

## Linna An, Ph.D in Chemistry

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## 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
- Project in progress: Machine learning models for small molecule-protein binding affinity ranking

**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: 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. G. Li<sup>#</sup>, **L. An**<sup>#</sup>, W. Yang<sup>#</sup>, L. Yang, T. Wei, J. Shi, J. Wang, J. Doonan, K. Xie, A. R. Fernie, E. S. Lagudah, R. A. Wing, C. Gao<sup>\*</sup>. Integrated biotechnological and AI innovations for crop improvement, 2025, in press.
2. Modeling protein-small molecule conformational ensembles with ChemNet, I. Anishchenko, Y. Kipnis, I. Kalvet, G. Zhou, R. Krishna, S. J Pellock, A. Lauko, G. R. Lee, **L. An**, J. Dauparas, F. DiMaio, David Baker, 2025, biorXiv, doi: <https://doi.org/10.1101/2024.09.25.614868>. ([Preprint link](#))

## PUBLICATIONS (#: equal contribution, \*:correspondence)

3. J. Dauparas, G. Lee, R. Pecoraro, **L. An**, I. Anishchenko, C. Glasscock, D. Baker<sup>\*</sup>, Atomic context-conditioned protein sequence design using LigandMPNN, 2025, **Nature Methods**, Accepted, <https://doi.org/10.1038/s41592-025-02626-1>. ([Link](#))
4. **L. An**<sup>\*</sup>, 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<sup>\*</sup>. Binding and sensing diverse small molecules using shape complementary pseudocycles, 2024, **Science**, 385, 276. ([link](#)).
5. **L. An**<sup>#</sup>, D. Hicks<sup>#</sup>, D. Zorine<sup>#</sup>, J. Dauparas, B. Wicky, L. Milles, A. Courbet, A. Bera, H. Nguyen, A. Kang, L. Carter, D. Baker<sup>\*</sup>. Hallucination of closed repeat proteins containing central pockets, **Nat. Struct. Mol. Biol.**, 2023, 30, 1755. ([Link](#))
6. **L. An**<sup>#</sup>, D. Cogan<sup>#</sup>, C. Navo, G. Jiménez-Osés, S. K. Nair, and W. A. van der Donk<sup>\*</sup>, Substrate-assisted enzymatic formation of lysinoalanine in duramycin, **Nat. Chem. Biol.** 2018, 10, 928. ([Link](#))
7. **L. An**<sup>#</sup>\* and G. R. Lee<sup>#</sup>\*, De novo protein design using the blueprint builder in Rosetta, *Current Protocols in Protein Science*, 2020, 102,1, e116. ([Link](#))
8. **L. An**, and W. A. van der Donk<sup>\*</sup>, Recent progress in lanthipeptide biosynthesis, discovery, and engineering, *Comprehensive Natural Products III*. 2019, 2, 119. ([Link](#))
9. **L. An**, M. Rehan H. Shah Gilani, G. L. Liang<sup>\*</sup>, Peptide-based nanostructures for cancer diagnosis and therapy, *Curr. Med. Chem.* 2014, 21, 2453. ([Link](#))
10. J. Acedo, I. Bothwell, **L. An**, A. Truth, C. Frazier, W. A. van der Donk<sup>\*</sup>, O-Methyltransferase-mediated Incorporation of a  $\beta$ -Amino Acid in Lanthipeptides, *J. Am. Chem. Soc.* 2019, 141, 42, 16790. ([Link](#))
11. **L. An**, "iGEM: Get & Give (& Share)", *Microbiology Today*, Web. 15 May 2018. ([Link](#))
12. Y. Liu<sup>#</sup>, Q. Miao<sup>#</sup>, P. Zou, L. Liu, X. Wang, **L. An**, X. Zhang, X. Qian, S. Luo, and G. Liang<sup>\*</sup>. Enzyme-controlled intracellular self-assembly of <sup>18</sup>F nanoparticles for enhanced

