Prof. Defang OUYANG

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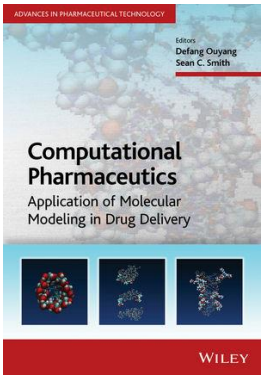

Brief Summary

Prof. Ouyang is a recognized leader in computational pharmaceutics field and the founding chair of the Computational Pharmacy Society (CPhS). He has published 2 books, 6 book chapters, over 100 peer-reviewed papers (e.g. *Acta Pharmaceutica Sinica B, Journal of Controlled Release, Biomaterials* et al.), and over 100 invited presentations (e.g. **US-FDA**). He had been granted 11 patents, which had been used in marketed pharmaceutical products. He edited **the first book <Computational Pharmaceutics>** (John Wiley & Sons Inc., 2015, as shown above) in this research area. He serves as the associate editor/editorial board of multiple SCI journals, such as <*Drug Delivery and Translational Research*>, <*Asian Journal of Pharmaceutical Sciences*>, <*Pharmaceutical Research*>, and <*Journal of Pharmaceutical Sciences* >. He successfully attracted 11 research grants (over 20 million MOP in total) in the past 6 years. He established **the first global artificial intelligence (AI)-based formulation platform** (https://formulationai.computpharm.org/), which attracts widely global users (e.g. **Boehringer Ingelheim**, Triastek and other companies). He successfully supervised over 30 PhD and master students. He built wide networks with industry, business, government agencies and professional bodies in the world.

Research interests

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":**

- **Artificial intelligence (AI)** for pharmaceutics: to develop novel 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/gene delivery: to integrate 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 **(14 research grants in recent 8 years with over 20 million MOP in total)**

- "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 Research Grant (MYRG-GRG2023-00077-ICMS-UMDF), 320,000 MOP, Macau (PI);
- "Investigation of the release mechanism of long-sustained release microspheres", 2023 Research Grant (MYRG-CRG2022-00008-ICMS), 1,520,000 MOP, Macau (PI);
- "PBPK modeling of oral peptide formulation", 2023, Industry 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, Shenzhen-Hongkong-Macau collaboration project, 1000,000 CNY, Shenzhen (PI);

- “Application of artificial intelligence in triptorelin long-sustained release microsphere”, 2022, Zhuhai Industrial-Academic collaboration project (ZH22017002210010PWC), 800,000 CNY, Zhuhai, (co-PI);
- “Preparation and evaluation of a highly-soluble Ginsenoside Rh2 formulation”, 2021, FDCT Research Grant (0108/2021/A), 721,000 MOP, Macau (PI);
- “Prediction of ternary cyclodextrin formulations by machine learning approaches”, 2020 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 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 Research Grant (MYRG2019-00041-ICMS), 750,000 MOP, Macau (PI);
- “Preparation and evaluation of highly-soluble andrographolide formulations”, 2018 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 Research Grant (MYRG2016-00038-ICMSQRCM), 1,474,000 MOP, Macau (PI)
- "Computational Prediction of Physical Stability of Solid Dispersions", 2016 Research Grant (MYRG2016-00040-ICMSQRCM), 662,500 MOP, Macau (PI);
- “Preparation and evaluation of a highly-soluble lutein formulation”, 2015 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 Royal Society Research Grants (RG120633), £14,950, Royal Society, UK (PI);

Publications

(Over 30 JCR Q1 papers with the corresponding author in recent 3 years, 10 representative papers in yellow)

Books (3)

1. **D. Ouyang**. ***Exploring Computational Pharmaceutics - AI and Modeling in Pharma 4.0*.** John Wiley & Sons Inc. & Chemical Industrial Press, 2024. (in press)
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 (6)

4. 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)

5. Feng Qian， **D. Ouyang.** Chapter 12: solid dispersions, cyclodextrin, microencapsule and microsphere. <Pharmaceutics Textbook> (2017). Chemical Industrial Press, Beijing. (in Chinese)
6. **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;
7. 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;
8. 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;
9. 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.

Selected peer-reviewed SCI papers

1. Zhuyifan, Ye, Nannan Wang, **Defang Ouyang***. Crystal structure prediction for organic compounds by machine learning algorithm, ***The Innovation***, 2024, (accepted);
2. 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;
3. 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***, 2023, https://doi.org/10.1007/s11095-023-03638-2;
4. Shunzhe Zheng, Guanting Li, Shuwen Fu, Nannan Wang, Han Qiao, Meng Li, Xuanbo Zhang, Kaiyuan Wang, Wei Sun, Chutong Tian, Zhonggui He, **Defang Ouyang***, Bingjun Sun*, Jin Sun*. Hybrid nanoassembly indicating a synthetic lethality relationship induces mitotic catastrophe-mediated tumor elimination, ***Chemical Engineering Journal***, 2023, 147802;
5. 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;
6. 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;
7. 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;
8. 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;
9. 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;
10. 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;

