Prof. Defang OUYANG

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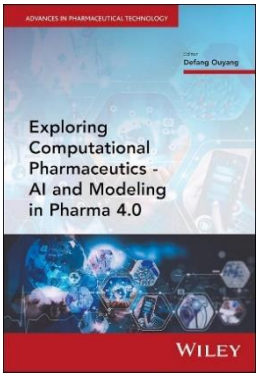

Brief Summary

Prof. Ouyang is a recognized leader in the field of computational pharmaceutics. He has authored two books, 10 book chapters, and over 100 peer-reviewed SCI papers, along with more than 150 invited presentations, including US-FDA. He edited the first book in this research domain <**Exploring Computational Pharmaceutics – AI and Modeling in Pharma 4.0**> (1st Edition in 2015 & 2nd edition in 2024). Additionally, he holds 12 patents that have been utilized in marketed medicinal products.

Since 2011, he has pioneered the integration of artificial intelligence, big data and multi-scale modeling techniques in the field of drug/gene delivery - "**computational pharmaceutics".** He has developed the crucial **"Rule of 5"** for effective AI drug delivery models and has published over 35 SCI papers in this pioneering area, ranking first and solidifying his status as a leader in the field. He also established the first global AI-based formulation platform "**FormulationAI**" (https://formulationai.computpharm.org/), which has attracted numerous major pharmaceutical companies and top academic institutions.

Prof. Ouyang serves as an associate editor and on the editorial boards of several SCI journals, such as *Drug Delivery and Translational Research*, *Asian Journal of Pharmaceutical Sciences, Pharmaceutical Research, Journal of Pharmaceutical Sciences*, and *npj Drug Discovery*. Furthermore, he participates as a reviewer for numerous international grants and chairs multiple international conferences. He is the founding chair of the Computational Pharmacy Society (CPhS). He has been recognized as "World's Top 2% Scientists" from 2020 to 2024.

Research interests

- **Artificial intelligence (AI)** for drug delivery: to develop advanced machine learning algorithms for the prediction of pharmaceutical formulations, such as lipid nanoparticle (LNP) for mRNA/siRNA delivery, long-term sustained release microsphere and various solubilization techniques for water insoluble drugs;
- **Multi-scale modeling** in drug formulations: to combine quantum mechanics (QM), molecular dynamics (MD), mathematical modeling and physiologically based pharmacokinetic (PBPK) modeling into drug and gene delivery systems;
- **Pharmacoinformatics**: big data analysis of pharmaceutical information from the literature, patent, clinical trial and marketed products.

Educational Background

2007 – 2010, PhD, School of Pharmacy, The University of Queensland, Australia

PhD thesis: “The Rational Design, Synthesis and Evaluation of Non-Viral Gene Delivery Systems Based on Computer-Aided Drug Design”

Supervisors: Dr. Harendra S. Parekh & Prof. Sean C. Smith

2002 – 2005, MPhil (Pharmaceutics), Shenyang Pharmaceutical University, China

Master thesis: “Development of oral sustained-release preparations of metformin/glipizide combination”

Supervisor: Prof. Weisan Pan

1996 – 2000, BSc (Pharmaceutics), Shenyang Pharmaceutical University, China

Career History

08/2021 – now, Associate professor, University of Macau, Macau

11/2014 – 08/2021, Assistant Professor, University of Macau, Macau

01/2011 – 10/2014, Lecturer in Pharmaceutics, School of Life and Health Sciences, Aston University, UK

2005 – 2007, Formulation scientist, Shenzhen Main Luck Pharmaceutical Inc., China

2000 – 2002, Engineer, Tianjin Huajin Pharmaceutical Company, China

Research grants **(12 research grants in recent 5 years with over 8 million MOP in total)**

- “Rational design of lipid nanoparticles for mRNA delivery”, 2024-2027, FDCT Research Grant (0071/2024/RIA1), 1,910,000 MOP, Macau (PI);
- “Artificial intelligence-driven protein formulation development”, 2025-2026, UM Research Grant (MYRG-GRG2024-00123-ICMS-UMDF), 200,000 MOP, Macau (PI);
- “Set Sail for New Horizons, Create the Future” Grant 2024 - Visiting Scholar Exchange Program”, 2024, Dr. Stanley Ho Medical Development Foundation (SHMDF-VSEP/2024/001), 100,000 MOP, Macau (PI);
- “Prediction of ternary solid dispersion formulations by integrated high-throughput screening and machine learning approaches”, 2024-2025 UM Research Grant (MYRG-GRG2023-00077-ICMS-UMDF), 320,000 MOP, Macau (PI);
- “Investigation of the release mechanism of long-sustained release microspheres”, 2023-2024, UM Research Grant (MYRG-CRG2022-00008-ICMS), 1,520,000 MOP, Macau (PI);

- “PBPK modeling of oral peptide formulation”, 2023, Industrial project (Peking University 3rd Hospital), 180,000 CNY, Macau (PI);
- “Prediction of 3D printing formulations”, 2022, Industrial project (Triastek), 100,000 CNY, Macau (PI);
- “Development and validation of molecular modeling platform for pharmaceutics”, 2022-2024, Shenzhen-Hongkong-Macau collaboration project, 1000,000 CNY, Shenzhen (PI);
- “Application of artificial intelligence in triptorelin long-sustained release microsphere”, 2022-2024, Zhuhai Industrial-Academic collaboration project (ZH22017002210010PWC), 800,000 CNY, Zhuhai, (co-PI);
- “Preparation and evaluation of a highly-soluble Ginsenoside Rh2 formulation”, 2021-2023, FDCT Research Grant (0108/2021/A), 721,000 MOP, Macau (PI);
- “Prediction of ternary cyclodextrin formulations by machine learning approaches”, 2020-2021 UM Research Grant (MYRG2020-00113-ICMS), 360,000 MOP, Macau (PI);
- “Joint Research for the Quality Evaluation Technology of Pharmaceutical Preparations for the Treatment of Major Diseases” 2020-2024, Strategic Technological Innovation Cooperation (2020YFE0201700), 12,690,000 CNY, the Ministry of Science and Technology of China (co-PI);
- "An Artificial Intelligence System for Oral Formulation Prediction of Poorly‐Soluble Drugs", 2019-2020, UM Research Grant (MYRG2019-00041-ICMS), 750,000 MOP, Macau (PI);
- “Preparation and evaluation of highly-soluble andrographolide formulations”, 2018-2020, FDCT Research Grant (0029/2018/A1), 1,002,000 MOP, Macau (PI);
- “Development of Chinese medicine database”, 2017 Guangdong-Macau Cooperation Industrial Park grant, 1,500,000 CNY, China (co-PI);
- “An intelligent system for cyclodextrin formulation development”, 2016-2017, UM Research Grant (MYRG2016-00038-ICMSQRCM), 1,474,000 MOP, Macau (PI)
- "Computational Prediction of Physical Stability of Solid Dispersions", 2016-2017, UM Research Grant (MYRG2016-00040-ICMSQRCM), 662,500 MOP, Macau (PI);
- “Preparation and evaluation of a highly-soluble lutein formulation”, 2015-2017, FDCT Research Grant (009/2015/A), 466,000 MOP, Macau (PI);
- “Investigation of molecular mechanism of glipizide/cyclodextrin formulations by molecular dynamics simulations”, 2014 UM Start-up grant (SRG2014 -00029-ICMS-QRCM), 150,000 MOP, Macau (PI);
- “Development of activated carbon-based oral drug delivery systems for taste-masking”, 2013-2014, Royal Society Research Grants (RG120633), £14,950, Royal Society, UK (PI);

