Rui Chen

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EDUCATION

China Pharmaceutical University (CPU) Sep. 2020 – Jun. 2023
M.Sc. in Pharmacy, **GPA:** 4.00 / 4.00 (88.54/100.00, Top 10%, Ranked 8/81)

Shandong University of Traditional Chinese Medicine (SDUTCM) Sep. 2016 – Jun. 2020
B.Sc. in Pharmaceutical Engineering, **GPA:** 3.29/4.00 **(**82.48/100, Top 3%, Ranked 7/247)

PUBLICATIONS

Papers:

Chen, R.; Huang, J.; Chen, Y; Qin, L.; Chen, H.; Wang, Y.; Huang, D.; Li, Z.; Ali, A. R.; Bian, J. *Identification of a Novel ASCT2 (SLC1A5) Inhibitor by Dynamic Pharmacophore-Based Virtual Screening.* (Status: In Submission)

Hu, T[1].; Zhang, H[1].; **Chen, R[1].**; Huang, J.; Liu, M.; Zhou, W.; Li, D.; Li, Z.; Wu, H.; Bian, J. *Discovery of CLKs Inhibitors for the Treatment of Non-small Cell Lung Cancer.* Eur. J. Med. Chem. 2024, 280, 116952 (First author, co-authored by 3)

Zhou, L.; Yu, B.; Gao, M.; **Chen, R**.; Li, Z.; Gu, Y.; Bian, J.; Ma, Y. *DNA Framework-Engineered Chimeras Platform Enables Selectively Targeted Protein Degradation.* Nat. Commun. 2023, 14 (1), 4510.

Wu, T.; Yu, B.; Xu, Y.; Du, Z.; Zhang, Z.; Wang, Y.; Chen, H.; Zhang, L. A.; **Chen, R**.; Ma, F.; Gong, W.; Yu, S.; Qiu, Z.; Wu, H.; Xu, X.; Wang, J.; Li, Z.; Bian, J. *Discovery of Selective and Potent Macrocyclic CDK9 Inhibitors for the Treatment of Osimertinib-Resistant Non-Small-Cell Lung Cancer.* J. Med. Chem. 2023, 66 (22), 15340–15361.

Wu, T.; Wu, X.; Xu, Y.; **Chen, R**.; Wang, J.; Li, Z.; Bian, J. *A Patent Review of Selective CDK9 Inhibitors in Treating Cancer.* Expert Opin. Ther. Pat. 2023, 33 (4), 309–322.

Wang, D.; Li, X.; Gong, G.; Lu, Y.; Guo, Z.; **Chen, R**.; Huang, H.; Li, Z.; Bian, J. *An Updated Patent Review of Glutaminase Inhibitors (2019-2022).* Expert Opin. Ther. Pat. 2023, 33 (1), 17–28.

Xie, Y.; Tian, Y.; Zhang, Y.; Zhang, Z.; **Chen, R**.; Li, M.; Tang, J.; Bian, J.; Li, Z.; Xu, X. *Overview of the Development of Selective Androgen Receptor Modulators (SARMs) as Pharmacological Treatment for Osteoporosis (1998-2021).* Eur. J. Med. Chem. 2022, 230, 114-119.

RESEARCH

Research Area: Discovery of novel anti-cancer drugs
Keywords: ASCT2, DON, PROTAC, LAT1, Drug Discovery, CADD, Virtual Screen

(1) **Discovery of novel ASCT2 inhibitors (Project Leader)** Oct. 2021 – Jun. 2023
Supervisor: Prof. Jinlei Bian

- Discovery of novel scaffold ASCT2 lead compounds through virtual screening and activity assaying workflows.
- Virtual screening workflows such as molecular dynamics simulations, molecular docking, and pharmacophore screening.
- Based on the lead compounds, studied the drug-target conformational relationship, combined with the protein crystal structure, through molecular docking and MD simulation, designed and synthesized 31 novel inhibitors.
- By screening for enzyme and cellular activity, obtained inhibitors with tumor cell inhibitory activity superior to positive drug V9302.
- Presented results to professors and produced a graduation thesis and paper.

(2) **Discovery of novel CLK2 inhibitors** Jun. 2022 – Jun. 2023
Supervisor: Prof. Jinlei Bian

- Discovery of novel CLK2 inhibitors based on structure-based drug design.
- Enhanced water solubility and formulation properties of the lead compound.
- Improved antiproliferative activity against H1299 cells.
- Co-first author, published in Eur. J. Med. Chem., under minor revision.