11. 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;
12. 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;
13. 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;
14. 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;
15. 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;
16. 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;
17. 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;
18. Wenwen Zheng, Yiyang, Wu, Hanlu Gao, **Defang Ouyang***. Traditional Chinese medicine injections: where we are after 80-year development. ***Chinese Medicine***, 2022, 17, 127;
19. Shuang Zhou, Jinbo Li, Jiang Yu, Yuequan Wang, Zhaomeng Wang, Zhonggui He, **Defang Ouyang**, Hongzhuo Liu*, Yongjun Wang*. Tumor microenvironment adrenergic nerves blockade liposomes for cancer therapy, ***Journal of Controlled Release***, 2022, 351, 656-666;
20. Songtao Dong, Yuan Zhang, Xiangnan Guo, Chuang Zhang, Zhaomeng Wang, Jiang Yu, Yubo Liu, Chang Li, Yuting Hu, Bingjun Sun, Mengchi Sun, Haotian Zhang, **Defang Ouyang**, Zhonggui He, Yongjun Wang*. Glutathione Pulse Therapy: Promote Spatiotemporal Delivery of Reduction‐Sensitive Nanoparticles at the "Cellular Level" and Synergize PD‐1 Blockade Therapy. ***Advanced Science***, 2022, 2202744;
21. Jinbo Li, Wenxu Cai, Jiang Yu, Shuang Zhou, Xianlu Li, Zhonggui He, **Defang Ouyang**, Hongzhuo Liu*, Yongjun Wang*. Autophagy inhibition recovers deficient ICD-based cancer immunotherapy. ***Biomaterials***, 2022, 287, 121651;
22. Junhuang Jiang, Han-Hsuan Peng, Zhenpei Yang, Xiangyu Ma, Sawittree Sahakijpijarn, Chaeho Moon, **Defang Ouyang**, Robert O. Williams III*. The Applications of Machine Learning (ML) in Designing Dry Powder for Inhalation by Using Thin-film-freezing Technology. ***International Journal of Pharmaceutics***, 2022, 626, 122179;
23. Jiawei Wang; Niloofar Heshmati Aghda; Junhuang Jiang; Ayishah Mridula Habib; **Defang Ouyang**, Mohammed Maniruzzaman*. 3D bioprinted microparticles: Optimizing loading efficiency using advanced DoE technique and machine learning modeling. ***International Journal of Pharmaceutics***, 2022, 122302;
24. Junhuang Jiang, Xiangyu Ma, **Defang Ouyang**, Robert O Williams*. Emerging Artificial Intelligence (AI) Technologies Used in the Development of Solid Dosage Forms, 2022, 14(11), 2257;

25. Wang, Wei, **Defang Ouyang***. Opportunities and challenges of physiologically based pharmacokinetic modeling in drug delivery. ***Drug Discovery Today,*** 2022, 27(8), 2100-2120;
26. Haoshi Gao, Stanislav Kan, Zhuyifan Ye, Yuchen Feng, Lei Jin, Xudong Zhang, Jiayin Deng, Ging Chan, Yuanjia Hu, Yongjun Wang, Dongsheng Cao, Yuanhui Ji, Mingtao Liang, Haifeng Li, **Defang Ouyang***. Development of in silico methodology for siRNA lipid nanoparticle formulations, ***Chemical Engineering Journal***, 2022, 442, 136310;
27. 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***, 2022, https://doi.org/10.1016/j.cclet.2022.05.028;
28. Yupeng Liu, Josh Haipeng Lei, Gang Wang, Zhiming Zhang, Jun Wu, Bohan Zhang, Huiqi Zhang, Enshan Liu, Liming Wang, Tzu‐Ming Liu, Guichuan Xing, **Defang Ouyang**, Chu‐Xia Deng, Zikang Tang, Songnan Qu. Toward Strong Near‐Infrared Absorption/Emission from Carbon Dots in Aqueous Media through Solvothermal Fusion of Large Conjugated Perylene Derivatives with Post‐Surface Engineering. ***Advanced Science***, 2022, 2202283
29. Cheng, Yu, Yuanhui Ji, and **Defang Ouyang**. FC-BBR/IND-induced glucose oxidase nanodrugs for targeted combination therapy, ***International Journal of Pharmaceutics,*** 611 (2022): 121349;
30. Yiping Huang, **Defang Ouyang**, Yuanhui Ji*. The Role of H‐bond in Solubilizing Drugs by Ionic Liquids: A Molecular Dynamics and Density Functional Theory Study, ***AIChE Journal***, 2022, e17672;
31. Junjun Li, Hanlu, Gao, **Defang Ouyang***. In silico formulation prediction of drug/cyclodextrin/polymer ternary complexes by machine learning and molecular modeling techniques, ***Carbohydrate Polymers***, 275 (2022): 118712;
32. 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; **(IF 14.903, JCR Q1)**
33. Zhuyifan Ye, **Defang Ouyang***. "Prediction of small-molecule compound solubility in organic solvents by machine learning algorithms." ***Journal of Cheminformatics***, 13.1 (2021): 1-13;
34. Wei Wang, Zhuyifan Ye, Hanlu Gao, **Defang Ouyang***. Computational pharmaceutics – a new paradigm of drug delivery, ***Journal of Controlled Release***, 2021, 338, 119-136; **(IF 11.467, JCR Q1)**
35. Nannan Wang, Huimin Sun, Jie Dong, **Defang Ouyang***. PharmDE: a new expert system for drug-excipient compatibility evaluation, ***International Journal of Pharmaceutics***, 2021, 607, 120962;
36. Yanqing Wang, Weijuan Huang, Nannan Wang, **Defang Ouyang**, Lifeng Xiao, Sirui Zhang, Xiaozheng Ou, Tingsha He, Rongmin Yu, Liyan Song*. Development of Arteannuin B Sustained-Release Microspheres for Anti-Tumor Therapy by Integrated Experimental and Molecular Modeling Approaches, ***Pharmaceutics***, 2021, 13(8), 1236;
37. Jie Dong, Hanlu Gao, **Defang Ouyang*.** PharmSD: a novel AI-based computational platform for solid dispersion formulation design, ***International Journal of Pharmaceutics***, 2021, 604, 120705;
38. Hongyu Chen, Guanghui Hu, **Defang Ouyang***. A numerical study of the distribution of chemotherapeutic drug Carmustine on brain glioblastoma, ***Pharmaceutical Research***, 2021, 1-14;
39. Wei Wang, **Defang Ouyang***. Prediction of Free Drug Absorption in Cyclodextrin Formulation by A Modified Physiologically Based Pharmacokinetic Model and Phase Solubility 3-D Surface Graph, ***Pharmaceutical Research***, 2021, 38 (7), 1157-1168;

