

Heqin Zhu

Ph.D. @ University of Science and Technology of China zhuheqin1@gmail.com +86 153 5141 6199

[heqin-zhu.github.io](https://github.com/heqin-zhu) [heqin-zhu](https://heqin-zhu.github.io) [Google Scholar](https://scholar.google.com/citations?user=HeqinZhu)

Research Interests

My research centers on AI biology, aiming at understanding biomolecular structures and designing functional molecules, including: **(1) Molecular design and drug discovery**; **(2) Multimodal biological foundation model**; **(3) Structure and function prediction**. Previously, I developed universal models for medical image analysis.

- **Structure and function prediction**: RNA secondary structure prediction: BPfold [I6] (*Nature Communications*), NC-fold [I9] (*ICLR 2026*), IRES identification [I7].
- **Structure-guided RNA foundation model**: structRFM [I8] (*Nature, Accepted*).
- **NA aptamer design**: NACraft [I10].
- **Medical Image Analysis**: Domain adaptation: GU2Net [I1, I2] (*MICCAI 2021, BMEF*), DATR [I4]; Few-shot learning: UOD [I5] (*MICCAI 2023*).

Education

Ph.D.	University of Science and Technology of China (USTC) , Biomedical Engineering	09/2023 – 06/2026
	• Advisor: Prof. Shaohua Kevin Zhou	
M.S.	Institute of Computing Technology (ICT), Chinese Academy of Sciences (CAS) & University of Chinese Academy of Sciences (UCAS) , Computer Science and Technology	09/2020 – 06/2023
	• Advisor: Prof. Shaohua Kevin Zhou	
B.S.	University of Science and Technology of China (USTC) , Computer Science and Technology	09/2016 – 06/2020
	• Hua Xia Talent Program in Computer Science and Technology	

Selected Research Projects

NACraft: Programmatic Nucleic-Acid Aptamer Design via All-Atom Structure-Model Feedback Code	Research Project 08/2026
• Lead developer; designed and implemented a training-free framework for de novo, similarity-guided, and target-selective RNA and DNA aptamer design through backpropagation of structure-model feedback. • Unified binding, sequence-similarity, and anti-binding objectives within a single differentiable optimization framework, followed by NA-MPNN refinement and independent AlphaFold 3 evaluation. • Achieved maximum AF3 ipTM values of 0.63–0.88 across five protein targets; 69.44% of paired candidates favoured EGFR over HER2, and NACraft outperformed ODesign on 10/11 NA-12 targets and 17/20 therapeutic target-length settings.	
structRFM: Fully Open Structure-Guided RNA Foundation Model Paper Code	Nature (Accepted)
• First author; developed the end-to-end pipeline spanning sequence-structure data construction, pre-training objective and model design, downstream adaptation, benchmarking, and open-source release. • Built the pre-training stack on 21 million RNA sequence-structure pairs, combining MUSES multi-source structural annotations with Structure-guided	

Masked Language Modeling (SgMLM) to capture local base-pair contexts while reducing annotation bias.

- Produced sequence-, nucleotide-, and pair-level representations; achieved state-of-the-art results on multiple RNA structure and function benchmarks and ranked among the top four in zero-shot homology classification.

BPfold: Generalizable RNA Structure Prediction with Thermodynamic Priors [Paper](#)
[🔗](#) | [Code](#) [🔗](#)

Nature Communications
07/2025

- **First author**; led the complete method pipeline, including motif-library construction, network architecture design, experimentation, result analysis, and reproducible software release.
- Built the core modeling chain from complete three-neighbor base-pair motif enumeration and de novo tertiary-structure energy estimation to thermodynamic energy maps, **base-pair attention**, and physically constrained contact-map refinement.
- Improved F1 and INF by **approximately 5%** over SPOT-RNA on bpRNA-TS0 and achieved the best **F1 of 0.689** on **10,791 RNAs from unseen families** in Rfam12.3–14.10.

USTC Course Resources [GitHub](#) [🔗](#) (16.2K GitHub stars)

2019 – Present

- **Project lead and maintainer**; led long-term repository maintenance and curation of student-authored course notes, examinations, code, and learning resources for the USTC community.

Selected Publications

I=Representative, J=Journal, C=Conference

denotes co-first author and * denotes co-corresponding author. For full list, please refer to [Google Scholar](#) [🔗](#).

