Jianyuan Deng

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GitHub| Google Scholar| LinkedIn| ResearchGate

EDUCATION

Stony Brook University, *Stony Brook, New York, United States* — *Aug. 2018 – May. 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 a set of representation learning models 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 (in Java) to simulate oral drug absorption with emphasis on transporters and enzymes

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 Journal of Cheminformatics & Bioinformatics

SELECTED PUBLICATIONS

- **J. Deng**, Z. Yang, H. Wang, I. Ojima, D. Samaras, F. Wang. "Taking a Respite from Representation Learning for Molecular Property Prediction." *arXiv preprint arXiv:2209.13492*. 2022.
- **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*