40. 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; **(IF 14.903, JCR Q1)**
41. Zhuyifan Ye; Wenmian Yang; Yilong Yang; **Defang Ouyang***. Interpretable Machine Learning Methods for Pharmaceutical Formulation Development, ***Food Frontier***, 2021, 2(2), 195-207;
42. Haoshi Gao, Yan Su, Wei Xiong, Hua Yu, **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;
43. Gao Hanlu, Wang Wei, Dong Jie, Ye Zhuyifan, **Defang Ouyang***. An integrated computational methodology with data-driven machine learning, molecular modeling and PBPK modeling to accelerate solid dispersion formulation design. ***European Journal of Pharmaceutics and Biopharmaceutics,*** 158 (2021) 336–346; **(IF 5.589, JCR Q1)**
44. Xiaoting Zhang, Qiuhong Rao, Zhenwen Qiu, Yisheng Lin, Lei Zhang, Qingzhong Hu, Tingting Chen, Zhimin Ma, Hanlu Gao, Dandong Luo, Jiaqi Zhao, **Defang Ouyang***, Zhenyu Jason Zhang*, Qingguo Li*. Using Acetone/Water Binary Solvent to Enhance the Stability and Bioavailability of Spray Dried Enzalutamide/HPMC-AS Solid Dispersions, ***Journal of Pharmaceutical Sciences***, 2020, 1-12;
45. Yan Ma, Liuting Zhong, Zhuo Peng, Xinyang Liu, **Defang Ouyang*** & Shixia Guan***.*** Development of a Highly Water-Soluble Lycopene Cyclodextrin Ternary Formulation by the Integrated Experimental and Modeling Techniques, ***AAPS PharmSciTech,*** *(2021) 22:5*;
46. S Zhang, Q Zhu, JY Chen, **D Ouyang**, JH Lu*. The pharmacological activity of epigallocatechin-3-gallate (EGCG) on Alzheimer's disease animal model: A systematic review, ***Phytomedicine***, 2020, 79, 153316;
47. Zhengfei Yang, Ran Xiao, Feijun Luo, Qinlu Lin, **Defang Ouyang**, Wenbin Zeng, Jie Dong*. Food bioactive small molecule database: deep boosting for the study of food molecular behaviors. ***Innovative Food Science & Emerging Technologies***, 2020, 102499;
48. Yuan He, Zhuyifan Ye, Xinyang Liu, Hai-Feng Li, Ying Zheng, **Defang Ouyang***. Can machine learning predict drug nanocrystals? ***Journal of Controlled Release***, 2020, 322, 274-285; **(IF 11.467, JCR Q1, Cover story)**
49. Haoshi Gao , Zhuyifan Ye, Hanlu Gao, Haifeng Li, **Defang Ouyang***. Predicting complexation rate of drug/phospholipid complex by machine learning method, ***Chemical Physics Letter***, 2020, 747, 137354;
50. Xing Yang, Yuan Luo, Sanpeng Li, Xiuli Xu, Yingxia Bao, Jiaming Yang, **Defang Ouyang**, Xingxing Fan, Ping Gong*, Lintao Cai*. Small Molecular Prodrug Amphiphile Self-Assembled AIE Dots for Cancer Theranostics, Frontiers in bioengineering and biotechnology, 2020, 8, 903;
51. Nikhila Miriyala, Daniel J Kirby, Aude Cumont, Ruoying Zhang, Baogui Shi, **Defang Ouyang**, Haitao Ye*, Synthesis of Carbon Onion and Its Application as a Porous Carrier for Amorphous Drug Delivery. ***Crystals***, 2020, 10 (4), 281;
52. Yiping Huang, Yuanhui Ji, Mao Zhang, **Defang Ouyang**. How Imidazolium‐Based Ionic Liquids Solubilize the Poorly Soluble Ibuprofen? A Theoretical Study, ***AIChE Journal***, 2020, DOI: 10.1002/aic.16940;
53. Conglian Yang, Kun Tu, Hanlu Gao, Liao Zhang, Yu Sun, Ting Yang, Li Kong, **Defang Ouyang***, Zhiping Zhang*. The novel platinum(IV) prodrug with self-assembly property and structure-transformable character against triple-negative breast cancer, ***Biomaterials***, 2020, 232, 119751; **(IF 15.304, JCR Q1)**
54. Mao Zhang, Yiping Huang, Dule Hao, Yuanhui Ji, **Defang Ouyang**. Solvation structure and molecular interactions of ibuprofen with ethanol and water: A theoretical study, ***Fluid Phase Equilibria***, 2020, 510, 112454;