- microPET imaging of tumor. *Theranostics*. 2015, 5, 1058. ([Link](#))
13. 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](#))
  14. 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](#))
  15. 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 <sup>19</sup>F nanoparticles confer respective “Off” and “On” <sup>19</sup>F NMR/MRI signals for legumain activity detection in zebrafish. *ACS Nano*. 2015, 9, 5117-5124. ([Link](#))
  16. 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 <sup>19</sup>F nanoparticles for MR imaging of caspase 3/7 in zebrafish. *ACS Nano*. 2015, 9, 761. ([Link](#))
  17. 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](#))
  18. 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](#))
  19. 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](#))
  20. B. You\*, P. Yin, and **L. An**. (2014), Multifunctional Electroactive Heteroatom-Doped Carbon Aerogels. *Small*, 10: 4352-4361. ([Link](#))
  21. 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](#))
  22. 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](#))

## FUNDING

1. CPRIT - Recruitment of First-Time, Tenure-Track Faculty Members (RFT) award, 2025/05 - 2029/05

## HONORS

2. 2024 Rising Stars in Biological Engineering, Princeton University, Omenn-Darling Bioengineering Institute, Princeton University, 09/2024
3. 2024 Rising Star in Engineering in Health, co-hosted by Boston University, Johns Hopkins University, Cornell University, Columbia University, 09/2024

4. 2024 UT Austin MBS Trailblazers of Tomorrow National Postdoctoral Symposium, 05/2024
5. New Frontiers Scholar Award, Corteva, Inc. 08/2019
6. Fuson Travel Award, University of Illinois at Urbana-Champaign, 07/2018

## SELECTED Presentations

1. 2024 Workshop on Neutrons in Structural Biology, 06/2024
  - Invited talk: De Novo Small Molecule Binder and Sensor Design
2. RosettaCon, 08/2023
  - Presentation: De Novo Small Molecule Binder Design with Shape Complimentary Sampling
3. 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
4. MRSEC seminar, invited seminar. Brandeis University 06/2023
7. Rosetta Conference, Seattle (*Invited conference, supported by RosettaCon travel grant*) 08/2022
  - Poster: De novo design of small molecule binder using pseudocyclic proteins
8. Foresight's Molecular Machines Workshop, San Francisco (*Invited conference*) 07/2022
  - Invited Talk: De novo design of small molecule binding proteins
9. 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 lantipeptide mining strategy
10. 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
11. Midwest Enzyme Chemistry Conference, Loyola University, 10/2017
  - Selected talk: Substrate-assisted enzymatic formation of lysinoalanine in duramycin
11. Enzymes Coenzymes and Metabolic Pathways Gordon Research Seminar & Gordon Research Conference, 07/2017
  - Poster: Mechanistic details of duramycin biosynthesis
12. Midwest Enzyme Chemistry Conference, University of Illinois at Chicago, 10/2016
  - Poster: Mode of action studies for the two-peptide lantibiotic haloduracin
13. The 3rd National Chemistry Majors Scientific Activity Exchange (*Supported by the Department Travel Award*) Sichuan University, 12/2013

## TEACHING & MENTORING

**Mentor** for rotation students, Haotian(Odin) Zhang (computer science), UW, fall/2024-present

**Mentor** for graduate students, Shajesh Sharma (bioengineering), UW, winter/2023-present

**Mentor** for rotation students, Valentina Alvarez (biochemistry), UW, summer/2023

**Mentor** for graduate students, Long Tran (chemical engineering), UW, winter/2022-present

**Mentor** for rotation student, Emma Mackey (biochemistry), UW, summer 2021

**Mentor** for graduate student, Chunyu Wu(biochemistry), UIUC, 09/2018-2019

**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

## SERVICES

**Women in Biology**, Seattle chapter, 2022- present

**Jupyter Summer Internship preparation committee**, Institute for Protein Design, 2022

**Women in Science**, Institute for Protein Design, 2020- present

**Conference Committee** , Allerton Conference, UIUC, 2017

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

**Women Chemists Committee**, Stoesser Lecture, UIUC, 2016 & 2015

## SKILLSETS

Computational skills: python (fluent), bash scripts, Fine tune of machine learning models, RosettaScripts (fluent), PyRosetta (fluent), machine learning-based protein design scripts (fluent), python-based data analysis (fluent).

Chemistry/Biochemistry related skills:

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

Others:

1. Accomplished user of Illustrator, Photoshop, Autodesk 3D Max, Endnote, ChemDraw, html language;
2. Open water scuba diving;
3. Bouldering.