

# 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*. (In Submission)

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, 114119.

## RESEARCH

**Research Area:** Discovery of novel anti-cancer drugs

**Keywords:** Drug Discovery, Computer-aided drug design (CADD), Virtual Screening, ASCT2, DON, PROTAC, LAT1

### (1) Discovery of novel ASCT2 inhibitors (Project Leader)

Oct. 2021 – Jun. 2023

Supervisor: Prof. Zhiyu Li, Prof. Jinlei Bian

- Discovery of novel scaffold ASCT2 lead compounds through virtual screening and activity assaying workflows.
- Help labs purchase and build high-performance computer hardware and build CADD workstations
- 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 DON inhibitors

Feb. 2022 – Jun. 2022

Supervisor: Prof. Zhiyu Li, 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.

### (3) Discovery of novel DNA framework-based PROTACs (DbTACs)

Apr. 2022 – Jul. 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 DbTACs 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.

### (4) 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.
- Determination of crystal form and improved the insoluble drug solubility.

**(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, Adobe illustrator, GraphPad, ChemDraw, MestReNove, etc.

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

**HONORS & AWARDS**

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|---|-----------|
| • 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**

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