55. Xiao-Wen Zhang, Jia-Yue Chen, **Defang Ouyang**, Jia-Hong Lu*. Quercetin in Animal Models of Alzheimer's Disease: A Systematic Review of Preclinical Studies, ***International Journal of Molecular Sciences***, 2020, 21, 493.
56. Qianqian Zhao, Haoshi Gao, Yan Su, Tianhe Huang, Jiahong Lu, Hua Yu, **Defang Ouyang***. Experimental Characterization and Molecular Dynamic Simulation of Ketoprofen-Cyclodextrin complexes, ***Chemical Physics Letter***, 2019, 736, 136802;
57. Chen Jia-Yue, Qi Zhu, Zhang Shuang, **Defang Ouyang**, Lu Jiahong*. Resveratrol in experimental Alzheimer's disease models: A systematic review of preclinical studies, ***Pharmacological Research***, 2019, 150, 104476;
58. Yan He, Hongfei Liu, Wangqing Bian, Yue Liu, Xinyang Liu, Shijing Ma, Xi Zheng, Zhiyun Du, Kun Zhang, **Defang Ouyang***. Molecular Interactions for the Curcumin-polymer Complex with Enhanced Anti-inflammatory Effects, ***Pharmaceutics***, 2019, 11(9), 442; **(IF 6.525, JCR Q1)**
59. Song, Ke; Wang, Zhaobo; Liu, Xue; Zhang, Guolin; Wang, Xin; **Ouyang, Defang**; Guo, Mingrui; Chen, Lijiang*. A Novel Dual Sensitive Polymer-Gambogic Acid Conjugate: Synthesis, characterization, and in vitro evaluation, ***Nanotechnology***, 2019, 30(50):505701;
60. Run Han, Hui Xiong, Zhuyifan Ye, Yilong Yang, Tianhe Huang, Qiufang Jing, Jiahong Lu, Hao Pan, Fuzheng Ren, Defang Ouyang*. Predicting physical stability of solid dispersions by machine learning techniques, ***Journal of Controlled Release***, 2019, 311-312, 16-25; **(IF 11.467, JCR Q1, cover story)**
61. Run Han, Tianhe Huang, Xunqing Yin, Haifeng Li, **Defang Ouyang***. Insight into the dissolution molecular mechanism of ternary solid dispersions by combined experiments and molecular simulations. ***AAPS PharmSciTech***, 2019, 20, 274;
62. Qianqian Zhao, Ye Zhuyifang, Yan Su, **Defang Ouyang***. Predicting Complexation Performance between Cyclodextrins and Guest Molecules by Integrated Machine learning and Molecular Modeling Techniques. ***Acta Pharmaceutica Sinica B***, 2019, 9(6), 1241-1252; **(IF 14.903, JCR Q1)**
63. Qiang Li, Qianqian Zhao, Qiufang Jing, Xiaosi Ma, Ning Chen, Guo-Bin Ren, **Defang Ouyang***, Fuzheng Ren*. Investigating molecular interactions of high-loaded glipizide-HPMCAS microparticles by integrated experimental and modeling techniques. ***European Journal of Pharmaceutical Sciences***, 2019, 131, 127-135;
64. Zhuyifan Ye, Yilong Yang, Xiaoshan Li, Dongsheng Cao, **Defang Ouyang***. An Integrated Transfer Learning and Multitask Learning Approach for Pharmacokinetic Parameter Prediction. ***Molecular Pharmaceutics***, 2019, 16 (2), 533−541; **(IF 5.364, JCR Q1)**
65. Liu, Lu; Fu, Li; Zhang, Jin-Wei; Wei, Hui; Ye, Wen-Ling; Deng, Zhen-Ke; Zhang, Lin; Cheng, Yan; **Ouyang, Defang**; Cao, Qian; Cao, Dong-Sheng*. A three-level hepatotoxicity prediction system based on adverse hepatic effects, ***Molecular Pharmaceutics***, 2019, 16 (1), 393–408;
66. Lin Hui-Heng; **Ouyang, Defang**; Hu, Yuanjia. Intelligent Classifier: a Tool to Impel Drug Technology Transfer from Academia to Industry, ***Journal of Pharmaceutical Innovation***, 2019, 14, 28-34;
67. Tianhe Huang, Qianqian Zhao, Yan Su, **Defang Ouyang***. Investigation of Molecular Aggregation Mechanism of Glipizide/Cyclodextrin Complexation by Combined Experimental and Molecular Modeling Approaches. ***Asian Journal of Pharmaceutical Sciences***, 2019, 14(6), 609-620; **(cover page)**
68. Hao Zhong, Ging Chan, Hao Hu, Yuanjia Hu, **Defang Ouyang*.** A comprehensive map on FDA-approved pharmaceutical products. ***Pharmaceutics***, 2018, 10(4), 263; **(IF 6.525, JCR Q1)**
69. Yilong Yang, Zhuyifan Ye, Yan Su, Qianqian Zhao, Xiaoshan Li, **Defang Ouyang***. Deep learning for in vitro prediction of pharmaceutical formulations. ***Acta Pharmaceutica Sinica B***, 2019;9(1):177–185; **(IF 14.903, JCR Q1)**