(3) **Discovery of novel DON inhibitors** Feb. 2022 – Jun. 2022
Supervisor: Prof. Jinlei Bian

- Participated in the design and synthesis of a series of DON ester prodrugs.
- Improved the original toxic effects of DON through the design of the prodrug, and improved the plasma stability and tolerability of DON.

(4) **Discovery of novel DNA-linker PROTAC** Apr. 2022 – Jun. 2023
Supervisor: Prof. Jinlei Bian

- Participated in the design and synthesis of the CDK9 inhibitor-based PROTAC warhead.
- Responsible for molecular docking of DNA to protein and small molecules to protein in the project.
- It was demonstrated that caged DNA could fix the length of PROTAC's linker well and play a good role in protein degradation.
- Contributed as an author to the article, which was published in *Nature Communication* in 2023.

(5) **Discovery of novel LAT1 inhibitors** Aug. 2021 – May. 2022

Supervisor: Prof. Jinlei Bian

- Participated in the research of LAT1 novel inhibitor program, molecular docking and designing novel backbone molecules for existing inhibitors.
- Supervised undergraduate students in writing reviews on glutamine inhibitors and participated as an author in articles published in Expert Opinion on Therapeutic Patents.

Research Area: Drug synthesis process optimization

Keywords: Process optimization, Crystallization process

(1) **Studies on the synthesis of standardized products related to psychotropic drugs** Oct. 2020 – Mar. 2021

Supervisor: Prof. Zhiyu Li

- Participated in the investigation of the synthesis process of some compounds of psychotropic substances in cooperation with the National Narcotics Control Office of China.
- Synthesis of standardized controls for several related psychotropic drugs.
- Completing the writing and typesetting and proofreading of the project closure report.

(2) **Study on patenting of novel JAK inhibitors** Apr. 2021 – Jan. 2022

Supervisor: Prof. Zhiyu Li

- Participated in the process optimization process of the new JAK inhibitor, optimized some process parameters and improved the overall yield.
- Improved recrystallization parameters for compound intermediates resulted in rapid synthesis of kilogram-sized products.

WORK EXPERIENCE

Jiangsu Aidea Pharmaceutical Co., Ltd. **Position:** Synthetic Scientist Jul. 2023 – Present

Research Area: Novel long-acting HIV inhibitors

(1) Research on novel integrase inhibitor ACC017

- Design and synthesis the novel HIV-1 integrase inhibitors, enhances the original drug activity.
- Improving the metabolism issue with new structure design, enhanced plasma stability of the drug.
- Improvement of insoluble drug solubility and determination of crystal form.

(2) Research on novel HIV-1 capsid inhibitor

- Design of novel HIV-1 capsid inhibitors using molecular dynamics simulations and molecular docking techniques.
- Synthesis of novel capsid inhibitors and assayed for biological activity.

(3) Research on new production processes ACC007

- Improved the original synthesis process and reduced the production cost.
- Optimize the production process and reduce waste due to operations in production.

PROFESSIONAL SKILLS

Experiment skills: Independently design experiments and obtain target compounds, and master specific experimental methods such as TLC, recrystallization, column chromatography, and structure analysis (HNMR, MS, HPLC, etc.).

CADD Skills: Knowledge of molecular docking, virtual screening, molecular dynamic simulation (MD) theory and methods, proficiency in CADD software such as Schrödinger, MOE, Discovery Studio (DS), Autodock, GROMACS, Pymol, VMD, etc.

Software Skills: Proficient in Office, Zotero, Ai, GraphPad, ChemDraw, MestReNove, etc.

Language: Chinese Mandarin (Level II, Grade A), English (IELTS 6.0).

HONORS & AWARDS

- The Second Prize, CPU Scholarship Oct. 2022
- The Second Prize, CPU Scholarship Oct. 2021
- The First Prize, CPU Freshman Graduate Student (Top 5%) Dec. 2020
- Shandong Province Outstanding Undergraduate Student Award (Top 1%) Jun. 2020
- SDUTCM Excellent Student Cadre Dec. 2019
- Provincial Team Silver Award, “Internet+” Innovation and Entrepreneurship Competition Sep. 2019
- Team Second Prize, the 1st SDUTCM Tai Chi Competition Apr. 2019
- The First Prize, SDUTCM Scholarship Dec. 2018
- SDUTCM Excellent Student Dec. 2018
- SDUTCM Excellent Student Cadre Dec. 2017
- Volunteer Activities for the Country People Excellent Student Oct. 2017

EXTRACURRICULAR ACTIVITIES

- Hosted and managed the innovation and entrepreneurship training program for university students 2022 – 2023
- Class monitor during the university 2016 – 2020