Xin Li

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EDUCATION

1/2013–5/2017 Ph.D. in Chemical Biology, Department of Chemistry, The University of Hong Kong.

9/2008–6/2012 B.Sc. in Pharmaceutical Sciences, Department of Pharmacy, Zhejiang University.

WORKING EXPERIENCE

6/2017–present Post-doctoral Fellow, Department of Chemistry, The University of Hong Kong.

ACADEMIC EXPERIENCE

8/2012–present Ph.D. student and Post-doctoral Fellow, Department of Chemistry, The University of Hong Kong. (Supervisor: Dr. Xiang David Li)

- Biochemical characterization for the decrotonylase activities of sirtuins.
  - *Characterization for the mechanism of sirtuin-catalyzed decrotonylation.*
  - *Substrate selectivity study of sirtuin-catalyzed decrotonylation.*
  - *Mutagenesis studies to investigate the roles played by the π-π interaction in the Sirt3-crotonyllysine recognition.*
- Developing cleavable chemical reporters for mapping the modification sites of fatty-acylation.
  - *Design and synthesis of selenoether-functionalized cleavable chemical reporters with terminal alkyne, azide, and alkene as bioorthogonal handles.*
  - *Metabolic labeling of chemical reporters in different cell lines.*
  - *Step-by-step analysis for the incompatibility of selenoether with Cu(I)-catalyzed azide-alkyne cycloaddition.*
- Developing chemical proteomics approaches to profile writers and readers of lysine acetylation (Kac). (Ongoing)
  - *Design and synthesis of photoaffinity probes to capture the endogenous writers and readers of Kac.*
  - *Pull-down experiments enriched multiple known writers and readers of Kac in cell lysates or living cells.*
  - *SILAC experiments for quantitative proteomic profiling of writers and writers of Kac.*
- Development of YEATS domain inhibitors (Ongoing).
  - *Structure-guided design of peptide-based YEATS domain inhibitors.*
  - *Inhibitory activity estimation using photo-crosslinking-based competition assay.*
  - *Direct binding measurements between inhibitors and YEATS domains using ITC and FP.*
  - *SAR study, new round of inhibitor design and structural optimization for better activity and drug-like properties.*
  - *High throughput screening and virtual screening of small molecule YEATS domain inhibitors (in collaboration with Richard Kao Lab, HKU, and Xuhui Huang Lab, HKUST).*
  - *Patent application.*

9/2009–6/2012 Undergraduate Research Assistant, Zhejiang University-Ecole Normale Super Paris Joint Laboratory of Medicinal Chemistry, Zhejiang University. (Supervisor: Prof. Yongzhou Hu)

- The 2nd Zhejiang Innovation Program for Undergraduates: Pharmacophore model construction of

p53–MDM2 binding inhibitors and its application in virtual screening.

- The 13th Student Research Training Program of Zhejiang University (SRTP): Synthesis and bioactivities evaluation of p53-MDM2 binding inhibitors. (Project leader)
- The 3rd Zhejiang Innovation Program for Undergraduates: Design, synthesis and bioactivities evaluation of MDM2 E3 ligase inhibitors. (Project leader)
- 2010 Zhejiang Innovation Program for Graduate Students: Design, synthesis and anti-tumor activities evaluation of PKB-MDM2 dual inhibitors. (The only undergraduate participant of the program for graduate students)
  - *Anti-tumor drug discovery targeting the p53-MDM2 pathway.*
  - *Pharmacophore model construction and novel leads identification by virtual screening.*
  - *Structure optimization of leads using rational and computer-aided drug design.*
  - *Synthesis, purification and structure validation of more than 30 target molecules in total.*
  - *SAR studies based on data of bioactivities evaluation.*

7/2011–9/2011 Short-term Intern, Department of Chemistry, University of California, Davis. (Advisor: Prof. Jacquelyn Gervay-Hague)

- Global Research Experience in Advanced Technologies (GREAT) Summer Research Program: Development of a Fluorescent High-throughput Screening Method for Sialyltransferase Inhibitors.
  - *One of 30 students selected from more than 200 applicants by Zhejiang University and University of California, Davis with good GPA and performances in research.*
  - *Training on operation of instruments like NMR, UV-Vis and LC-MS.*
  - *Training on critical thinking and reasoning, scientific writing, poster and oral presentation skills.*

CONFERENCE ATTENDANCE

4/2017 Abstract: Design, synthesis, and biological evaluation of peptide-based YEATS domain inhibitors. 1st Symposium on Chromatin Biology of Chinese Society for Cell Biology, Shenzhen, Guangdong, China.

12/2015 Abstract: Developing chemical tools to study histone acetyltransferases, The 2015 International Chemical Congress of Pacific Basin Societies (PAC CHEM™), Honolulu, HI, USA.

9/2012 Poster presentation: Pharmacophore model construction of p53-MDM2 binding inhibitors and its application in the discovery of a novel lead. 22nd International Symposium on Medicinal Chemistry (ISMC2012), Berlin, Germany.

11/2010 Poster presentation: Design, synthesis and biological evaluation of inhibitors of MDM2 E3 Ligase. 2010 Yangtze River Delta Symposium on Medicinal Chemistry, Shanghai, China.