70. Jie Dong, Ning-Ning Wang, Zhi-Jiang Yao, Lin Zhang, Yan Cheng, **Defang Ouyang**, Ai-Ping Lu, Dong-Sheng Cao*. ADMETlab: a platform for systematic ADMET evaluation based on a comprehensively collected ADMET database. ***Journal of Cheminformatics***, 2018, 10(1), 29;
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73. Tenglan Chan, **Defang Ouyang***. Investigating the molecular dissolution process of binary solid dispersions by molecular dynamics simulations. ***Asian Journal of Pharmaceutical Sciences*** 2018, 13(3), 248-254. **(IF 9.273, JCR Q1)**
74. Qianqian Zhao, Nikhila Miriyala, Yan Su, Weijie Chen, Xuejiao Gao, Ling Shao, Ru Yan, Haifeng Li, Xiaojun Yao, Dongsheng Cao, Yitao Wang, **Defang Ouyang***. Computer-Aided Formulation Design for a Highly Soluble Lutein−Cyclodextrin Multiple-Component Delivery System. ***Molecular Pharmaceutics,*** 2018, 15(4), 1664-1673. **(IF 5.364, JCR Q1)**
75. Run Han, Yilong Yang, Xiaoshan Li, **Defang Ouyang***, Predicting Oral Disintegrating Tablet Formulations by Neural Network Techniques. ***Asian Journal of Pharmaceutical Sciences,*** 2018, 13(4), 336-342. **(IF 9.273, JCR Q1)**
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83. Weijie Chen, **Defang Ouyang***. Investigation of molecular dissolution mechanism of ketoprofen binary and ternary solid dispersions by molecular dynamics simulations. ***Molecular Simulation***. 2017, 43(13-16), 1074-1080.
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Pharmacy education paper (4)

106. Zhong Hao, **Defang Ouyang***. The gap analysis between academia, industry and government in Chinese pharmaceutical field from 2000 to 2018, ***Scientometrics***, 2020, 122(2), 1113-1128; **(SSCI, IF 2.770, JCR Q1)**
107. Weixiang Zhang, Hao Zhong, Yitao Wang, Ging Chan, Yuanjia Hu, Hao Hu, **Defang Ouyang***. Academic career progression of Chinese-origin pharmacy faculty members in western countries. ***Pharmacy***, 2018, 6, 104;
108. Weixiang Zhang, Yitao Wang, **Defang Ouyang***. Diversity of Pharmacy Faculty Members between UK and US. ***Indian Journal of Pharmaceutical Education and Research****, 2017; 51(1):20-24;*
109. **D. Ouyang***, How to help first-year pharmacy to gain the big picture. ***Journal of Asian Association of Schools of Pharmacy***. 2012, 1(4) 194 - 202;

Patents (11 patents with commercialization)

110. **D. Ouyang**, T. Lu. A highly-soluble ginsenoside Rh2 formulation and its preparation method. CN 202311611678.9
111. **D. Ouyang**. A development and prediction evaluation method for pharmaceutical combination. CN202110172942.8
112. **D. Ouyang**, Y Su. A highly-soluble andrographolide formulation and its preparation method. CN201811652632.0
113. **D. Ouyang**, Q Zhao. A prediction system and method for in silico formulation design and evaluation. CN201710429764.6;
114. **D. Ouyang**, Y Yang, Y Ye. A new algorithm to predict drug delivery systems. CN 201710429823.X;
115. **D, Ouyang,** Q Zhao. Preparation and method of lutein-containing combination. CN201710355210.6；
116. **D. Ouyang**, Q. Zuo, C. Wang, H. Zhang, Y. Bao. Instant pirarubicin HCl freeze-drying powdery injection and its production. CN200610157023;
117. **D. Ouyang**, J. Zeng, N. Yu, Y. Bao. Stable injection docetaxel. CN200610032942;
118. J. Zeng, **D. Ouyang**, H. Zhang, Y. Bao. Method for removing organic solvent from viscous liquid. CN200610061698;
119. **D. Ouyang**, W. Pan. Combination of metformin/glipizide controlled-release tablet and its preparation method: CN200510045949;
120. 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;
121. Pan W，Li W，**D. Ouyang**. Preparation and method of venlafaxine hydrochloride osmotic pump controlled release tablet. CN200510046231；

Teaching

Prof. Ouyang has wide teaching and curriculum development experiences in pharmaceutical sciences, 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.

- 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)
- Computational pharmacy (MPhil, module coordinator)
- Pharmacokinetics (MPhil)
- Advanced medicinal administration (PhD)

PhD supervision

Prof. Ouyang had successfully supervised 1 postdoc, 7 PhD students (as below) and 26 master students. Currently his research group includes 2 postdoc, 10 PhD students, 5 master students and 1 research assistant.

- 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)

Awards

- 2024, Dr. Stanley Ho Medical Development Foundation Visiting Scholar;

- 2021, Excellent Scientific Paper Award of Chinese Science Association;
- 2019, Student Travel Grant of 2019 Asian Association of Schools of Pharmacy (AASP) Conference, Korea (as the Supervisor);
- 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);
- 2017 & 2018, Student Travel Grant of 17th Meeting of Consortium for Globalization of Chinese Medicine (CGCM), CGCM, Asia (as the Supervisor);
- 2016, Student Poster Award of 52nd Annual Meeting of the Drug Information Association, Drug Information Association (USA), US (as the Supervisor);
- 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

Academic Leadership

- **Associate editor of <Drug Delivery and Translational Research>** (IF 5.671)
- Editorial board of <Asian Journal of Pharmaceutical Sciences> (IF 9.273);
- Editorial board of <Pharmaceutical Research> (IF 4.58);
- Scientific Advisor of <Journal of Pharmaceutical Sciences> (IF 3.784);
- Topic editor of Special Issue "The Use of Bio/Chemoinformatics Tools in Drug-Formulation to Reach Better Pharmacological Responses" of <Frontiers in Pharmacology> (IF 5.988)
- Topic editor of Special Issue "Gene Therapy" of <Pharmaceutics> (IF 6.525);
- **Grant reviewer of Canada First Research Excellence Fund (CFREF), BBSRC (UK), French National Research Agency (ANR) French Funding Program, and National Science Centre Poland;**
- Organizing committee and session chair of multiple international conferences, including
    - 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;
- 2015 Outstanding reviewer of <International Journal of Pharmaceutics>;
- 2019 Outstanding reviewer of <Journal of Pharmaceutical Sciences>;
- 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.;