Awards

- 2020 - 2024, World's Top 2% Scientists;
- 2024, University of Macau Academic Award Scheme;
- 2024, Dr. Stanley Ho Medical Development Foundation Visiting Scholar;
- 2021, Excellent Scientific Paper Award of Chinese Science Association;
- 2019 Outstanding reviewer of <Journal of Pharmaceutical Sciences>;
- 2018, 3rd Prize in National Competition & 2nd Prize in Macau Regional, Bank of China Trophy One Million Dollar Entrepreneurship Competition, Hong Kong University of Science and Technology, China (as the Supervisor);

- 2015 Outstanding reviewer of <International Journal of Pharmaceutics>;
- 2015, 2nd Prize of 2015 Challenge Cup, China Science and Technology Association, China (as the Supervisor);
- 2013, Science Capital Business Plan Award, UK;
- 2011, Dean's Award for Research Higher Degree Excellence, The University of Queensland, Australia;
- 2009, Research Higher Degree Award in the Therapeutic Targeting category, School of Pharmacy, The University of Queensland, Australia;
- 2007, Faculty of Health Science Tuition Fee-Waiver Scholarship & School of Pharmacy International Living Allowance Scholarship, The University of Queensland, Australia;
- 2005, Excellent Master Thesis Award, Shenyang Pharmaceutical University, China

Teaching

Prof. Ouyang has wide teaching and curriculum development experiences in pharmaceutical sciences and bioengineering, at the undergraduate (MPharm) and postgraduate level (Master and PhD). He obtained **the Post-Graduate Certificate in Higher Education Practice (PgCHEP, UK) and is the Fellow of Higher Education Academy in the UK**. He is also interested in pharmacy education and published 4 pedagogical papers.

- Computational pharmacy (MPhil, module coordinator)
- Professional Studies: Effective Learning, Career Management and IT (MPharm, 1st year, module coordinator, 150 undergraduates)
- Pharmaceutical Formulation I: Liquid-Based Dosage Forms (MPharm, 1st year, 150 undergraduates)
- Spectroscopic Analysis of Medicines (MPharm, 2nd year, 150 undergraduates)
- Pharmaceutical Formulation III (MPharm, 3rd year, 150 undergraduates)
- Advanced Drug Delivery and Targeting (MPharm, 4th year, 150 undergraduates)
- Principles of Drug Analysis and Validation (MSc, module coordinator)
- Application of Computer Technology in Pharmacy (MSc, module coordinator)
- Pharmacokinetics (MPhil)
- Advanced medicinal administration (PhD)

PhD supervision

Prof. Ouyang had successfully supervised 1 postdoc, 7 PhD students (as below) and 29 master students. Currently his research group includes 2 postdoc, 12 PhD students and 10 master students.

- Wei Wang, PhD thesis "Computational modeling for mRNA lipid nanoparticle formulation design" (2019-2023, University of Macau, supervisor);
- Zhuyifan Ye, PhD thesis "Application of advanced machine learning algorithms in drug delivery" (2018-2022, University of Macau, supervisor);
- Haoshi Gao, PhD thesis "Integrated in silico formulation design of lipid based drug delivery systems" (2018-2022, University of Macau, co-supervisor with Prof. Haifeng Li);

- Qianqian Zhao, PhD thesis “Investigation of Molecular Mechanism of Cyclodextrin Solubilization and Development of a Predictive Model with Machine Learning Techniques” (2015-2018, University of Macau, supervisor);
- Miriyala, N., PhD thesis “Porous carbon carriers for amorphous drug delivery” (2013-2017, Aston University, co-supervisor with Dr Daniel Kirby);
- Thu Pham, PhD thesis “Design and characterisation of orally dissolving films as a potential new dosage form for paediatrics” (2013-2016, Aston University, supervisor)
- Karnaker R Tupally, PhD thesis “Engineering novel disulfide-bridged amino acid for the development therapeutic and carrier peptide and a novel FRET probe synthesis” (2012-2016, University of Queensland, co-supervisor with Dr Harendra Parekh)

Academic Leadership

- Founding chair of the Computational Pharmacy Society (CPhS)
- Associate editor of <*Drug Delivery and Translational Research*>
- Editorial board of <*Asian Journal of Pharmaceutical Sciences*>;
- Editorial board of <*Pharmaceutical Research*> (IF 4.58);
- Editorial board of <*npj Drug Discovery*>
- Scientific Advisor of <*Journal of Pharmaceutical Sciences*>;
- Guest editor of Virtual Special Issue (VSI) “Computational Methods in Drug Delivery” of <*Molecular Pharmaceutics*>
- Topic editor of Special Issue “The Use of Bio/Chemoinformatics Tools in Drug-Formulation to Reach Better Pharmacological Responses” of <*Frontiers in Pharmacology*>
- Topic editor of Special Issue "Gene Therapy" of <*Pharmaceutics*>;
- Grant reviewer of Canada First Research Excellence Fund (CFREF), BBSRC (UK), French National Research Agency (ANR) French Funding Program, and National Science Centre Poland;
- Examiner of PhD thesis from University of Texas at Austin (US, 2), University of Helsinki (Finland, 1), University of Queensland (Australia, 1), Monash University (Australia, 1), University of Auckland (New Zealand, 1), CUHK (HK, 1), HKBU (2) and UM (over 10);
- Chair and organizing committee of multiple international conferences, including
    - **1st Symposium on Computational Pharmaceutics – AI and Modeling in Pharma 4.0 (14-15 December, 2024, Macau)**
    - Macau Symposium on Artificial Intelligence and Health (30-31 October, 2023, Macau)
    - Bioinformatics: “Omics” Approach and Data Analysis Session, 17th Meeting of the Consortium for Globalization of Chinese Medicine (8-10 August, 2018, Sarawak, Malaysia);
    - Biophysics symposium in 2018 Joint Annual Conference of Physical Societies in Guangdong-Hong Kong-Macau Greater Bay Area（26-29 July 2018, Macau）
    - Mini-Symposium on Computational Pharmaceutics in The 10th International Conference on Computational Physics (ICCP10) (16-20 January 2017, Macau),
    - 7th International Conference on Computational Systems-Biology and Bioinformatics 2016 (19-22 December, 2016, Macau),
    - Computational Pharmaceutics Workshop in the Controlled Release Society Annual Meeting 2014 (12th - 16th July, Chicago, USA),

