis. Project received Gold Award in iGEM World Jamboree at MIT

Patent

• D. Baker, **L. An**, S. Majumder, M. Said and L. Tran, 2023, DE NOVO DESIGNED SMALL MOLECULE BINDERS VIA EXTENSIVE SHAPE COMPLIMENTARY SAMPLING, 63/610,726.

Preprints (#: equal contribution, *: (co)correspondence)

1. **L. An***, M. Seid#, L. Tran#, S. Majumder#, I. Goreshnik, G. Lee, J. Dauparas, I. Anishchenko, B. Coventry, A. Bera, A. Kang, P. M. Levine, V. Alvarez, A. Pillai, C. Norn, D. Feldman, D. Zorine, D. R. Hicks, X. Li, M. G. Sanchez, D. K. Vafeados, P. J. Salveson, A. A. Vorobieva, and D. Baker*. Binding and sensing diverse small molecules using shape complementary

- pseudocycles, 2023, under review. Preprint: https://doi.org/10.1101/2023.12.20.572602.
- 2. J. Dauparas, G. Lee, R. Pecoraro, **L. An**, I. Anishchenko, C. Glasscock, D. Baker*, Atomic context-conditioned protein sequence design using LigandMPNN, 2023, *submitted*. Preprint: https://doi.org/10.1101/2023.12.22.573103

PUBLICATIONS (#: equal contribution, *:correspondence)

- 3. **L. An**#*, D. Hicks#, D. Zorine#, J. Dauparas, B. Wicky, L. Milles, A. Courbet, A. Bera, H. Nguyen, A. Kang, L. Carter, D. Baker*. Hallucination of closed repeat proteins containing central pockets, *Nat. Struct. Mol. Biol.*, 2023, 30, 1755. (Link)
- 4. **L. An**#, D. Cogan#, C. Navo, G. Jiménez-Osés, S. K. Nair, and W. A. van der Donk*, Substrate-assisted enzymatic formation of lysinoalanine in duramycin, *Nat. Chem. Biol.* 2018, 10, 928. (Link)
- 5. **L. An**#* and G. R. Lee#*, De novo protein design using the blueprint builder in Rosetta, *Current Protocols in Protein Science*, 2020, 102,1, e116. (Link)
- 6. **L. An**, and W. A. van der Donk*, Recent progress in lanthipeptide biosynthesis, discovery, and engineering, *Comprehensive Natural Products III.* 2019, 2, 119. (Link)
- 7. **L. An**, M. Rehan H. Shah Gilani, G. L. Liang*, Peptide-based nanostructures for cancer diagnosis and therapy, *Curr. Med. Chem.* 2014, 21, 2453. (Link)
- 8. J. Acedo, I. Bothwell, **L. An**, A. Trouth, C. Frazier, W. A. van der Donk*, O-Methyltransferase-mediated Incorporation of a β-Amino Acid in Lanthipeptides, *J. Am. Chem. Soc.* 2019, 141, 42, 16790. (<u>Link</u>)
- 9. **L. An**, "iGEM: Get & Give (& Share)", *Microbiology Today*, Web. 15 May 2018. (Link)
- 10. Y. Liu#, Q. Miao#, P. Zou, L. Liu, X. Wang, **L. An**, X. Zhang, X. Qian, S. Luo, and G. Liang*. Enzyme-controlled intracellular self-assembly of 18F nanoparticles for enhanced microPET imaging of tumor. *Theranostics*. 2015, 5, 1058. (Link)
- 11. Y. Yuan#, L. Wang#, W. Du, Z. Ding, J. Zhang, T. Han, **L. An**, H. Zhang, and G. Liang*. Intracellular self-assembly of taxol nanoparticles for overcoming multi-drug resistance. *Angew. Chem. Int. Ed.* 2015, 54, 9700. (Link)
- 12. Y. Yuan, J. Zhang, Q. Cao, **L. An**, G. Liang*. Intracellular disassembly of self-quenched nanoparticles turns NIR fluorescence on for sensing furin activity in cells and in tumors. *Anal. Chem.* 2015, 87, 6180. (Link)
- 13. Y. Yuan, S. Ge, H. Sun, X. Dong, H. Zhao, **L. An**, J. Zhang, J. Wang, B. Hu, G. Liang*. Intracellular self-assembly and disassembly of 19F nanoparticles confer respective "Off" and "On" 19F NMR/MRI signals for legumain activity detection in zebrafish. *ACS Nano*. 2015, 9, 5117-5124. (<u>Link</u>)
- 14. Y. Yuan#, H. Sun#, S. Ge#, M. Wang, H. Zhao, L. Wang, L. An, J. Zhang, H. Zhang, B. Hu, J. Wang, G. Liang*. Controlled intracellular self-assembly and disassembly of 19F nanoparticles for MR imaging of caspase 3/7 in zebrafish. ACS Nano. 2015, 9, 761. (Link)
- 15. W. Wang#, J. Qian#, A. Tang#, **L. An**, K. Zhong, G. Liang*. Using magnetic resonance imaging to study enzymatic hydrogelation. Anal. Chem. 2014, 86, 5955-5961. (Link)
- 16. Y. Yuan, J. Zhang, **L. An**, Q. Cao, Y Deng, G. Liang*. Oligomeric nanoparticles functionalized with NIR-emitting CdTe/CdS QDs and folate for tumor-targeted imaging. Biomaterials. 2014,

