

# Xiaoqiong Xia

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## RESEARCH INTERESTS

Deep learning; Drug discovery; Drug target interaction; Drug response; Molecule generation; Molecular representation; CADD; Omics analysis; Knowledge graph.

## EDUCATION

- ♦ Ph.D., Institutes of Biomedical Sciences, Fudan University (GPA: 3.27/4) 2019.09-2024.06  
Supervisor: Professor Lei Liu
- ♦ B.S., Biomedical engineering, China Medical University (TOP 1) 2015.09-2019.06

## RESEARCH EXPERIENCES

1. **Develop a structure-based molecular generation model (primary researcher) 2022.12–present**
  - Used MGLTools and AutoDock-GPU to build a virtual screening process for molecular fragments on a Linux system and screen high-scored molecular fragments efficiently.
  - Developed a fragment growth model using a diffusion algorithm to generate reasonable candidate molecules with high affinity to the target.
  - Used the GROMACS tool to perform molecular dynamics simulation of the receptor-ligand complex.
    - The project helps accelerate drug development.
2. **Develop a cancer-drug response prediction model (primary researcher) 2022.06–2023.09**
  - Used pre-trained models ChemBERTa and GIN, MLP to learn the drug's structural information.
  - Applied MLP to learn multi-omics profiles of cell lines.
  - Fused multimodal features based on multi-head attention mechanisms.
  - Transfer learning improves the model's generalization to predict drug cell line response (IC50).
    - The model could accelerate drug discovery and precision medicine.
3. **Develop a multimodal fusion DTI prediction model (primary researcher) 2020.09–2022.12**
  - Used deep learning modules such as CNN/Transformer, GNNs, and TransE to integrate structural information, knowledge graphs, and gene expression profiles of drugs and proteins to predict drug-target interactions accurately.
    - The model helps in drug repurposing and drug discovery. The paper was published in Bioinformatics.
4. **Multimodal reasoning based on knowledge graph embedding (Cooperative) 2020.09–2023.07**
  - Constructed RDKG-115, a rare disease knowledge graph based on 372,384 high-quality literature and 4 biomedical datasets: DRKG, Pathway Commons, PharmKG, and PMapp.
  - Developed a trimodal KGE model containing structure, category, and description embeddings using reverse-hyperplane projection.
  - Utilized this model to infer 4199 reliable new inferred triplets from RDKG-115.

- The project provides a paradigm for large-scale screening of drug repurposing and discovery for rare diseases.

## **PUBLICATIONS**

1. **Xiaoqiong Xia**, Chaoyu Zhu, Fan Zhong, Lei Liu. MDTips: A Multimodal-data based Drug-Target interaction prediction system fusing knowledge, gene expression profile and structural data. *Bioinformatics*. 2023 Jun 22.
2. **Xiaoqiong Xia**, Chaoyu Zhu, Fan Zhong, Lei Liu. TransCDR: a deep learning model for enhancing the generalizability of cancer drug response prediction through transfer learning and multimodal data fusion. *computer methods and programs in biomedicine*. Under review.
3. Chaoyu Zhu, Zhihao Yang, **Xiaoqiong Xia**, Nan Li, Fan Zhong, Lei Liu. Multimodal reasoning based on knowledge graph embedding for specific diseases. *Bioinformatics*. 2022 Apr 12.
4. Chaoyu Zhu, **Xiaoqiong Xia**, Nan Li, Fan Zhong, Lei Liu. RDKG-115: Assisting Drug Repurposing and Discovery for Rare Diseases by Trimodal Knowledge Graph Embedding. *Computers in Biology and Medicine*. 2023 Jul 17.
5. Gang Liu, Zhenhao Liu, Xiaomeng Sun, **Xiaoqiong Xia**, Yunhe Liu, Lei Liu. Pan-Cancer Genome-Wide DNA Methylation Analyses Revealed That Hypermethylation Influences 3D Architecture and Gene Expression Dysregulation in HOXA Locus During Carcinogenesis of Cancers. *Frontiers in cell and developmental biology*. 2021 Mar 18.
6. **Xiaoqiong Xia**, Mengyu Zhou, Hao Yan, Sijia Li, Xianzheng Sha, Yin Wang. Network analysis of aging acceleration reveals systematic properties of 11 types of cancers. *FEBS Open Bio*. 2019 Jul.

## **SKILLS**

- ♦ Familiar with Linux systems, proficient in R, Python, and PyTorch framework to build, train, and test models and GPU acceleration.
- ♦ Familiar with CNN/RNN/Transformer model, GCN/GAT/EGNN model and diffusion model.
- ♦ Proficient in utilizing PyG and DGL Python packages for graph representation.
- ♦ Proficient in PyMOL, MOE, AutoDock, RDKit, and GROMACS for molecular docking and molecular dynamics simulation.
- ♦ Familiar with open-source databases for compound/gene/protein/perturbation expression profiles and omics data analysis processes.
- ♦ Good English reading and writing skills, CET-6:558.
- ♦ Excellent written, communication skills, and collaborative ability.

## **AWARDS**

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| • Academic scholarship, Fudan University                                     | 2020-2023 |
| • Excellent student of “CAS CLUB AI Pharmaceutical Elite Class”              | 2023      |
| • “Huixiang Technology – Kai Si” Outstanding Talent Scholarship              | 2023      |
| • Outstanding student, Fudan University                                      | 2021      |
| • Excellent Student Cadre of Biomedical Research Institute, Fudan University | 2021      |
| • Outstanding Graduate of Liaoning Province                                  | 2019      |
| • National Scholarship   | 2018      |
| • National Encouragement Scholarship   | 2017      |

## **REFERENCES**

- Prof. Lei Liu  
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