- Member of The Controlled Release Society (CRS), American Chemical Society (ACS), Asian Association of Schools of Pharmacy (AASP), Computational Pharmacy Society;
- Reviewer of over 20 SCI journals: <Journal of Controlled Release>, <Molecular Pharmaceutics>, <International Journal of Pharmaceutics>, <Journal of Pharmaceutical Sciences>, <Journal of Pharmacy and Pharmacology>, <Drug Development and Industrial Pharmacy>, <American Journal of Pharmaceutical Education>, <BMC Biotechnology>, <Journal of Biomaterial Application>, <Pharmaceutics>, <Bioconjugate Chemistry>, <BMC Biotechnology>, <Chemical Communications>, <Colloids and Surfaces B Biointerfaces>, <International Journal of Molecular Sciences>, <Journal of Photochemistry and Photobiology B Biology>, <Pharmaceutics>, <Chemical Physics Letter>, <Journal of Physical Chemistry Letter> <Journal of Liposome Research>, <Drug Delivery>, <Biomacromolecules>, <Chinese Medicine> etc.;

Publications

Books (3)

1. **D. Ouyang**. ***Exploring Computational Pharmaceutics - AI and Modeling in Pharma 4.0*.** Wiley (English version) & Chemical Industrial Press (Chinese version), 2024.
2. **D. Ouyang**, S. Smith. Computational Pharmaceutics - application of molecular modeling in drug delivery. John Wiley & Sons Inc., 2015.
3. **Ouyang D**, Pan Weisan. <Practical Pharmaceutical Patents> (2006). The People Medical Press, Beijing. ISBN: 7117080914. (in Chinese)

Book chapters (10)

4. N Wang, W Wang, H Zhong, **D Ouyang**. Introduction to Computational Pharmaceutics. <Exploring Computational Pharmaceutics - AI and Modeling in Pharma 4.0>2024, 1-9;
5. Z Ye, **D Ouyang**. Opportunities and Challenges of Artificial Intelligence (AI) in Drug Delivery. <Exploring Computational Pharmaceutics: AI and Modeling in Pharma 4.0>2024, 10;
6. KR Tupally, P Seal, P Pandey, RJ Lohman, S Smith, **D Ouyang**, H Parekh. Integration of Dendrimer - Based Delivery Technologies with Computational Pharmaceutics and Their Potential in the Era of Nanomedicine. <Exploring Computational Pharmaceutics - AI and Modeling in Pharma 4.0> 2024, 328-378;
7. W Wang, Y Wang, **D Ouyang**. Model-informed Drug Development (MIDD) Regarding Regulatory Requirements and Thinking. <Exploring Computational Pharmaceutics - AI and Modeling in Pharma 4.0> 2024, 574-592;
8. Zhuyifan Ye, **D. Ouyang**. Application of artificial intelligence techniques in pharmaceutical excipients and pharmaceutical big data. <Test techniques of pharmaceutical excipients and pharmaceutical packaging materials>, 2019, 239-255 (in Chinese)
9. Feng Qian， **D. Ouyang.** Chapter 12: solid dispersions, cyclodextrin, microencapsule and microsphere. <Pharmaceutics Textbook> (2017). Chemical Industrial Press, Beijing. (in Chinese)
10. **Ouyang, D**., Smith, S.C. Introduction to Computational Pharmaceutics. Computational Pharmaceutics - the application of molecular modeling in drug delivery. John Wiley & Sons Inc., 2015. p1-5;
11. Thakur, S.S., Parekh, H.S., Schwable, C.H., Gan, Y., **Ouyang, D**. Solubilization of Poorly Soluble Drugs: Cyclodextrin-Based Formulations. Computational Pharmaceutics - the application of molecular modeling in drug delivery. John Wiley & Sons Inc., 2015. P31-51;

12. Ke, P., Qi, S., Sadowski, G., **Ouyang, D**. Solid Dispersion - a Pragmatic Method to Improve the Bioavailability of Poorly Soluble Drugs. Computational Pharmaceutics - the application of molecular modeling in drug delivery. John Wiley & Sons Inc., 2015. P81-100;
13. Shah, Neha, **Ouyang, Defang**, Mutalik, Srinivas and Parekh, Harendra (2011). Dendrimers as carriers for the effective delivery of drugs and genes. In P.D. Gupta and N. Udupa (Ed.), Nanotechnology in health care (pp. 367-391) Jaipur, India: S.P. Publications.

Patents (12 patents with commercialization)

1. **D Ouyang**, W Wang, J Lin. Ionizable lipids and their screening methods and applications. PCT/CN2024/096356;
2. **D Ouyang**, Z Ye, N Wang. Method, device, equipment, and storage medium for predicting organic crystal structures. CN116130018A;
3. **D Ouyang**, T Lu, H Gao, H Gao, Z Ye, W Wang. Method for developing pharmaceutical composition and predicting and evaluating pharmaceutical composition. CN114913927A
4. **D. Ouyang**, T. Lu. A highly-soluble ginsenoside Rh2 formulation and its preparation method. CN 202311611678.9
5. **D. Ouyang**. A development and prediction evaluation method for pharmaceutical combination. CN202110172942.8
6. **D, Ouyang,** Q Zhao. Preparation and method of lutein-containing combination. CN201710355210.6；
7. **D. Ouyang**, Q. Zuo, C. Wang, H. Zhang, Y. Bao. Instant pirarubicin HCl freeze-drying powdery injection and its production. CN200610157023;
8. **D. Ouyang**, J. Zeng, N. Yu, Y. Bao. Stable injection docetaxel. CN200610032942;
9. J. Zeng, **D. Ouyang**, H. Zhang, Y. Bao. Method for removing organic solvent from viscous liquid. CN200610061698;
10. **D. Ouyang**, W. Pan. Combination of metformin/glipizide controlled-release tablet and its preparation method: CN200510045949;
11. W.Pan, W. Li, S. Nie, H. Guo, **D. Ouyang**, Z. Zhang, G. Du. Single-chamber, double-layered osmotic pump control-release system with holes on two sides. CN200510045951;
12. Pan W， Li W， **D. Ouyang**. Preparation and method of venlafaxine hydrochloride osmotic pump controlled release tablet. CN200510046231；

Selected peer-reviewed SCI papers (Over 120 SCI papers, 10 representative papers in yellow)

1. N Wang, J Dong, **D Ouyang***. AI-directed formulation strategy design initiates rational drug development. ***Journal of Controlled Release***, 2025, 378, 619-636;
2. S Deng, Y Wu, Z Ye, **D Ouyang***. In silico prediction of metabolic stability for ester-containing molecules: Machine learning and quantum mechanical methods. ***Chemometrics and Intelligent Laboratory Systems***, 2025, 257, 105292
3. S Wang, D Liu, **D Ouyang***. Quantitative analysis of excipients to the permeability of BCS class III drugs. ***International Journal of Pharmaceutics***, 2025, 668, 124958;
4. H Zhong, T Lu, R Wang, **D Ouyang***. Quantitative Analysis of Physical Stability Mechanisms of Amorphous Solid Dispersions by Molecular Dynamic Simulation. ***The AAPS Journal***, 2025, 27 (1), 1-13;
5. W Wang, K Chen, T Jiang, Y Wu, Z Wu, H Ying, H Yu, J Lu, J Lin, **D Ouyang***. Artificial intelligence-driven rational design of ionizable lipids for mRNA delivery. ***Nature Communications***, 2024, 15, 10804;
6. Z Wu, N Wang, Z Ye, H Xu, G Chan, **D Ouyang***. FormulationBCS: A Machine Learning Platform Based on Diverse Molecular Representations for Biopharmaceutical Classification System (BCS)