HONORS AND AWARDS

2015 Best Oral Presentation in Postgraduate Research Seminar Award, Department of Chemistry, The University of Hong Kong

2012 Second-Class Research and Innovation Scholarship (Given to those who performed well in research work, Top 5%).

2011 First-award of university level and second-award of province level in 12th "Challenge Cup" Competition for Research and Technologies of College Students (Top 2%);

2010 Kwang-Hua Scholarship and Pharmacy Scholarship (Given to students who devote themselves to study of pharmacy-related majors, Top 5%);

2010 Third-Class Scholarship for Outstanding Merits (Top 10%).

SKILLS

- Organic and medicinal chemistry: small molecule synthesis and solid-phase peptide synthesis, including purification and analysis (HPLC, IR, UV-Vis, NMR and MS), rational drug design, mainstream computational chemistry and drug design software: Catalyst, Discovery Studio, Sybyl, PyMol.
- Biochemistry and molecular cell biology: molecular cloning, protein expression and purification, enzymatic kinetics study, isothermal titration calorimetry, fluorescence polarization, cell culture (including SILAC), immunoblotting.
- Proteomics: affinity-based or photo-cross-linking-based pull-down, quantitative proteomics sample preparation and data analysis by MaxQuant.

PUBLICATIONS

13. X. Bao, Y. Xiong, **X. Li**, X. D. Li, Chemical reporter facilitates the detection and identification of lysine HMGylation on histones. Manuscript submitted.
12. Y. Zhou, L. Chen, J. Peng, L. Xie, L. Meng, J. Zhang, X. D. Li, **X. Li***, X. Huang*, X. Li*, A dynamic approach to fragment-based ligand discovery enabled by DNA dynamic assembly and DNA encoding. Manuscript under revision. (*co-corresponding author)
11. **X. Li**[#], X.-M. Li[#], Y. Jiang, Z. Liu, Y. Cui, K. Y. Fung, S. H. E. van der Beelen, G. Tian, L. Wan, X. Shi, C. D. Allis, H. Li, Y. Li, X. D. Li, Targeting π-π-π stacking: structure-guided development of YEATS domain inhibitors. Manuscript under revision. (#co-first author)
10. Y. Chen, T. L. Li, X. Lin, **X. Li**, X. D. Li, Z. Guo, Crystal structure of the thioesterification conformation of *Bacillus subtilis O*-succinylbenzoyl-CoA synthetase reveals a distinct substrate-binding mode. *J. Biol. Chem.*, **2017**, *292*, 12296-12310.
9. Y. Cui[#], **X. Li**[#], J. Lin. Q. Hao, X. D. Li, Histone ketoamide adduction by 4-oxo-2-nonanal is a reversible posttranslational modification regulated by Sirt2. *ACS Chem. Biol.*, **2017**, *12*, 47-51. (#co-first author)
8. **X. Li**, X. D. Li, Chemical proteomics approaches to examine novel histone posttranslational modifications. *Curr. Opin. Chem. Biol.*, **2015**, *24*, 80-90.
7. Z. Liu, T. Yang, **X. Li**, T. Peng, H. C. Hang, X. D. Li, Integrative chemical biology approaches for identification and characterization of "erasers" for fatty-acid-acylated lysine residues within proteins. *Angew. Chem. Int. Edit.*, **2015**, *54*, 1149-1152.
6. X. Bao[#], Y. Wang[#], **X. Li**[#], X.-M. Li[#], Z. Liu, T. Yang, C. F. Wong, J. Zhang, Q. Hao, X. D. Li, Identification of 'erasers' for lysine crotonylated histone marks using a chemical proteomics approach. *eLife*, **2014**, *3*. (#co-first author)
5. C. Hu, **X. Li**, W. Wang, R. Zhang, L. Deng, Metal-*N*-heterocyclic carbene complexes as anti-tumor agents. *Curr. Med. Chem.*, **2014**, *21*, 1220-1230.
4. X. Dou, **X. Li**, T. Liu, C. Hu, L. Zhang, Q. He, B. Yang, Y. Hu, Synthesis and biological evaluation of novel pyrimido[4,5-b]quinoline-2,4-dione derivatives as MDM2 ubiquitin ligase inhibitors. *Med. Chem.*, **2013**, 9, 581-587.
3. C. Hu, **X. Li**, W. Wang, L. Zhang, L. Tao, X. Dong, B. Yang, Y. Hu, Design, synthesis, and biological evaluation of imidazoline derivatives as p53–MDM2 binding inhibitors. *Bioorg. Med. Chem.*, **2011**, *19*, 5454-5461.
2. S. Yuan, P. Zhang, X. Huang, **X. Li**, Q. Teng, Electronic structures and spectroscopic characters of modified oligo(alkylenedioxypyrrole). *Chin. J. Chem. Phys.*, **2011**, 29, 888-892.
1. P. Zhang, X. Huang, **X. Li**, Q. Teng, DFT Study on Electronic: Structures and spectroscopic sroperties of oligo(silanylenediethynylanthracene). *Chin. J. Chem. Phys.*, **2011**, 24, 25-30.