

Jianyuan Deng

✉ jianyuan.deng@stonybrook.edu | ☎ +1 (631) 202-9572 | Stony Brook NY, 11790
GitHub | Google Scholar | LinkedIn | ResearchGate

EDUCATION

- Stony Brook University**, Stony Brook, New York, United States Aug. 2018 – Nov. 2023
Doctor of Philosophy (Ph.D.) in Biomedical Informatics, GPA: 3.9/4.0
- The Chinese University of Hong Kong**, Hong Kong SAR, China Aug. 2014 – Oct. 2016
Master of Philosophy (M.Phil.) in Pharmacy, GPA: 3.7/4.0
- Sun Yat-Sen University**, Guangzhou, China Sep. 2010 – Jun. 2014
Bachelor of Science (B.Sc.) in Pharmaceutical Sciences, GPA: 4.0/5.0 (Rank 1/113)

WORK EXPERIENCE

- ML Engineer Intern** – Insitro, South San Francisco, CA, United States May. 2022 – Aug. 2022
- AI Scientist Intern** – Genentech, South San Francisco, CA, United States May. 2021 – Aug. 2021
- Research Assistant** – The Chinese University of Hong Kong, Hong Kong SAR, China Nov. 2016 – Jun. 2018

RESEARCH PROJECTS

- De novo Drug Design with Deep Generative and Predictive Neural Networks** Nov. 2019 - Now
- Implemented a deep reinforcement learning framework to design molecules with multiple desired properties
 - Conducted a comprehensive survey on the applications and techniques in AI-driven drug discovery
 - Evaluated various molecular representations and model architectures for molecular property prediction
- Mining Electronic Health Records for Opioid Overdose Patterns and Opioid Prescriptions** Feb. 2019 - Dec. 2020
- Implemented Python and R scripts to process and analyze large-scale electronic health records
 - Designed and conducted a retrospective cross-sectional study on the temporal trends and risk factors of opioid overdose
- Identification of Key Pharmacological Components in Drug-Drug Interactions** Nov. 2018 - Dec. 2019
- Implemented Python scripts to parse the DrugBank database in XML format
- Patient Outcome Prediction based on Electronic Health Records with Deep Learning** Sep. 2018 - Jun. 2019
- Implemented Python scripts to retrieve medication details from RxNav APIs
- In Silico Drug Absorption Tract for Human Oral Drug Absorption** Aug. 2015 – Jun. 2018
- Developed an agent-based model to simulate oral drug absorption with emphasis on transporters and enzymes
 - Implemented a graphical user interface for the drug absorption model using a multi-agent simulation toolkit MASON

TECHNICAL STRENGTHS

- Skills:** Machine Learning (PyTorch, scikit-learn); Big Data Analytics (relational database); Data Visualization (ggplot2)
- Programming Languages:** Python, R, PostgreSQL, Git, Java
- Professional Activities:** Reviewer for Bioinformatics, Journal of Cheminformatics, PLOS One

SELECTED PUBLICATIONS

- J. Deng**, Z. Yang, H. Wang, I. Ojima, D. Samaras, F. Wang. "Unraveling Key Elements Underlying Molecular Property Prediction: A Systematic Study." *arXiv preprint arXiv:2209.13492*. 2022. In-principle acceptance to Nature Communications.
- J. Deng**, Z. Yang, I. Ojima, D. Samaras, F. Wang. "Artificial Intelligence in Drug Discovery: Applications and Techniques." *Briefings in Bioinformatics*. 2022.
- J. Deng**, W. Hou, X. Dong, J. Hajagos, M. Saltz, J. Saltz, F. Wang. "A Large-Scale Observational Study on the Temporal Trends and Risk Factors of Opioid Overdose: Real-World Evidence for Better Opioids." *Drugs - Real World Outcomes*. 2021.
- X. Dong, **J. Deng**, W. Hou, S. Rashidian, R.N. Rosenthal, M. Saltz, J. Saltz, F. Wang. "Predicting Opioid Overdose Risk of Patients with Opioid Prescriptions Using Electronic Health Records Based on Temporal Deep Learning." *J Biomed Inform.* 116(2021), pp.103725, 2021.
- J. Deng**, Z. Yang, Y. Li, D. Samaras, F. Wang. "Towards Better Opioid Antagonists Using Deep Reinforcement Learning." *arXiv preprint arXiv:2004.04768*, 2020.
- J. Deng**, F. Wang. "An Informatics-based Approach to Identify Key Pharmacological Components in Drug-Drug Interactions." *AMIA Jt Summits Transl Sci Proc*, 2020, pp.142, 2020.
- J. Deng**, A. Jhandey, X. Zhu, Z. Yang, K.F.P. Yik, Z. Zuo, T.N. Lam. "In Silico Drug absorption tract: An Agent-based Biomimetic Model for Human Oral Drug Absorption." *PloS One*, 13(8), pp.e0203361, 2018.
- J. Deng**, X. Zhu, Z. Chen, C.H. Fan, H.S. Kwan, C.H. Wong, K.Y. Shek, Z. Zuo, T.N. Lam. "A Review of Food-Drug Interactions on Oral Drug Absorption." *Drugs*, 77(17), pp.1833-1855, 2017.
- X. Zhu, **J. Deng**, Z. Zuo, T.N. Lam. "An Agent-based Approach to Dynamically Represent the Pharmacokinetic Properties of Baicalein." *AAPS J*, 18(6), pp.1475-1488, 2016.

HONORS & SCHOLARSHIPS

- Postgraduate Scholarship** - The Chinese University of Hong Kong 2014-2016
- LIU Yongsheng Outstanding Medical Student Scholarship** - Sun Yat-Sen University 2013
- National Scholarship** - China Ministry of Education 2011, 2012
- First-Class Scholarship** - Sun Yat-Sen University 2011, 2012, 2013