

Ziqi Chen

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EDUCATION

The Ohio State University, Columbus, US

PhD student

Aug. 2019 - current

Master student

Aug. 2018 - May 2019

Department of Computer Science and Engineering

Wuhan University, Wuhan, China

Sept. 2014 - Jun. 2018

Bachelor of Engineering

School of Computer Science

RESEARCH INTEREST

My research focuses on generative AI (genAI) for science (**genAI4Science**). I have developed innovative generative models for several key problems in the design of (1) small molecule drugs, including lead optimization, 3D ligand generation and retrosynthesis prediction; and (2) biologic drugs, including binding peptide generation and T-cell receptor sequence optimization.

PUBLICATION

* below indicates equal contributions.

1. Frazier Baker, **Ziqi Chen**, and Xia Ning. RLSynC: Offline-online reinforcement learning for synthesis completion. *arXiv*, 2023
2. **Ziqi Chen**, Bo Peng, Srinivasan Parthasarathy, and Xia Ning. Shape-conditioned 3D molecule generation via equivariant diffusion models. *arXiv:2308.11890*, 2023
3. Yonghyun Nam, Anastasia Lucas, Jae-Seung Yun, Seung Mi Lee, Ji Won Park, **Ziqi Chen**, Brian Lee, Xia Ning, Li Shen, Anurag Verma, and Dokyoon Kim. Development of complemented comprehensive networks for rapid screening of repurposable drugs applicable to new emerging disease outbreaks. *Journal of Translational Medicine*, 21(1), Jun. 2023
4. **Ziqi Chen**, Oluwatosin R. Ayinde, James R. Fuchs, Huan Sun, and Xia Ning. G²retro as a two-step graph generative models for retrosynthesis prediction. *Communications Chemistry*, 6(102), May 2023
5. **Ziqi Chen**, Martin Renqiang Min, Hongyu Guo, Chao Cheng, Trevor Clancy, and Xia Ning. T-cell receptor optimization with reinforcement learning and mutation polices for precision immunotherapy. In *Research in Computational Molecular Biology. RECOMB 2023. Lecture Notes in Computer Science*, pages 174–191. Springer Nature Switzerland, Apr. 2023
6. **Ziqi Chen***, Baoyi Zhang*, Hongyu Guo, Prashant Emani, Trevor Clancy, Chongming Jiang, Mark Gerstein, Xia Ning, Chao Cheng, and Martin Renqiang Min. Binding peptide generation for MHC class I proteins with deep reinforcement learning. *Bioinformatics*, 39(2):btad055, Jan. 2023
7. **Ziqi Chen***, Bo Peng*, Vassilis N. Ioannidis, Mufei Li, George Karypis, and Xia Ning. A knowledge graph of clinical trials (CTKG). *Scientific Reports*, 12(4724), Mar. 2022
8. **Ziqi Chen**, Martin Renqiang Min, Srinivasan Parthasarathy, and Xia Ning. A deep generative model for molecule optimization via one fragment modification. *Nature Machine Intelligence*, 3:1040–1049, Dec. 2021

9. **Ziqi Chen**, Martin Renqiang Min, and Xia Ning. Ranking-based convolutional neural network models for peptide-MHC class I binding prediction. *Frontiers in Molecular Biosciences*, 8:634836, May 2021

PATENT APPLICATION

1. Xia Ning and **Ziqi Chen**. Generative AI methods and systems for small molecule structure generation, Application No. 63/519,833, Date of Application: Aug. 2023
2. Xia Ning and **Ziqi Chen**. Retrosynthesis prediction system and method using graph generative models, Application No. PCT/US2023/017546, Date of Application: Apr. 2023
3. Renqiang Min, Hans Peter Graf, and **Ziqi Chen**. Peptide search system for immunotherapy, U.S. Patent US20230083313A1, Mar. 2023
4. Renqiang Min, Hans Peter Graf, and **Ziqi Chen**. Binding peptide generation for MHC class I proteins with deep reinforcement learning, U.S. Patent US20230083313A1, Mar. 2023

WORK EXPERIENCE

Meta Platforms, Menlo Park, US

May 2022 - Aug. 2022

Software Engineer Intern, Machine Learning

- I explored reinforcement learning algorithms to improve feed ranking in Facebook.
- I developed a deep Q-learning model to personalize feed re-ranking using predictions from a multi-task learning framework. A/B testing results demonstrate notable improvements in user engagement metrics with this model.
- I developed a model based on off-policy reinforcement learning algorithm for slate re-ranking.
- I built data pipelines for personalized feed re-ranking and slate ranking.

NEC Labs America, Princeton, US

May 2021 - Aug. 2021

Research Intern

- I developed a framework PepPPO based on proximal policy optimization (PPO) to optimize random initial peptides through mutating amino acids step by step until the mutated peptides can be predicted to be presented by a given MHC class I protein. This work is accepted by Bioinformatics.
- I developed a framework TCRPPO based on PPO to learn a mutation policy to optimize CDR3 sequences of β chains in T-cell receptors for any given peptide sequences. I also developed a reward function that combines the likelihoods of mutated sequences being valid TCRs with the probabilities of mutated sequences recognizing peptides from a peptide-TCR interaction predictor. This work is accepted by Research in Computational Molecular Biology 2023.

ACADEMIC ACHIEVEMENT

Second-class scholarship of Wuhan University

2015, 2016 and 2017

TECHNICAL STRENGTH

Program Languages	Python, Shell Script, Java, SQL
Software & Tools	Pytorch, Numpy
OS	Linux, Windows