Class Prediction. Molecular Pharmaceutics, 2024, https://doi.org/10.1021/acs.molpharmaceut.4c00946;

7. Y Han, M Wang, Y Chen, **D Ouyang**, Y Zheng, Y Hu*. Profiling patent compounds in lipid nanoparticle formulations of siRNA. ***Molecular Therapy Nucleic Acids***, 2024, 35 (4);
8. W Wang, S Deng, J Lin, **D 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;
9. Ana M López-Estévez, Y Zhang, María Medel, Iker Arriaga, Lucía Sanjurjo, Cristian Huck-Iriart, Nicola GA Abrescia, María J Vicent, **Defang Ouyang**, Dolores Torres, María José Alonso*. Engineering hyaluronic acid-based nanoassemblies for monoclonal antibody delivery–design, characterization, and biological insights. ***Nano Research***, 2024, 17 (10), 9111-9125;
10. X Tan, Q Liu, Y Fang, Y Zhu, F Chen, W Zeng, **D Ouyang**, J Dong*. Predicting Peptide Permeability Across Diverse Barriers: A Systematic Investigation. ***Molecular Pharmaceutics***, 2024, 21 (8), 4116-4127
11. X Tan, Q Liu, Y Fang, S Yang, F Chen, J Wang, **D Ouyang**, J Dong, W Zeng*. Introducing enzymatic cleavage features and transfer learning realizes accurate peptide half-life prediction across species and organs, ***Briefings in Bioinformatics***, 2024, 25 (4), bbae350;
12. T Lu, T Wu, H Zhong, X Li, Y Zhang, H Yue, Y Dai, H Li, **D Ouyang***. Computer-driven formulation development of Ginsenoside Rh2 ternary solid dispersion. ***Drug Delivery and Translational Research***, 2024, 1-17
13. F Gao, Z Ma, X Luo, Y Wang, X Liu, M Tang, J Chen, L Tu, **D Ouyang**, J Zheng, C Li*. Self-Assembled Micelles Based on Ginsenoside Rg5 for the Targeted Treatment of PTX-Resistant Tumors. ***Molecular Pharmaceutics***, 2024, 21, 7, 3502–3512;
14. G Zhou, S Fu, Y Zhang, S Li, Z Guo, **D Ouyang**, T Ying, Y Lu, Q Zhao*. Antibody Recognition of Human Epidermal Growth Factor Receptor-2 (HER2) Juxtamembrane Domain Enhances Anti-Tumor Response of Chimeric Antigen Receptor (CAR)-T Cells. ***Antibodies***, 2024, 13 (2), 45;
15. F Chen, H Zhong, G Chan, **D Ouyang***. A Comprehensive Analysis of Biopharmaceutical Products Listed in the FDA's Purple Book. ***AAPS PharmSciTech***, 2024, 25 (5), 88;
16. Z Ye, Y Bao, Z Chen, H Ye, Z Feng, Y Li, Y Zeng, Z Pan, **D Ouyang**, K Zhang, X Liu, Y He*. Recent advances in the metal/organic hybrid nanomaterials for cancer theranostics. ***Coordination Chemistry Reviews***, 2024, 504, 215654;
17. Y Liu, B Wang, Y Zhang, J Guo, X Wu, **D Ouyang**, S Chen, Y Chen, S Wang, G Xing, Z Tang, S Qu*. Perylenedioic Acid‐Derived Carbon Dots with Near 100% Quantum Yield in Aqueous Solution for Lasing and Lighting. ***Advanced Functional Materials***, 2024, 2401353;
18. M Liu, R Zhang, H Huang, P Liu, X Zhao, H Wu, Y He, R Xu, X Qin, Z Cheng, H Liu, O Ergonul, F Can, **D Ouyang**, Z Wang, Z Pang, F Liu*. Erythrocyte‐Leveraged Oncolytic Virotherapy (ELeOVt): Oncolytic Virus Assembly on Erythrocyte Surface to Combat Pulmonary Metastasis and Alleviate Side Effects. ***Advanced Science***, 2024, 11 (5), 2303907;
19. X Lou, J Wang, X Jin, X Wang, B Qin, D Liu, X Shi, **D Ouyang**, Z He, J Sun, H Li, M Sun*. An oral bacterial pyroptosis amplifier against malignant colon cancer. ***Nano Today***, 2024, 54, 102091;
20. Y Wu, X Ding, Y Wang, **D Ouyang***. Harnessing the power of machine learning into tissue engineering: current progress and future prospects. ***Burns & Trauma***, 2024, 12, tkae053;
21. H Ling, Q Zhang, Q Luo, **D Ouyang**, Z He, J Sun, M Sun*. Dynamic immuno-nanomedicines in oncology. ***Journal of Controlled Release***, 2024, 365, 668-687;
22. S Zheng, G Li, S Fu, N Wang, H Qiao, M Li, X Zhang, K Wang, W Sun, C Tian, Z He, **D Ouyang**, B Sun, J Sun*. Hybrid nanoassembly indicating a synthetic lethality relationship induces mitotic catastrophe-mediated tumor elimination. ***Chemical Engineering Journal***, 2024, 479, 147802;