Representative Papers

- [I10] **Heqin Zhu**, Jiaqi Wang, Weibo Zhao, YuZhi Xu, Huang Su, Jianmin Wang, Qinghan Wang, Yuntao Yu, Ziyi You, Gang Du, Pheng Ann Heng*, Liqin Zhang*, and Odin Zhang*. "NACraft: Programmatic nucleic-acid aptamer design via all-atom structure-model feedback" (In submission). [bioRxiv [🔗](#); Code [🔗](#)]
- [I9] **Heqin Zhu**#, Ruifeng Li#, Ao Chang, Mingqian Li, Hongyang Chen*, Peng Xiong*, and S. Kevin Zhou*. "Toward Accurate RNA Non-Canonical Structure Prediction: The NC-Bench Benchmark and the NCfold Framework." (ICLR 2026). [bioRxiv [🔗](#); Code [🔗](#)]
- [I8] **Heqin Zhu**, Ruifeng Li, Feng Zhang, Fenghe Tang, Tong Ye, Xin Li, Yunjie Gu, Peng Xiong*, and S. Kevin Zhou*. "A fully open structure-guided RNA foundation model for robust structural and functional inference." (Nature, Accepted). [bioRxiv [🔗](#); Code [🔗](#)]
- [I7] Feng Zhang#, **Heqin Zhu**#, Jiayin Gao, Jie Hu, Ke Chen, Shaohua Kevin Zhou*, and Peng Xiong*. "IRESeek: structure-informed deep learning method for accurate identification of internal ribosome entry sites in circular RNAs." NAR Genomics and Bioinformatics 7, no. 4 (2025): lqaf210. (NAR Genomics and Bioinformatics). [Paper [🔗](#); Code [🔗](#)]
- [I6] **Heqin Zhu**, Fenghe Tang, Quan Quan, Ke Chen, Peng Xiong*, and S. Kevin Zhou*. "Deep generalizable prediction of RNA secondary structure via base pair motif energy." Nature Communications 16, (2025): 5856. (Nat. Commun., 2025). [Paper [🔗](#); Code [🔗](#)]
- [I5] **Heqin Zhu**, Quan Quan, Qingsong Yao, Zaiyi Liu, and S. Kevin Zhou. "Uod: Universal one-shot detection of anatomical landmarks." In International Conference on Medical Image Computing and Computer-Assisted Intervention, pp. 24-34. Cham: Springer Nature Switzerland, 2023. (MICCAI 2023). [Paper [🔗](#); Code [🔗](#)]
- [I4] **Heqin Zhu**, Qingsong Yao, and S. Kevin Zhou. "Datr: Domain-adaptive transformer for multi-domain landmark detection." arxiv preprint arxiv:2203.06433 (2022). (Preprint). [Paper [🔗](#); Code [🔗](#)]
- [I3] **Heqin Zhu**, Xu Sun, Yuexiang Li, Kai Ma, S. Kevin Zhou*, and Yefeng Zheng*. "DFTR: Depth-supervised fusion transformer for salient object detection." arxiv preprint arxiv:2203.06429 (2022). (Preprint). [Paper [🔗](#); Code [🔗](#)]
- [I2] **Heqin Zhu**, Qingsong Yao, Li Xiao, and S. Kevin Zhou. "Learning to Localize Cross-Anatomy Landmarks in X-Ray Images with a Universal Model." BME Frontiers 2022 (2022): 9765095. (BMEF 2022). [Paper [🔗](#); Code [🔗](#)]
- [I1] **Heqin Zhu**, Qingsong Yao, Li xiao, and S. Kevin Zhou. "You only learn once: Universal anatomical landmark detection." In Medical Image Computing and Computer Assisted Intervention, pp. 85-95. Springer International Publishing, 2021. (MICCAI 2021). [Paper [🔗](#); Code [🔗](#)]

Journal Papers

- [J4] Quan Quan#, Qingsong Yao#, **Heqin Zhu**, and S. Kevin Zhou. "IGU-Aug: Information-guided unsupervised augmentation and pixel-wise contrastive learning for medical image analysis." IEEE Transactions on Medical Imaging (2024). (TMI 2024).
- [J3] Quan Quan#, Qingsong Yao#, **Heqin Zhu**, Qiyuan Wang, and S. Kevin Zhou. "Which images to label for few-shot medical image analysis?." Medical Image Analysis 96 (2024): 103200. (MIA 2024).
- [J2] Huang Zhen#, Han Li#, Shitong Shao, **Heqin Zhu**, Huijie Hu, Zhiwei Cheng, Jianji Wang, and S. Kevin Zhou. "PELE scores: pelvic X-ray landmark detection with pelvis extraction and enhancement." International Journal of Computer Assisted Radiology and Surgery 19, no. 5 (2024): 939-950. (IJCARs 2024).
- [J1] Pengbo Liu, Hu Han, Yuanqi Du, **Heqin Zhu**, Yinhao Li, Feng Gu et al. "Deep learning to segment pelvic bones: large-scale CT datasets and baseline models." International Journal of Computer Assisted Radiology and Surgery 16 (2021): 749-756. (IJCARs 2021).

