YUNPENG XIA

Now in ***Chunfu Xu Lab, National Institute of Biological Sciences, Beijing 102206, China***
Phone: +86 15195870821 *Email: xiayunpeng@nibs.ac.cn* *Interests: AI Assited Drug Discovery*

OBJECTIVE

AI technology has demonstrated some potential and initial applications in biopharmaceuticals. **My vision** is to apply artificial intelligence technologies in drug discovery and screening to achieve a new paradigm in drug discovery. **My current research** focus includes RNA binding sites prediction, RNA-targeting drug disocvery, histone modification, and small molecule binder design with generative AI.

EDUCATION

Nanjing University of Science and Technology — *Jiangsu, China*

M.S. in Software Engineering, School of Computer Science and Technology — *Sep. 2021 – Apr. 2024*

- **Core Courses**: Principles and Methods of Artificial Intelligence (A)、Data Mining (A)、Advanced Engineering Mathematics (A)、Formal Language and Automata (A+)、Pattern recognition technology (A-)
- **Academic Records:** GPA:3.83/4.0 | Ranking: 16/113
- **Honors:** Scholarship of Academic Excellence (Top 20%) in 2021 & 2022 | Third Prize in the 2023 Artificial Intelligence Innovation Competition | Outstanding graduate in 2024.

Nanjing Institute of Technology — *Jiangsu, China*

B.S. in Software Engineering, School of Computer Science and Engineering — *Sep. 2017 – Jun. 2021*

- **Core Courses:** Linear Algebra (A+)、Data Structure (A+)、Compilation Principle (A-)、Linux System (A-)
- **Academic Records**: GPA:3.8/5.0 | Ranking: 6/40
- **Honors:** Scholarship of Academic Excellence (Top 10%) in 2020 | Second Prize in 2020 Programming Competition | Third Prize in 2019 Mathematical Modeling Competition.

RESEARCH EXPERIENCE

NUSTBIO Lab, Nanjing University of Science and Technology — ***Jiangsu, China***

Research assistant, supervised by Prof. Dong-Jun Yu — *Sep 2021 – Aug 2023*

Task: Prediction of N6-methyladenosine modification sites.
Solution and Key Contributions: In applying the attentional mechanism to methylation modification site prediction, it was found that the attentional mechanism has fitness with different features. To solve this problem, we matched different attention mechanisms for different features and converted the search results of Blastn tool into sequence similarity features. By combining this feature with other features, the model's performance is effectively improved.
Relevant Outputs: First author of one paper in **TCBB** (CCF B & SCI Q1); co-authored one paper (**TCBB**)

GENTEL Lab, Shanghai Jiao Tong University — ***Shanghai, China***

Research assistant, supervised by Prof. Shuangjia Zheng — *Aug 2023 – Apr 2024*

Task: Prediction of binding affinity and interaction between small molecules and RNA.
Solution and Key Contributions: We use graph neural network to construct the pairwise interaction map between RNA and small molecules and optimise the predicted interaction by using geometric constraints. Wet experiments have now demonstrated the effectiveness of the model in screening small molecules targeting RNA, and the model has been verified to work well for predicting interaction matrices on available crystal structure data.
Relevant Outputs: First author of one paper (Model's name: GerNA-Bind).

Chunfu Xu Lab, National Institute of Biological Sciences — ***Beijing, China***

Research assistant, supervised by Prof. Chunfu Xu — *Apr 2024 – Present*

Task: Constructing Deep learning algorithms for designing small molecule targeted protein using surface fingerprint information.

PUBLICATIONS

Note: * denotes equal contribution; † denotes corresponding author.

- ***Y Xia**[*]**,** Y Zhang[*], D Liu, Y Zhu, Z Wang, J Song[†], D Yu[†]*. BLAM6A-Merge: Leveraging Attention Mechanisms and Feature Fusion Strategies to Improve the Identification of RNA N6-methyladenosine Sites[J], **IEEE/ACM Transactions on Compute Biology and Bioinfomatics,** *doi: 10.1109/TCBB.2024.3418490*
- *D Liu, Z Liu, **Y Xia**, Z Wang, J Song[†], D Yu[†].* TransC-ac4C: Identification of N4-acetylcytidine (ac4C) sites in mRNA using deep learning[J], **IEEE/ACM Transactions on Compute Biology and Bioinfomatics,** *doi: 10.1109/TCBB.2024.3386972*

SELECTED HONORS

Competition

2019 ***Yunpeng Xia**, Lu Fang, Kanghui Li.* Optimization of a Backpropagation Neural Network Model Using Genetic Algorithm for Valuation of Prospective Listing Companies on the STAR Market, **Mathematical Modeling "May Day Cup".** (2rd Prize)

2022 ***Yunpeng Xia**, Weilong Zhang, Xuanming Chang.* Intelligent Writing Assistant Platform, **The 11th China Software Cup College Student Software Design Competition.** (2rd Prize)

2023 *Keyi Liu, **Yunpeng Xia**, Zhen Guo.* Blood Glucose Prediction Employing Attention Mechanism and Enhanced LSTM Network, **The 5th Huawei Cup China Graduate Artificial Intelligence Innovation Competition.** (2rd Prize)

Copyright of Computer software

2023 *Dong-Jun Yu, **Yunpeng Xia***. N6-methyladenosine modification sites prediction system V1.0.

SKILLS

Programming: Python (Pytorch, TensorFlow, Scikit-learn. etc.), R, C++
Language: Chinese (Native), English (CET-6: 479)

RESEARCH INTERESTS

Tools: Protein Surface Fingerprint, Protein Language Models, Geometric Deep Learning.
Research Area: Drug Discovery and Therapeutics, Small Molecule Binder Design, RNA Binding Sites Prediction.