23. Zhuyifan, Ye, Nannan Wang, **Defang Ouyang***. Crystal structure prediction for organic compounds by machine learning algorithm, ***The Innovation***, 2024, 5(2), 100562;
24. Jie Dong, Zheng Wu, Huanle Xu, and **Defang Ouyang***. FormulationAI: a novel web-based platform for drug formulation design driven by artificial intelligence. ***Briefings in Bioinformatics***, 2024, 25(1): bbad419;
25. Xinyang Liu, Wei Wang, Jingsi Chen, Dunjin Chen, Yong Tao, Defang Ouyang*. PBPK/PD Modeling of Nifedipine for Precision Medicine in Pregnant Women: Enhancing Clinical Decision-Making for Optimal Drug Therapy, ***Pharmaceutical Research***, 2024, 41, 63-75;
26. Junhuang Jiang, Anqi Lu, Xiangyu Ma, **Defang Ouyang**, Robert O Williams III. The applications of machine learning to predict the forming of chemically stable amorphous solid dispersions prepared by hot-melt extrusion, ***International Journal of Pharmaceutics: X***, 2023, 5, 100164;
27. Ying Tian, Yiquan Zhang, Jiawei Zhao, Fuxiao Luan, Yingjie Wang, Fan Lai, **Defang Ouyang**, Yong Tao. Combining MSC Exosomes and Cerium Oxide Nanocrystals for Enhanced Dry Eye Syndrome Therapy, ***Pharmaceutics***, 2023, 15 (9), 2301;
28. Junhuang Jiang, **Defang Ouyang**, Robert O Williams III. Predicting Glass-Forming Ability of Pharmaceutical Compounds by Using Machine Learning Technologies, ***AAPS PharmSciTech***, 2023, 24 (5), 103;
29. Qinghan Tang, Fei Xu, Xuchao Wei, Jingyue Gu, Pengli Qiao, Xuemin Zhu, Shaoping Yin, **Defang Ouyang**, Jie Dong, Junhong Yao, Yiwei Wang, Jun Chen. Investigation of β-caryophyllene as terpene penetration enhancer: Role of stratum corneum retention, ***European Journal of Pharmaceutical Sciences***, 2023, 183, 106401;
30. Yudi Song, Wei Wang, Xinyang Liu, Jingsi Chen, Dunjin Chen, Xiaoyi Wang, Wei Li, **Defang Ouyang***. Physiologically based pharmacokinetic modeling for multiple oral administration labetalol in pregnant women, ***Pharmaceutical Research***, 2023, 40, 1765–1775;
31. Nannan Wang, Hongyu Chen, Yunsen Zhang, Wei Wang, Zhuyifan Ye, **Defang Ouyang***. How can machine learning and multiscale modeling help ocular drug delivery? ***Advanced Drug Delivery Review***, 2023, 114772;
32. 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;
33. Wenwen Zheng, Junjun Li,Yu Wang, Zhuyifan Ye, Hao Zhong, Hung Wan Kot, **Defang Ouyang*** , Ging Chan*. Quantitative analysis for Chinese and US-listed pharmaceutical companies by the LightGBM algorithm. ***Current Computer-Aided Drug Design***, 2023, 19 (6), 405-415;
34. Jiayin Deng, Zhuyifan Ye, Wenwen Zheng, Jian Chen, Haoshi Gao, Zheng Wu, Ging Chan, Yongjun Wang, Dongsheng Cao, Yanqing Wang, Simon Ming-Yuen Lee, **Defang Ouyang***. Machine learning in accelerating microsphere formulation development. ***Drug Delivery and Translational Research***, 2023, 13, 966-982;
35. Yifan Cai, Xin Ji, Yunsen Zhang, Chang Liu, Zichen Zhang, Yongjiu Lv, Xiaochun Dong, Haisheng He, Jianping Qi, Yi Lu, **Defang Ouyang***, Weili Zhao*, Wei Wu*. Near-infrared fluorophores with absolute aggregation-caused quenching and negligible fluorescence re-illumination for in vivo bioimaging of nanocarriers, ***Aggregate***, 2023, 4 (2), e277;
36. Jianzhong Zhu, Cheng Chen, Jie Dong, Shasha Cheng, Guodong Li, Chunming Wang, **Defang Ouyang**, Chung-Hang Leung, Ligen Lin. Artificial intelligence-aided discovery of prolyl hydroxylase 2 inhibitors to stabilize hypoxia inducible factor-1α and promote angiogenesis, ***Chinese Chemical Letters***, 2023, 34 (2), 107514;
37. Sena Karaosmanoglu, Yunsen Zhang, Wenli Zhou, **Defang Ouyang***, Michael Chen*. Synthesis of Carrier-Free Paclitaxel–Curcumin Nanoparticles: The Role of Curcuminoids. ***Bioengineering***, 2022, 9 (12), 815;

38. Meiqi He, Wenwen Zheng, Nannan Wang, Hanlu Gao, **Defang Ouyang*,** Zunnan Huang*. Molecular dynamics simulation of drug solubilization behavior in surfactant/co-solvent injections. ***Pharmaceutics***, 2022, 14, 2366;
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Pharmacy education paper (4)

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Invited lectures and talks (over 100)

1. AI-driven drug delivery – revolution and challenge. Innovation Webinar (21 December 2024, online)
2. AI for drug delivery. School of Biomedical and Pharmaceutical Sciences, Guangdong University of Technology (20 December 2024, Guangzhou, China)
3. Computational pharmaceutics – a new paradigm of drug delivery. 7th Symposium on Biophysics Postgraduate Research in Hong Kong (17 December, 2024, HongKong, China)
4. Computational pharmaceutics – yesterday, today and tomorrow. 1st Symposium on Computational Pharmaceutics – AI and Modeling in Pharma 4.0 (14-15 December 2024, Macau, China)
5. AI for DMPK and drug delivery. 14th Drug Metabolism Committee Annual Meeting of Chinese Pharmacology Association (6-8 December 2024, Shanghai, China)
6. AI for drug delivery. Nanjing University of Chinese Medicine (26 November, 2024, Nanjing, China)
7. Opportunity and Challenge of AI in drug delivery. University of Science and Technology of China (10 November 2024, Hefei, China)
8. Opportunities and Challenges of Artificial Intelligence in Pharmaceutical Formulation and Excipients. 2024 Pharmaceutical Excipient Committee Annual Meeting of Chinese Pharmaceutical Association (8-10 November 2024, Hefei, China)
9. AI for drug delivery. 2024 Industrial Pharmaceutics Committee Annual Meeting of Chinese Pharmaceutical Association (26-28 October, 2024, Lianyungang, China)
10. Computational pharmaceutics – a new paradigm of drug delivery. 17th Pharmaceutical Preparation Conference (27-29 September, 2024, Hangzhou, China)
11. AI-driven rational design of lipid nanoparticles for mRNA delivery. 10th Symposium in Quantitative Pharmacology 2024 (26-28 September, 2024, Fuzhou, China)
12. AI for drug delivery. 2024 China Pharmceutical Industry Information Annual Meeting (6-8 September, 2024, Chengdu, China)
13. AI-driven rational design of lipid nanoparticles for mRNA delivery. Translation and Early Clinical Research Discussion of Complex Injections (26-28 Auguest, 2024, Dali, China)
14. Opportunities and Challenges of Artificial Intelligence in Pharmaceutical Formulation. Science Day 2024 of Global Development of Boehringer Ingelheim (20 June, 2024, Shanghai, China)
15. Opportunity and challenge of quantitative pharmacology and AI in advanced formulations R&D. Xiangjiang Pharmaceutical Symposium (14-16 June, 2024, Changsha, China)
16. Opportunity and Challenge of AI in drug delivery. School of Biological Sciences, University of California Irvine (14 May, 2024, Irvine, USA)
17. Opportunity and Challenge of AI in drug delivery. Department of Pharmaceutics, University of Florida (21 May 2024, Gainesville, USA)
18. Opportunity and Challenge of AI in drug delivery. Computational Medicine Program Seminar, University of North Carolina at Chapel Hill (7 May 2024, NC, USA)
19. Opportunity and Challenge of AI in drug delivery. Industrial & Molecular Pharmaceutics Seminar, Department of Industrial & Molecular Pharmaceutics, Purdue University (25 April 2024, USA)
20. Opportunity and Challenge of AI in drug delivery. College of Pharmacy, University of Kentucky (16 April 2024, Lexington, USA)