Invited lectures and talks (over 120)

1. 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)
2. Opportunity and Challenge of AI in drug delivery. Frointer Symposium of NSFC-FDCT (6-7, December, 2023, Harbin, China)
3. Computational pharmaceutics. School of Pharmacy, Harbin Medical University (5 December, 2023, Harbin, China)
4. Opportunity and Challenge of AI in drug delivery. International Conference on Theoretical and High Performance Computational Chemistry 2023 (24-26 November, 2023, Haikou, China)
5. Opportunity and Challenge of AI in drug delivery. 5th International Conference on Nanomedicine of China (November 4–7, 2023, Guangzhou, China)
6. Opportunity and Challenge of AI in drug delivery. Macau Symposium on Artificial Intelligence and Health (30-31 October, 2023, Macau)
7. 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)
8. 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)
9. Opportunity and Challenge of AI in drug delivery. 9th UK-China International Particle Technology Forum (21st- 24th August, 2023, University of Greenwich, London, UK)
10. Opportunity and Challenge of AI in drug delivery. School of Engineering, The University of Edinburgh (16 August, 2023, Edinburgh, UK)
11. Opportunity and Challenge of AI in biologics formulations. 2023 Biopharmaceutical Bioprocess Development Summit (3-5 August, 2023, Shanghai, China)

12. Opportunity and Challenge of AI in drug delivery. Tongxieyi Conference (29 July, 2023, Shenzhen, China)
13. 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)
14. Opportunity and Challenge of AI in drug delivery. 6th Asian Symposium on Pharmaceutical Science and Technology (3-4 June, 2023, Zhengzhou, China)
15. 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)
16. Opportunity and Challenge of AI in drug delivery. 15th China Pharmaceutical Strategy Conference 2023 (18-20 March, 2023, Shijiazhuang, China)
17. Artificial intelligence in drug delivery. Artificial Intelligence (AI) and Machine Learning Webinar of Academy of Pharmaceutical Sciences (APS) UK (15 Feburary 2023, online)
18. Predicting lipid nanoparticle for mRNA vaccine by machine learning algorithm. 15th China Pharmaceutical Conference 2022 (23 December, 2022, Shanghai, China)
19. Computational pharmaceutics – a new paradigm of drug delivery. University of Helsinki, Finland (10 November, 2022, Helsinki, Finland)
20. Computational pharmaceutics – a new paradigm of drug delivery. Drug Research Academy, University of Copenhagen, Denmark (9 November, 2022, Copenhagen, Denmark)
21. Predicting lipid nanoparticle of mRNA vaccine by machine learning algorithm. 2nd Innovation Symposium of mRNA therapeutics in 2022. (26-27 September, 2022, Shanghai, China)
22. Opportunity and challenge of artificial intelligence (AI) in drug delivery. XXVII EFMC International Symposium on Medicinal Chemistry (4-8 September, 2022, Nice, France)
23. Artificial intelligence in pharmaceutical excipients and formulation development. 2022 Gushu Dialogue (24-26 August, 2022, Soochow, China)
24. Predicting lipid nanoparticle of mRNA vaccine by machine learning algorithm. 5th Symposium of Pharmaceutics and Particle Design (9-10 July, 2022, Changsha, China)
25. Opportunity and challenge of artificial intelligence (AI) in drug delivery. 4th Cloud Symposium of Asian Journal Pharmaceutical Sciences (7th July, 2022, online)
26. Computational pharmaceutics – from AI to PBPK modeling. Young Symposium of South China Quantitative Pharmacology (5th July, 2022, online)
27. AI-driven lipid nanoparticle (LNP) design for mRNA therapeutics. 2022 Symposium of mRNA delivery systems and manufacture. (2nd July, 2022, online)
28. AI-driven lipid nanoparticle (LNP) design for mRNA therapeutics. 3rd Cell Therapy and Regenerative Medicine Conference (20-21 April, 2022, Shenzhen, China)
29. Computational pharmaceutics. Centre for Pharmaceutical Oncology (CPO) seminars. Leslie Dan Faculty of Pharmacy, University of Toronto (16 March, 2022, online)
30. Invited lectures, Wuhan Technology University (12/26 March, 2022, online)
31. Opportunity and challenge of artificial intelligence (AI) in drug delivery. 2022 ExciPerience (9-11 March, 2022, online)
32. Computational pharmacy – From molecular simulation, PBPK simulation to artificial intelligence. 8th International Symposium in Quantitative Pharmacology (5-6 December, 2021, Beijing, China)
33. Application of computational tools in clinical medication for pregnant women. Invited lecture from Guangzhou Medical University Third Hospital (27 January, 2022, Guangzhou, China)

