Defang OUYANG
Associate professor

Academic Qualifications

- PhD, The University of Queensland, Australia (2010)
- MSc, Shenyang Pharmaceutical University, China (2005)
- BSc, Shenyang Pharmaceutical University, China (2000)

Teaching

- HSCI4011 Pharmacoinformatics
- CMED7020 Computational Pharmacy
- CMED7035 Application of Computer Technology in Pharmacy
- CMED8011 Advanced topics in Medicinal Administration

Research

Prof. Ouyang has a multidisciplinary background in pharmaceutics & computer modelling, with experience in academia and industry. He obtained his bachelor (2000) and master (2005) in pharmaceutics from Shenyang Pharmaceutical University, China. He completed his PhD in pharmacy at The University of Queensland, Australia, in 2010 and progressed directly to his faculty position (Lecturer in Pharmaceutics, PI) at Aston University (UK). From the end of 2014, he moved to the University of Macau.

Since 2011, he has pioneered the integration of multi-scale modeling, artificial intelligence and big data techniques in the field of drug delivery – "**computational pharmaceutics**". He has published 2 books, 5 book chapters and over 140 refereed SCI journal papers, along with more than 150 invited talks. He held over 10 approved patents, which had been used in medicinal products. He edited the first book in this research domain <**Exploring Computational Pharmaceutics – AI and Modeling in Pharma 4.0**> (Wiley, 1st Edition in 2015 & 2nd edition in 2024). He has developed the crucial "Rule of 5" for effective AI drug delivery models and successfully built the first global artificial intelligence (AI)-based formulation platform "**FormulationAI**" (https://formulationai.computpharm.org/).

He serves as the associate editor of <*Drug Delivery and Translational Research*>, the editorial board or scientific advisor of <*Asian Journal of Pharmaceutical Sciences*>, <*Pharmaceutical Research*>, and <*Journal of Pharmaceutical Sciences*>. He successfully trained 6 PhD and over 30 master students. He has been recognized as "World's Top 2% Scientists" from 2020 to 2024.

His research focused on computational pharmaceutics, including:

- Artificial intelligence (AI) in drug delivery: to develop advanced machine learning algorithms for drug delivery systems;
- Multi-scale modeling in drug formulations: to integrate quantum mechanics (QM), molecular dynamics (MD) and physiologically based pharmacokinetic (PBPK) modeling into pharmaceutical formulations;
- Pharmacoinformatics: big data analysis of pharmaceutical information from the literature, patent, clinical trial and marketed products.

Publication

10 representative publications in recent 5 years

1. Nannan Wang, Jie Dong, **Defang Ouyang***. AI-directed formulation strategy design initiates rational drug development. ***Journal of Controlled Release***, 2025, 378, 619-636;
2. Wei Wang, Kepan Chen, Ting Jiang, Yiyang Wu, Zheng Wu, Hang Ying, Hang Yu, Jing Lu, Jinzhong Lin & **Defang Ouyang***. Artificial intelligence-driven rational design of ionizable lipids for mRNA delivery. ***Nature Communications***, 2024, 15, 10804;
3. Wei Wang, Shiwei Deng, Jinzhong Lin, **Defang Ouyang***. Modeling on in vivo disposition and cellular transportation of RNA lipid nanoparticles via quantum mechanics/physiologically-based pharmacokinetic approaches. ***Acta Pharmaceutica Sinica B***, 2024, 14 (10), 4591-4607;
4. Zhuyifan, Ye, Nannan Wang, **Defang Ouyang***. Crystal structure prediction for organic compounds by machine learning algorithm, ***The Innovation***, 2024, 5(2), 100562;
5. Nannan Wang, Yunsen Zhang, Wei Wang, Zhuyifan Ye, Hongyu Chen, Guanghui Hu, and **Defang Ouyang***. How can machine learning and multiscale modeling benefit ocular drug development? ***Advanced Drug Delivery Reviews***, 2023: 114772;
6. Run Han, Zhuyifan Ye, Yunsen Zhang, Yaxin Cheng, Ying Zheng, **Defang Ouyang***. Predicting liposome formulations by the integrated machine learning and molecular modeling approaches. ***Asian Journal of Pharmaceutical Sciences***, 2023, 18 (3), 100811;
7. Wei Wang, Shuo Feng, Zhuyifan Ye, Hanlu Gao, Jinzhong Lin, **Defang Ouyang*.** Prediction of lipid nanoparticles for mRNA vaccines by the machine learning algorithm, ***Acta Pharmaceutica Sinica B***, 2022, 12 (6), 2950-2962;
8. Wei Wang, Zhuyifan Ye, Hanlu Gao, **Defang Ouyang*.** Computational pharmaceutics-A new paradigm of drug delivery. ***Journal of Controlled Release***. 2021, 338, 119-136;
9. Haoshi Gao, Haoyue Jia, Jie Dong, Xinggang Yang, Haifeng Li, **Defang Ouyang***. Integrated in silico formulation design of self-emulsifying drug delivery systems. ***Acta Pharmaceutica Sinica B***, 2021, 11(11), 3585-3594;
10. Haoshi Gao, Yan Su, Wei Wang, Wei Xiong, Xiyang Sun, Yuanhui Ji, Hua Yu, Haifeng Li, and **Defang Ouyang***. Integrated computer-aided formulation design: A case study of andrographolide/cyclodextrin ternary formulation. ***Asian Journal of Pharmaceutical Sciences*** 2021,16(4): 494-507;

Professional Society

- Computational Pharmacy Society (CPS)
- American Chemical Society (ACS)
- Asian Association of Schools of Pharmacy (AASP)

Academic Services

- Fellow of the Higher Education Academy (UK);
- Associate editor of "Drug Delivery and Translational Research";
- Editorial board of "Asian Journal of Pharmaceutical Sciences", "Pharmaceutical Research" and "npj Drug Discovery";
- Scientific Advisor of "Journal of Pharmaceutical Sciences";
- Grant reviewer of BBSRC (UK), French National Research Agency (ANR), Canada First Research Excellence Fund, and National Science Centre Poland;
- Reviewer of over 20 SCI journals;

Contact Details

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