21. Opportunity and Challenge of AI in drug delivery. 8th Pharmaceutical Frontier Forum of Acta Pharmaceutica Sinica (29 March – 1st April 2024, Chongqing, China)
22. Opportunity and challenge of AI in biopharmaceutical formulations. 9th Biopharmaceutical Stability Conference (21-23 March, 2024, Shanghai, China)
23. Opportunity and Challenge of AI in drug delivery. 5th Annual Meeting of Chinese American Society of Nanomedicine and Nanobiotechnology (December 8-10, 2023, Guangzhou, China)
24. Opportunity and Challenge of AI in drug delivery. Frointer Symposium of NSFC-FDCT (6-7, December, 2023, Harbin, China)
25. Computational pharmaceutics. School of Pharmacy, Harbin Medical University (5 December, 2023, Harbin, China)
26. Opportunity and Challenge of AI in drug delivery. International Conference on Theoretical and High Performance Computational Chemistry 2023 (24-26 November, 2023, Haikou, China)
27. Opportunity and Challenge of AI in drug delivery. 5th International Conference on Nanomedicine of China (November 4–7, 2023, Guangzhou, China)
28. Opportunity and Challenge of AI in drug delivery. Macau Symposium on Artificial Intelligence and Health (30-31 October, 2023, Macau)
29. An artificial intelligence decision system for solubilization strategies of small molecule drug candidates: lessons from approved drugs by partially supervised learning. 81st FIP World Congress of Pharmacy and Pharmaceutical Sciences (24 - 28 September, 2023, Brisbane, Australia)
30. Opportunity and Challenge of AI in drug delivery. Keynote speaker, "Data-driven techniques and tools in formulation studies" Nordic POP network workshop (24th – 25th August, 2023, Helsinki, Finland)
31. Opportunity and Challenge of AI in drug delivery. 9th UK-China International Particle Technology Forum (21st- 24th August, 2023, University of Greenwich, London, UK)
32. Opportunity and Challenge of AI in drug delivery. School of Engineering, The University of Edinburgh (16 August, 2023, Edinburgh, UK)
33. Opportunity and Challenge of AI in biologics formulations. 2023 Biopharmaceutical Bioprocess Development Summit (3-5 August, 2023, Shanghai, China)
34. Opportunity and Challenge of AI in drug delivery. Tongxieyi Conference (29 July, 2023, Shenzhen, China)
35. Development and valication of the AI solubilization platform for water-insoluble drugs. 17th National Conference on Computer Chemistry of China (21-24 July, 2023, Xining, China)
36. Opportunity and Challenge of AI in drug delivery. 6th Asian Symposium on Pharmaceutical Science and Technology (3-4 June, 2023, Zhengzhou, China)
37. Development and valication of the AI solubilization platform for water-insoluble drugs. 9th National Conference on Computational Biology and Bioinformatics (12-15 May, 2023, Xuzhou, China)
38. Opportunity and Challenge of AI in drug delivery. 15th China Pharmaceutical Strategy Conference 2023 (18-20 March, 2023, Shijiazhuang, China)
39. Artificial intelligence in drug delivery. Artificial Intelligence (AI) and Machine Learning Webinar of Academy of Pharmaceutical Sciences (APS) UK (15 Feburary 2023, online)
40. Predicting lipid nanoparticle for mRNA vaccine by machine learning algorithm. 15th China Pharmaceutical Conference 2022 (23 December, 2022, Shanghai, China)

41. Computational pharmaceutics – a new paradigm of drug delivery. University of Helsinki, Finland (10 November, 2022, Helsinki, Finland)
42. Computational pharmaceutics – a new paradigm of drug delivery. Drug Research Academy, University of Copenhagen, Denmark (9 November, 2022, Copenhagen, Denmark)
43. Predicting lipid nanoparticle of mRNA vaccine by machine learning algorithm. 2nd Innovation Symposium of mRNA therapeutics in 2022. (26-27 September, 2022, Shanghai, China)
44. Opportunity and challenge of artificial intelligence (AI) in drug delivery. XXVII EFMC International Symposium on Medicinal Chemistry (online, 4-8 September, 2022, Nice, France)
45. Artificial intelligence in pharmaceutical excipients and formulation development. 2022 Gushu Dialogue (24-26 August, 2022, Soochow, China)
46. Predicting lipid nanoparticle of mRNA vaccine by machine learning algorithm. 5th Symposium of Pharmaceutics and Particle Design (9-10 July, 2022, Changsha, China)
47. Opportunity and challenge of artificial intelligence (AI) in drug delivery. 4th Cloud Symposium of Asian Journal Pharmaceutical Sciences (7th July, 2022, online)
48. Computational pharmaceutics – from AI to PBPK modeling. Young Symposium of South China Quantitative Pharmacology (5th July, 2022, online)
49. AI-driven lipid nanoparticle (LNP) design for mRNA therapeutics. 2022 Symposium of mRNA delivery systems and manufacture. (2nd July, 2022, online)
50. AI-driven lipid nanoparticle (LNP) design for mRNA therapeutics. 3rd Cell Therapy and Regenerative Medicine Conference (20-21 April, 2022, Shenzhen, China)
51. Computational pharmaceutics. Centre for Pharmaceutical Oncology (CPO) seminars. Leslie Dan Faculty of Pharmacy, University of Toronto (16 March, 2022, online)
52. Invited lectures, Wuhan Technology University (12/26 March, 2022, online)
53. Opportunity and challenge of artificial intelligence (AI) in drug delivery. 2022 ExciPerience (9-11 March, 2022, online)
54. Computational pharmacy – From molecular simulation, PBPK simulation to artificial intelligence. 8th International Symposium in Quantitative Pharmacology (5-6 December, 2021, Beijing, China)
55. Application of computational tools in clinical medication for pregnant women. Invited lecture from Guangzhou Medical University Third Hospital (27 January, 2022, Guangzhou, China)
56. Computational pharmaceutics – a new paradigm of drug delivery. International Frontier Symposium of Pharmaceutical Engineering. (13 January, 2022, online)
57. Invited lectures, Central South University (November 2021, online)
58. AI-leading the database development for pharmaceutical excipient and formulation. Chinese Drug Regulatory Conference (13-15 October, 2021, Beijing, China)
59. Artificial Intelligence in Pharmaceutics. FY 2021 Generic Drug Science and Research Initiatives Public Workshop, US-FDA (June 23, 2021, online);
60. Artificial intelligence of pharmaceutics. 10th International Conference on Molecular Simulations and Artificial Intelligence Application (29-30 May, 2021, Soochow, China)
61. Artificial intelligence of pharmaceutics. 13rd National Microanalysis Conference of China Chemical Society (23-25 April, 2021, Southern University of Science and Technology, Shenzhen, China)
62. Computational pharmaceutics – from molecular modeling to artificial intelligence. Series Academic Forum of China Pharmaceutical Society and Chinese Clinical Pharmacology Journal. (24 April, 2021, online)