34. Computational pharmaceutics – a new paradigm of drug delivery. International Frontier Symposium of Pharmaceutical Engineering. (13 January, 2022, online)
35. Invited lectures, Central South University (November 2021, online)
36. AI-leading the database development for pharmaceutical excipient and formulation. Chinese Drug Regulatory Conference (13-15 October, 2021, Beijing, China)
37. Artificial Intelligence in Pharmaceutics. FY 2021 Generic Drug Science and Research Initiatives Public Workshop, US-FDA (June 23, 2021, online);
38. Artificial intelligence of pharmaceutics. 10th International Conference on Molecular Simulations and Artificial Intelligence Application (29-30 May, 2021, Soochow, China)
39. Artificial intelligence of pharmaceutics. 13rd National Microanalysis Conference of China Chemical Society (23-25 April, 2021, Southern University of Science and Technology, Shenzhen, China)
40. Computational pharmaceutics – from molecular modeling to artificial intelligence. Series Academic Forum of China Pharmaceutical Society and Chinese Clinical Pharmacology Journal. (24 April, 2021, online)
41. Prediction of solid dispersion formulations by the integrated computational methodology. 32nd Annual Meeting of Chinese Chemical Society (19-22 April, 2021, Zhuhai, China)
42. Artificial intelligence of pharmaceutics. Hainan Free Trade Port 1st International Pharmaceutical Innovation Symposium and Investment Trade Conference (16-18 April, 2021, Haikou, China)
43. Computational pharmaceutics – a new paradigm of drug delivery. The first Greater Bay Area Biophysics and New Drug Discovery Forum (10-12 April, Zhuhai, China)
44. Rational design of mRNA lipid delivery systems by machine learning approach. mRNA Pharmaceutical Technique Innovation Symposium. (11 March, 2021, Shanghai Zhangjiang, China)
45. Computational pharmaceutics – a new paradigm of drug delivery. Asian Pharmaceutics Online Symposium, 1st Conference Computational pharmaceutics (online, 12 December, 2020)
46. 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)
47. The opportunity and challenge of artificial intelligence in pharmaceutics. 7th China Pharmaceutical Festival (11-12 November, 2020, Nanjing, China)
48. The opportunity and challenge of artificial intelligence in pharmaceutics. Changchun University of Chinese Medicine (2 November, 2020, Changchun, China)
49. 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)
50. Artificial intelligence in pharmaceutics. 8th Symposium of Medical Artificial Intelligence (online meeting, August 30, 2020)
51. Past, present and future of pharmaceutics. 7th Medical and Humanity Summer Camp (online meeting, August 22, 2020)
52. 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)
53. Computational pharmaceutics – from molecular modeling to artificial intelligence. Anhui Medical University (19 January, 2020, Hefei, China)

54. Computational prediction of physical stability of solid dispersions. 15th National Computational Chemistry Conference (15-17 November 2019, Shanghai, China)
55. Prediction of physical stability of solid dispersions by machine learning. 4th National Biological Particle Conference. (9-10 November 2019, Shenzhen, China)
56. Artificial intelligence in pharmaceutics. 9th China Pharmaceutical and Biotechnological Symposium. (25-27 October 2019, Shenzhen, China)
57. Computational pharmaceutics – from molecular modeling to artificial intelligence. Guangdong Pharmaceutical University (26 September 2019, Guangzhou, China)
58. Artificial intelligence in pharmaceutics. Southern University of Science and Technology (16 September 2019, Shenzhen, China)
59. Big data analysis of Chinese pharmaceutical industry and artificial intelligence in pharmaceutics. 2019 Guangdong-HK-Macau Intellectual Property Symposium (30 June, 2019, Zhuhai, China)
60. Artificial intelligence and deep learning in pharmaceutics. Chinese Pharmaceutical Quality Conference (4-5 June, 2019, Chendu, China)
61. Big data analysis of Chinese pharmaceutical industry. National Platelet Day (25 April, 2019, Shenzhen, China)
62. Artificial intelligence, big data and future education. China Education Society (9 April 2019, Macau, China)
63. Neutron scattering in pharmaceutics. Symposium of small angle neutron scattering users (7-8 April 2019, Dongguan, China)
64. Big data analysis of Chinese pharmaceutical industry from 2000 – 2018. CKPC college Inspiring seminar. (3 April 2019, Macau, China)
65. Big data analysis of global progress in pharmaceutics and future perspective. 2019 Zhanjiang-HK-Macau Medical Symposium (5 January 2019, Zhanjiang, China)
66. Transfer learning for the prediction of pharmacokinetic properties. 2018 Chinese Quantitative Pharmacology Conference (17-18 November 2018, Changsha, China)
67. Computational pharmaceutics. 2018 Postgraduate Lectures in Pharmaceutics at Shenyang Pharmaceutical University (3 November, 2018, Shenyang, China)
68. Artificial intelligence in Inhalation formulations. 2018 National Inhalation Drug Delivery Association Conference (19-21 October, 2018, Nanjing, China)
69. Artificial intelligence for pharmaceutical formulations. 2018 Chinese Pharmaceutical Innovation and Investment Conference (18-20 September, 2018, Soochow, China)
70. Artificial intelligence and big data in pharmaceutical formulations and excipients. 3rd China Drug Administration Conference 2018. (6-7 September, 2018, Beijing, China)
71. 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)
72. 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)
73. Big data analysis of the literature and patent of solid dispersions. 2018 Macau International Symposium of Intellectual Property.（6 August 2018, Macau, China）