Conference Papers

- [C4] Fenghe Tang, Chengqi Dong, Wenxin Ma, Zikang Xu, **Heqin Zhu**, Zihang Jiang, Rongsheng Wang, Yuhao Wang, Chenxu Wu, and Shaohua Kevin Zhou. "U-Bench: A Comprehensive Understanding of U-Net through 100-Variant Benchmarking." arXiv preprint arXiv:2510.07041 (2025). (Under review).
- [C3] Xinyi Wang, Zikang Xu, **Heqin Zhu**, Qingsong Yao, Yiyong Sun, and S. Kevin Zhou. "SIX-Net: Spatial-Context Information miX-up for Electrode Landmark Detection." In International Conference on Medical Image Computing and Computer-Assisted Intervention, pp. 338-348. Cham: Springer Nature Switzerland, 2024. (MICCAI 2024).
- [C2] Fenghe Tang, Ronghao Xu, Qingsong Yao, Xueming Fu, Quan Quan, **Heqin Zhu**, Zaiyi Liu, and S. Kevin Zhou. "Hyspark: Hybrid sparse masking for large scale medical image pre-training." In International Conference on Medical Image Computing and Computer-Assisted Intervention, pp. 330-340. Cham: Springer Nature Switzerland, 2024. (MICCAI 2024).
- [C1] Yuanyuan Lyu, Haofu Liao, **Heqin Zhu**, and S. Kevin Zhou. "A 3 DSegNet: anatomy-aware artifact disentanglement and segmentation network for unpaired segmentation, artifact reduction, and modality translation." In International Conference on Information Processing in Medical Imaging, pp. 360-372. Cham: Springer International Publishing, 2021. (IPMI 2021).

Experience

Tencent, JARVIS Lab, Research Intern

Shenzhen, China

- Developed a depth-supervised feature-fusion transformer for salient object detection [13].

07/2021 – 11/2021

Talks and Presentations

Multimodal AI for RNA modeling and foundation model

PDF 

06/15/2026, virtual, MSD R&D China Innovation Collaboration Center (MCICC)

12/2025, Suzhou, China, USTC Course on Digital Healthcare Technology and Applications

Structure-guided RNA foundation model for structure and function prediction

PDF 

06/13/2026, Hefei, China, The 7th USTC Academic Forum for Engineering Graduate Students & the "Dechuang ǔ Jingjian Innovation" Doctoral Academic Forum.

- Outstanding Academic Presentation Award, 1st of 10

Deep generalizable prediction of RNA secondary structure via base pair motif energy

PDF 

05/2025, Changchun, China, The 3rd National Conference on Biomolecular Structure Prediction and Simulation

- Outstanding Academic Presentation Award, 2nd of 12

Research Mentorship

Ao Chang, Ph.D. Student: Motif-informed RNA language pre-training using Mamba

2025 – 2026

Haobin Chen, M.S. Student: LLM-based agents for retrieving lncRNA knowledge from the literature

2025 – 2026

Duofan Tu, M.S. Student: Medical agents for clinical diagnosis

2024 – 2026

Feng Zhang, M.S. Student: IRES identification in circular RNAs

2024 – 2026

- IRESeek: a structure-informed deep learning method for accurate identification of internal ribosome entry sites in circular RNAs

Xiaoqian Zhou, M.S. Student: Anatomical landmark detection in medical images

2022 – 2024

- Hybrid attention network: an efficient approach for anatomy-free landmark detection

Zhen Huang, M.S. Student: Anatomical landmark detection in X-ray images

2021 – 2023

- **Pele Scores:** pelvic X-ray landmark detection with pelvis extraction and enhancement

Teaching Experience

- Open Practice in Electronic Information, USTC, 2023
- Biomolecular Structure Modeling, USTC, 2024

Academic Service

- **Academic Reviewer:** Neurips, MICCAI, TCSVT
- **Volunteer Activities**
 - Medical Augmented Reality Summer School (Suzhou, 2024)
 - Dushu Lake Symposium on Medical Image Computing (Suzhou, 2023)

Honors and Awards

President's Excellent Award , Chinese Academy of Sciences	2026
Provincial Outstanding Graduate (Ph.D., Class of 2026) , Anhui Province	2026
Outstanding Graduate (Ph.D., Class of 2026), USTC	2026
Outstanding Academic Presentation Award (1st of 10), The 7th USTC Academic Forum for Engineering Graduate Students	2026
National Scholarship for Doctoral Students , Ministry of Education of China	2025
Second Prize for Oral Presentation, The 3rd National Conference on Biomolecular Structure Prediction and Simulation	2025
Suzhou Industrial Park Scholarship, USTC	2025
Merit Student Award, UCAS & ICT	2023
Graduate Academic Scholarship, UCAS & ICT and USTC	2020 – 2025
Outstanding Student Award, USTC	2018 – 2019
Institute of Chemistry Excellence Scholarship, USTC	2017

Technical Skills

Methods: Foundation models, multimodal learning, large language models, diffusion models

Programming & Tools: Python, PyTorch, C++, Git, $\LaTeX$, Matplotlib

References

S. Kevin Zhou, Professor, University of Science and Technology of China

skevinzhou@ustc.edu.cn

Peng Xiong, Professor, University of Science and Technology of China

xiongxp@ustc.edu.cn

Wanxiang Shen, Professor, Zhejiang University

shenwx25@zju.edu.cn