63. Prediction of solid dispersion formulations by the integrated computational methodology. 32nd Annual Meeting of Chinese Chemical Society (19-22 April, 2021, Zhuhai, China)
64. Artificial intelligence of pharmaceutics. Hainan Free Trade Port 1st International Pharmaceutical Innovation Symposium and Investment Trade Conference (16-18 April, 2021, Haikou, China)
65. Computational pharmaceutics – a new paradigm of drug delivery. The first Greater Bay Area Biophysics and New Drug Discovery Forum (10-12 April, Zhuhai, China)
66. Rational design of mRNA lipid delivery systems by machine learning approach. mRNA Pharmaceutical Technique Innovation Symposium. (11 March, 2021, Shanghai Zhangjiang, China)
67. Computational pharmaceutics – a new paradigm of drug delivery. Asian Pharmaceutics Online Symposium, 1st Conference Computational pharmaceutics (online, 12 December, 2020)
68. In silico prediction of solid dispersion formulations by the integrated computational tools. 2020 Annual Meeting of Quantitative Pharmacology of China Pharmacological Society (27-28 November, 2020, Zhengzhou, China)
69. The opportunity and challenge of artificial intelligence in pharmaceutics. 7th China Pharmaceutical Festival (11-12 November, 2020, Nanjing, China)
70. The opportunity and challenge of artificial intelligence in pharmaceutics. Changchun University of Chinese Medicine (2 November, 2020, Changchun, China)
71. In silico prediction of solid dispersion formulations by the integrated computational tools. 11st Annual Meeting of Chinese Particle Society (24-25 October, 2020, Xiamen, China)
72. Artificial intelligence in pharmaceutics. 8th Symposium of Medical Artificial Intelligence (online meeting, August 30, 2020)
73. Past, present and future of pharmaceutics. 7th Medical and Humanity Summer Camp (online meeting, August 22, 2020)
74. Integrated computer-aided formulation design: A case study of andrographolide/ cyclodextrin ternary formulation. The 3rd Worldwide Chinese Computational Biology Conference (Online meeting, August 3-6, 2020)
75. Computational pharmaceutics – from molecular modeling to artificial intelligence. Anhui Medical University (19 January, 2020, Hefei, China)
76. Computational prediction of physical stability of solid dispersions. 15th National Computational Chemistry Conference (15-17 November 2019, Shanghai, China)
77. Prediction of physical stability of solid dispersions by machine learning. 4th National Biological Particle Conference. (9-10 November 2019, Shenzhen, China)
78. Artificial intelligence in pharmaceutics. 9th China Pharmaceutical and Biotechnological Symposium. (25-27 October 2019, Shenzhen, China)
79. Computational pharmaceutics – from molecular modeling to artificial intelligence. Guangdong Pharmaceutical University (26 September 2019, Guangzhou, China)
80. Artificial intelligence in pharmaceutics. Southern University of Science and Technology (16 September 2019, Shenzhen, China)
81. Big data analysis of Chinese pharmaceutical industry and artificial intelligence in pharmaceutics. 2019 Guangdong-HK-Macau Intellectual Property Symposium (30 June, 2019, Zhuhai, China)
82. Artificial intelligence and deep learning in pharmaceutics. Chinese Pharmaceutical Quality Conference (4-5 June, 2019, Chendu, China)

83. Big data analysis of Chinese pharmaceutical industry. National Platelet Day (25 April, 2019, Shenzhen, China)
84. Artificial intelligence, big data and future education. China Education Society (9 April 2019, Macau, China)
85. Neutron scattering in pharmaceutics. Symposium of small angle neutron scattering users (7-8 April 2019, Dongguan, China)
86. Big data analysis of Chinese pharmaceutical industry from 2000 – 2018. CKPC college Inspiring seminar. (3 April 2019, Macau, China)
87. Big data analysis of global progress in pharmaceutics and future perspective. 2019 Zhanjiang-HK-Macau Medical Symposium (5 January 2019, Zhanjiang, China)
88. Transfer learning for the prediction of pharmacokinetic properties. 2018 Chinese Quantitative Pharmacology Conference (17-18 November 2018, Changsha, China)
89. Computational pharmaceutics. 2018 Postgraduate Lectures in Pharmaceutics at Shenyang Pharmaceutical University (3 November, 2018, Shenyang, China)
90. Artificial intelligence in Inhalation formulations. 2018 National Inhalation Drug Delivery Association Conference (19-21 October, 2018, Nanjing, China)
91. Artificial intelligence for pharmaceutical formulations. 2018 Chinese Pharmaceutical Innovation and Investment Conference (18-20 September, 2018, Soochow, China)
92. Artificial intelligence and big data in pharmaceutical formulations and excipients. 3rd China Drug Administration Conference 2018. (6-7 September, 2018, Beijing, China)
93. Computational pharmaceutics - from molecular modeling to artificial intelligence and big data. International Graduate Students Conference on Pharmaceutical Science 2018. (29 - 30 August, 2018, Surabaya, Indonesia)
94. Computational pharmaceutics - from molecular modeling to artificial intelligence and big data. 17th Meeting of the Consortium for Globalization of Chinese Medicine. (8-10 August, Sarawak, Malaysia)
95. Big data analysis of the literature and patent of solid dispersions. 2018 Macau International Symposium of Intellectual Property.（6 August 2018, Macau, China）
96. Computational pharmaceutics. 2018 Joint Annual Conference of Physical Societies in Guangdong-Hong Kong-Macau Greater Bay Area. University of Macau （26-29 July 2018, Macau, China）
97. Computational Pharmaceutics – from molecular modeling to artificial intelligence and big data. School of Biomedical Sciences and Pharmacy, The University of Newcastle (20 July 2018, Newcastle, Australia)
98. Computational Pharmaceutics – from molecular modeling to artificial intelligence and big data. School of Chemical Engineering, The University of Adelaide (19 July 2018, Adelaide, Australia)
99. Computational Pharmaceutics – from molecular modeling to artificial intelligence and big data. School of Pharmacy, The University of Queensland (16 July 2018, Brisbane, Australia);
100. Computational Pharmaceutics. The 2nd Worldwide Chinese Computational Biology and Molecular Simulation Conference, Sun Yat-sen University (7-10 June 2018, Guangzhou, China)
101. Computational Pharmaceutics. School of Pharmacy, Zhejiang University (30 March, 2018 Hangzhou, China)
102. Computational Pharmaceutics – from molecular modeling to artificial intelligence and big data. The 7th Innovative Drug Delivery Solutions (28-30 March, 2018, Hangzhou, China)