74. 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）
75. 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)
76. Computational Pharmaceutics – from molecular modeling to artificial intelligence and big data. School of Chemical Engineering, The University of Adelaide (19 July 2018, Adelaide, Australia)
77. Computational Pharmaceutics – from molecular modeling to artificial intelligence and big data. School of Pharmacy, The University of Queensland (16 July 2018, Brisbane, Australia);
78. Computational Pharmaceutics. The 2nd Worldwide Chinese Computational Biology and Molecular Simulation Conference, Sun Yat-sen University (7-10 June 2018, Guangzhou, China)
79. Computational Pharmaceutics. School of Pharmacy, Zhejiang University (30 March, 2018 Hangzhou, China)
80. Computational Pharmaceutics – from molecular modeling to artificial intelligence and big data. The 7th Innovative Drug Delivery Solutions (28-30 March, 2018, Hangzhou, China)
81. 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)
82. 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)
83. Computational Pharmaceutics – from molecular modeling to artificial intelligence and big data. School of Pharmacy, China Pharmaceutical University (21 November 2017, Nanjing, China)
84. Computational Pharmaceutics – from molecular modeling to artificial intelligence and big data. 14th National Computer Chemistry Conference (17-20 November, 2017, Nanjing, China)
85. Computational Pharmaceutics – from molecular modeling to artificial intelligence and big data. 2017 China Pharmaceutical Conference (28-30 October, 2017, Shanghai, China)
86. Big data analysis of global advances in pharmaceutics and drug delivery 1980 – 2014. Yaodu college online live course. (17 October, 2018)
87. 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)
88. 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)
89. 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)
90. Computational Pharmaceutics – the development of aging medicine. 1st Beijing-Hongkong-Macau-Taiwan Aging Summer School, Peking University (29 June, 2017, Beijing, China)
91. Computational pharmaceutics – application of molecular modeling in formulation development. School of Pharmacy, Zhengzhou University (27 June, 2017, Zhengzhou, China)
92. Computational pharmaceutics – application of computer in clinical pharmacy. Henan Young Pharmacist Symposium 2017 (24 June, 2017, Zhengzhou, China)

93. 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)
94. Computational Pharmaceutics – a new paradigm of drug delivery. Chengdu Medical College (11 April, 2017, Chengdu, China)
95. Computational Pharmaceutics – a new paradigm of drug delivery. West China School of Pharmacy, Sichuan University (11 April, 2017 Chengdu, China)
96. Computational Pharmaceutics – In silico formulation design for better medicine. School of Pharmacy, Southwest University (10 April 2017, Chongqing, China)
97. Past, today and future of pharmaceutics. CKPC college lunch-sharing seminar. (29 March 2017, Macau, China)
98. Computational pharmaceutics. Listening to the Voice from the Western: Opinions on Data Integrity, CSV and Governance Affairs. (24 March 2017, Hong Kong, China)
99. 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)
100. Computational Pharmaceutics – a new paradigm of drug delivery. UM HPC Sharing Seminar (25 November 2016, Macau, China)
101. Computational Pharmaceutics – application of molecular modeling to drug delivery. 4th International Conference on Molecular Simulation (ICMS 2016) (24-26 Oct 2016, Shanghai, China)
102. Big Data Analysis of Global Progress in Pharmaceutics and Drug Delivery. 2016 Scientific Data Conference (25-26 August 2016, Shanghai, China)
103. 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)
104. Computational pharmaceutics - In silico formulation design for better medicine. 4th Asian Symposium on Pharmaceutical Science and Technology (28-29 April 2016, Shenyang, China)
105. Computational pharmaceutics - In silico formulation design for better medicine. The 13th National Symposium of Computer & Computational Chemistry. (20 – 21 November 2015, Guangzhou, China)
106. 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)
107. 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)
108. 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)
109. 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)
110. Computational pharmaceutics – In silico formulation design for better medicine. School of Pharmacy, Guangzhou Medical University (11 June 2015, Guangzhou, China)

111. Computational pharmaceutics – In silico formulation design for better medicine. School of Pharmacy, Sun Yat-sen University (28 April 2015, Guangzhou, China)
112. Computational pharmaceutics. Faculty of Science and Technology, University of Macau (4th February 2015, Macau)
113. Computational pharmaceutics – application of molecular dynamics simulation in drug delivery. Controlled Release Society Annual Meeting 2014 (12^{th} - 16^{th} July, Chicago, USA)
114. How to help first-year pharmacy student to gain the big picture. 2014 Manchester Pharmacy Education Conference (30^{th} June, Manchester, UK)
115. Professional development for first-year pharmacy students. CERA-UK Conference 2014 (12^{th} -13^{th} June 2014, London, UK)
116. Computational pharmaceutics – *In silico* formulation design for better medicines. LHS research day, Aston University (Birmingham, UK, 28^{th} May 2014)
117. Computational pharmaceutics – *In silico* formulation design for better medicines. Leicester Pharmacy School, De Montfort University (Leicester, UK, 20^{th} May 2014)
118. Computational pharmaceutics – application of computer modeling in drug delivery. Making Pharmaceutics Conference & Exhibition (Birmingham, UK, 29th April, 2014)
119. Oral fast dissolving films for paediatric formulations. Science Capital Business Plan Session: Innovative Healthcare 2013 Meeting. (Birmingham, UK, 25th September, 2013)
120. Computational pharmaceutics - virtual screening in formulation development. NanoFormulation 2013. (Manchester, UK, 18-21 June, 2013)
121. Computational pharmaceutics. Formulated Products-Meeting the Product and Process Design Challenge' Competition Briefing Event. (London, UK, 1st May, 2013)
122. Computational pharmaceutics. Nutrition for Life Birmingham Workshop. (Birmingham, UK, 10th April, 2013)
123. Computational pharmaceutics. School of Chemical Engineering, University of Birmingham, UK. (Birmingham, UK, 13th December, 3012)
124. Computational pharmaceutics - the application of molecular modeling in drug delivery. 5th Midlands Biophysics Network Symposium. (Birmingham, UK, 18th April 2012).
125. Computational pharmaceutics. Aston Research Centre for Healthy Ageing (ARCHA) seminar, Aston University (Birmingham, UK, December 7th, 2011).
126. 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).
127. 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).
128. Structure, Dynamics and Energetics of siRNA-Cationic Vector Complexation by Molecular Dynamics Simulations. RACI Student Symposium. (Brisbane, Australia, October 2, 2009).