- 35, 7881. (Link)
- 17. Y. Yuan, S. Jiang, Q. Miao, J. Zhang, M. Wang, **L. An**, Q. Cao, Y. Guan, Q. Zhang, G. Liang*, Fluorescent switch for fast and selective detection of mercury (II) ions in vitro and in living cells and a simple device for its removal. Talanta. 2014, 125, 204. (Link)
- 18. B. You*, P. Yin, and **L. An**. (2014), Multifunctional Electroactive Heteroatom-Doped Carbon Aerogels. Small, 10: 4352-4361. (<u>Link</u>)
- 19. Y. Deng, Y. Luo, **L. An**, Y. Yue, M. Rehan H. Shah Gilani, G. Liang*. Covalently conjugating fluorescence probes to nanoparticles for signal enhancement, Chem. Lett. 2013, 42, 10, 130424. (Link)
- 20. Y. Yuan., X. Wang, B. Mei, D. Zhang, **L. An**, X. He, J. Jiang, G. Liang*, Labeling thiols on proteins, living cells, and tissues with enhanced emission induced by FRET, Sci. Rep. 2013, 3, 3523 (Link)

SELECTED CONFERENCES & HONORS

- 1. RosettaCon, 08/2023
 - Presentation: De Novo Small Molecule Binder Design with Shape Complimentary Sampling
- 2. Biosynthesis, Biocatalysis, and New Methods in Enzymology, Gordon Research Seminar & Gordon Research Conference, 07/2023
 - Presentation & Poster: De Novo Small Molecule Binder Design with Shape Complimentary Sampling
- 3. MRSEC seminar, invited seminar. Brandeis University 06/2023
- 4. Rosetta Conference, Seattle (Invited conference, supported by RosettaCon travel grant) 08/2022
 - Poster: De novo design of small molecule binder using pseudocyclic proteins
- 5. Foresight's Molecular Machines Workshop, San Francisco (Invited conference) 07/2022
 - Invited Talk: De novo design of small molecule binding proteins
- 6. New Frontiers in Natural Products Discovery conference (*Supported by New Frontiers Scholar Award*), Corteva, Inc. 08/2019
 - Selected poster: A proof of concept target-guided lanthipeptide mining strategy
- 7. Natural Products and Bioactive Compounds Gordon Research Seminar & Gordon Research Conference (Supported by Fuson Travel Award), 07/2018
 - Talk & poster: Substrate-assisted enzymatic formation of lysinoalanine in duramycin
- 8. Midwest Enzyme Chemistry Conference, Loyola University, 10/2017
 - Selected talk: Substrate-assisted enzymatic formation of lysinoalanine in duramycin
- 6. Enzymes Coenzymes and Metabolic Pathways Gordon Research Seminar & Gordon Research Conference, 07/2017
 - Poster: Mechanistic details of duramycin biosynthesis
- 7. Midwest Enzyme Chemistry Conference, University of Illinois at Chicago, 10/2016
 - Poster: Mode of action studies for the two-peptide lantibiotic haloduracin
- 8. The 3rd National Chemistry Majors Scientific Activity Exchange (Supported by the Department Travel Award) Sichuan University, 12/2013

TEACHING, MENTORING & SERVICES

Mentor for rotation students, Valentina Alvarez, UW, summer/2023

Mentor for (rotation) graduate students, Long Tran, UW, winter/2022-present

Mentor for rotation student, Emma Mackey, UW, summer 2021

Graduate Mentor for rotation student, Chunyu Wu (later joined lab), UIUC, 09/2018

Teaching Assistant for Enzymatic Reaction Mechanisms (graduate level) for Prof. J. A. Gerlt, UIUC, 01-05/2016

Teaching Assistant for General Chemistry (leading discussion and lab sessions) for Dr. K. Marville, and Dr. J. A. Martinez, UIUC, 01-05/2016, 01-06/2014, 08-12/2014

Graduate Mentor for Women Chemists Committee (WCC), UIUC, 2017

Conference Committee, Allerton Conference, UIUC, 2017

Women Chemists Committee, 2016 & 2015 Women Welcome Retreat, UIUC, 2016 & 2015

Women Chemists Committee, 2016 Stoesser Lecture, UIUC, 2015

SKILLSETS

Computational skills:

- 1. Fluent use of python, bash scripts
- 2. Use of RosettaScripts, PyRosetta scripts.
- 3. Application and tuning of machine learning scripts, including AlphaFold2, RoseTTAFold, RFDiffusion, etc.

Chemistry/Biochemistry related skills:

- 1. Peptide/Protein expression and purification using biological system or chemical methods;
- 2. Analytical methods development and use of HPLC, UV-vis, LC-HRMS (Q-TOF), GC-MS, MALDI, SEC;
- 3. Natural product discovery using bioinformatics & genome mining, semi-synthesis and purification, and structure elucidation using NMR and LC-MSⁿ;
- 4. Plasmid construction and gene manipulation for Escherichia coli and Bacillus subtilis.

Others:

- 1. Accomplished user of Illustrator, Autodesk 3D Max, ChemDraw, Matlab, html language, Microsoft Word, Excel, PowerPoint;
- 2. Open water scuba diving.