103. Computational Pharmaceutics – from molecular modeling to artificial intelligence and big data. International Forum on Intelligent Supercomputing and Biopharmaceutical Innovation 2017 (17 December, 2017, Jiangmen, China)
104. Computational Pharmaceutics – from molecular modeling to artificial intelligence and big data. 2017 GD-HK-Macau Artificial Intelligence Heart & Brain Medical Imaging Symposium (16 December, 2017, Nansha, Guangzhou, China)
105. Computational Pharmaceutics – from molecular modeling to artificial intelligence and big data. School of Pharmacy, China Pharmaceutical University (21 November 2017, Nanjing, China)
106. Computational Pharmaceutics – from molecular modeling to artificial intelligence and big data. 14th National Computer Chemistry Conference (17-20 November, 2017, Nanjing, China)
107. Computational Pharmaceutics – from molecular modeling to artificial intelligence and big data. 2017 China Pharmaceutical Conference (28-30 October, 2017, Shanghai, China)
108. Big data analysis of global advances in pharmaceutics and drug delivery 1980 – 2014. Yaodu college online live course. (17 October, 2018)
109. Computational Pharmaceutics – from molecular modeling to artificial intelligence and big data. 7th Information Committee Annual Meeting of World Federation of Chinese Medicine Societies (13-16 October, 2017, Jiaxing, China)
110. Computational Pharmaceutics – from molecular modeling to artificial intelligence and big data. School of Pharmacy, East China University of Science and Technology (18 September, 2017, Shanghai, China)
111. Computational Pharmaceutics – from molecular modeling to artificial intelligence and big data. Packaging Material and Pharmaceutical Excipient Department, National Institutes for Food and Drug Control (4 July, 2017, Beijing, China)
112. Computational Pharmaceutics – the development of aging medicine. 1st Beijing-Hongkong-Macau-Taiwan Aging Summer School, Peking University (29 June, 2017, Beijing, China)
113. Computational pharmaceutics – application of molecular modeling in formulation development. School of Pharmacy, Zhengzhou University (27 June, 2017, Zhengzhou, China)
114. Computational pharmaceutics – application of computer in clinical pharmacy. Henan Young Pharmacist Symposium 2017 (24 June, 2017, Zhengzhou, China)
115. Big Data Analysis of Global Progress in Pharmaceutics and Drug Delivery from 1980-2014. Symposium on Industrial and Physical Pharmacy 2017 (24-25 April, 2017, Shenyang, China)
116. Computational Pharmaceutics – a new paradigm of drug delivery. Chengdu Medical College (11 April, 2017, Chengdu, China)
117. Computational Pharmaceutics – a new paradigm of drug delivery. West China School of Pharmacy, Sichuan University (11 April, 2017 Chengdu, China)
118. Computational Pharmaceutics – In silico formulation design for better medicine. School of Pharmacy, Southwest University (10 April 2017, Chongqing, China)
119. Past, today and future of pharmaceutics. CKPC college lunch-sharing seminar. (29 March 2017, Macau, China)
120. Computational pharmaceutics. Listening to the Voice from the Western: Opinions on Data Integrity, CSV and Governance Affairs. (24 March 2017, Hong Kong, China)

121. Computational pharmaceutics – A New paradigm of formulation development. Mini-Symposium on Computational Pharmaceutics, The 10th International Conference on Computational Physics (ICCP10). (16-20 January 2017, Macau, China)
122. Computational Pharmaceutics – a new paradigm of drug delivery. UM HPC Sharing Seminar (25 November 2016, Macau, China)
123. Computational Pharmaceutics – application of molecular modeling to drug delivery. 4th International Conference on Molecular Simulation (ICMS 2016) (24-26 Oct 2016, Shanghai, China)
124. Big Data Analysis of Global Progress in Pharmaceutics and Drug Delivery. 2016 Scientific Data Conference (25-26 August 2016, Shanghai, China)
125. Big Data Analysis of Global Literature and Patents in Pharmaceutics and Drug Delivery Area. The 8th Hongkong Intellectual Property (IP) Seminar (4-5 August 2016, Hongkong, China)
126. Computational pharmaceutics - In silico formulation design for better medicine. 4th Asian Symposium on Pharmaceutical Science and Technology (28-29 April 2016, Shenyang, China)
127. Computational pharmaceutics - In silico formulation design for better medicine. The 13th National Symposium of Computer & Computational Chemistry. (20 – 21 November 2015, Guangzhou, China)
128. Progress of Information and Tracing System of Chinese Medicine. 5th Information Committee Meeting – Big Data and Information Internationalization of Chinese Medicine, World Federation of Chinese Medicine Societies. (19 – 20 November 2015, Shenzhen, China)
129. Computational pharmaceutics - Yielding Insights into Mechanism and Function in Drug Delivery. School of Bioscience and Bioengineering, South China University of Technology. (5 November 2015, Guangzhou, China)
130. Two-decades progress in pharmaceutics and drug delivery: a global view of big data. 7th Asian Association of Schools of Pharmacy (AASP) Conference. (30 October - 1 November, Taipei, Taiwan, China)
131. Computational pharmaceutics – In silico formulation design for better medicine. 7th Asian Association of Schools of Pharmacy (AASP) Conference. (30 October - 1 November, Taipei, Taiwan, China)
132. Computational pharmaceutics – In silico formulation design for better medicine. School of Pharmacy, Guangzhou Medical University (11 June 2015, Guangzhou, China)
133. Computational pharmaceutics – In silico formulation design for better medicine. School of Pharmacy, Sun Yat-sen University (28 April 2015, Guangzhou, China)
134. Computational pharmaceutics. Faculty of Science and Technology, University of Macau (4th February 2015, Macau)
135. Computational pharmaceutics – application of molecular dynamics simulation in drug delivery. Controlled Release Society Annual Meeting 2014 (12th - 16th July, Chicago, USA)
136. How to help first-year pharmacy student to gain the big picture. 2014 Manchester Pharmacy Education Conference (30th June, Manchester, UK)
137. Professional development for first-year pharmacy students. CERA-UK Conference 2014 (12th -13th June 2014, London, UK)
138. Computational pharmaceutics – *In silico* formulation design for better medicines. LHS research day, Aston University (Birmingham, UK, 28th May 2014)

139. Computational pharmaceutics – *In silico* formulation design for better medicines. Leicester Pharmacy School, De Montfort University (Leicester, UK, 20th May 2014)
140. Computational pharmaceutics – application of computer modeling in drug delivery. Making Pharmaceutics Conference & Exhibition (Birmingham, UK, 29th April, 2014)
141. Oral fast dissolving films for paediatric formulations. Science Capital Business Plan Session: Innovative Healthcare 2013 Meeting. (Birmingham, UK, 25th September, 2013)
142. Computational pharmaceutics - virtual screening in formulation development. NanoFormulation 2013. (Manchester, UK, 18-21 June, 2013)
143. Computational pharmaceutics. Formulated Products-Meeting the Product and Process Design Challenge' Competition Briefing Event. (London, UK, 1st May, 2013)
144. Computational pharmaceutics. Nutrition for Life Birmingham Workshop. (Birmingham, UK, 10th April, 2013)
145. Computational pharmaceutics. School of Chemical Engineering, University of Birmingham, UK. (Birmingham, UK, 13th December, 3012)
146. Computational pharmaceutics - the application of molecular modeling in drug delivery. 5th Midlands Biophysics Network Symposium. (Birmingham, UK, 18th April 2012).
147. Computational pharmaceutics. Aston Research Centre for Healthy Ageing (ARCHA) seminar, Aston University (Birmingham, UK, December 7th, 2011).
148. The Effect of pH on PAMAM Dendrimer-siRNA Complexation – Endosomal Considerations as Determined by Molecular Dynamics Simulation. 7th Annual Conference of the ARC Centre of Excellence for Functional Nanomaterials (ARCCFN). (Gold Coast, Queensland, Australia, November 25-26, 2010).
149. Structure, Dynamics and Energetics of siRNA-polymer Complexation: A Molecular Dynamics Study. 6th Annual Conference of the ARC Centre of Excellence for Functional Nanomaterials (ARCCFN). (Coffs Harbor, New South Wales, Australia, November 9-11, 2009).
150. Structure, Dynamics and Energetics of siRNA-Cationic Vector Complexation by Molecular Dynamics Simulations. RACI Student Symposium. (Brisbane, Australia, October 2, 2009).