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EDUCATION

The Scripps Research Institute <i>Ph.D. Program</i> Advisor: Prof. Stefano Forli; Current Focus: AI for Drug Discovery Recipient of the Kellogg Fellowship , funded by the Kellogg Family and the ALSAM Foundation	San Diego, California, US <i>Aug 2025 - May 2029</i>
University of Illinois Urbana-Champaign (UIUC) <i>M.S. in Information Sciences</i> Course: ML for Bioinformatics, Text Information Systems, Large Language Models, Data Mining	Illinois, US <i>Aug 2023 - May 2025</i>
Peking University (PKU) <i>B.Econ. in Economics Minor</i> Course: Statistics, Applied Econometrics, Causal Inference Models	Beijing, China <i>Sep 2021 - Jul 2023</i>
Beijing Normal University (BNU) <i>B.S. in Computer Science and Education</i> Course: Data Structure, Database, WebDev, OOP, Information Retrieval, Intelligent System, Data Mining	Beijing, China <i>Sep 2017 - Jul 2021</i>

PUBLICATIONS

Google Scholar: <https://scholar.google.com/citations?hl=en&user=pXY2xYkAAAAJ>

[Ongoing] Jian, J., ..., & Chen, Q. The AI Scientist in Health: Potential, Challenges, and the Road Ahead.

[BPS'26] Torres-Paris, C., ..., Jian, J., Holcomb, M., Forli, S., & Racki, L.R. Allosterically inhibiting *Pseudomonas aeruginosa*'s polyphosphate kinase 2A by disrupting its oligomerization. *Biophysical Society Annual Meeting (2026)*. Jian

[ACL'26 Submitted] Wang, Q., ..., Jian, J., Guo, X., & Li, R. Human-AI Co-Discovery. *in submission*

[Published] Hou, R., Zhou, D., & **Jian, J.** GeoCM: Exploring Consistency Models and EGNNS for Molecular 3D Structure Prediction. *UIUC Machine Learning for Bioinformatics Workshop* (2024).

[AIED'24] Xiao, Y. & **Jian, J.** Which Animal Would You Like to See on Your Flashcards? Designing Visual Aids Together with Kids Using GIMs. *The 25th International Conference on Artificial Intelligence in Education*.

RESEARCH EXPERIENCE

[TechRxiv'25] Exploring Agentic Multimodal Large Language Models: *June 2025 – Nov 2025*
A Survey for AIScientists

Advisor: Prof. Qingyu Chen (Yale), Prof. Zhiyong Lu (NIH), Prof. Qingyun Wang (William & Mary)

- Lead author of a survey framing AIScientists from a machine learning centric and agentic multimodal LLM perspective.

[arXiv'24] GeoCM: Exploring Consistency Models and EGNNS for *Oct 2024 – Present*
Molecular 3D Structure Prediction

Advisor: Prof. Ge Liu (UIUC)

- Utilized **Equivariant Graph Neural Networks (EGNN)** and **Consistency Models (CM)** to train a self-supervised model to predict molecular 3D structures.
- Established two metrics **Coverage Rate** and **Matching Error** to compare GeoCM models against other models, demonstrating GeoCM claimed a new **SOTA**.

[Big Data'24] Fast and Accurate Drug Discovery Framework *Jan 2024 – Oct 2024*

Advisor: Prof. Yang Zhang (UIUC) and Dr. Jin Chen (Cleveland Clinic)

- Developed an enhanced parallel **Monte Carlo Tree Search** framework, considering aptamers' high-affinity and specificity for target proteins, achieving **98-fold** computational efficiency and **7.59-fold** improved sequence quality.

[arXiv'24] Team of AI-made Scientists (TAIS) *Aug 2023 – Feb 2024*

Advisor: Prof. Haohan Wang (UIUC)

- ML can discover disease-predictive genes from gene expression data. We introduced **TAIS**, a LLM-based framework for automatic streamlining ML analysis, outperforming **GPT4/MetaGPT/AutoGPT**.
- Fetched data from the **GEO/TAGC** database. Created the **GenoTEX**, a NEW benchmark for evaluating the exploration of genomics data, with aligning gene symbols, logging, and statistical corrections.
- Created several **agents** as scientists, via autonomously creating codes (**template-based prompting**), execution (**subprocess**), outputs/errors capture (**logger**), and built communication within (**Data Engineer, Code Reviewer, and Domain Expert agents**).

[Bachelor's Thesis] Semi-automatic Knowledge Graph Construction *Sep 2020 - Jul 2021*

Advisor: Prof. Qinhua Zheng (BNU)

- Developed a **semi-automatic** ML paradigm for **knowledge graph creation** for addressing time-consuming issues by combining **supervised ML** with **human-in-the-loop** incorporation.
- Developed a benchmark dataset for educational entities by annotating transcriptions using BIO tagging.
- Iterated a supervised **BiLSTM-CRF** model for **entity recognition** and dynamic term re-ranking (**mutual information and human feedback**), improving F1-score (0.54 → **0.76**).

PROFESSIONAL EXPERIENCE

Software Developer Intern *May 2024 – Aug 2024*

Supervisor: David Bachtler and Ian Cowen, ReDirect

- Engineered subscription functionality using Flutter framework and implemented unit testing.

Teaching Assistant, IS 589 Independent Study *Aug 2023 – Dec 2023*

Supervisor: Prof. Haohan Wang, University of Illinois Urbana-Champaign

- Developed and published a comprehensive ML tutorial, the “Gold-Standard-Pipeline-Guide”, teaching students to analyze gene expression data for disease-related gene discovery. [GitHub]
- The resource has been forked by 9 students who applied it to their own research projects.

Research Assistant

Supervisor: Prof. Mackenzie Alston, University of Illinois Urbana-Champaign

Aug 2023 – Aug 2024

– Conducted literature review (randomized controlled trials) using Zotero and scraped 2000+ emails.
Head on Online Learning Department & Teacher Volunteer *May 2019 – Aug 2022*

China Starry Night (NGO) [Web]

- Designed online educational videos to help intangible cultural heritage artisans in rural regions share traditional crafts, enabling younger generations to preserve cultural treasures.
- Courses published on Bilibili (China's leading video platform) garnered 10,000+ views.
- Presented at the 5th China Education Innovation Expo (National Award - Top 1%).

SELECTED PROJECTS

- **Demo of ChemTutor: AI Q&A system with Chemistry Textbooks** [[Code](#)] *2024*
#LLM #Q&A system #RAG #LangChain
- **HMM-DRL Model for Data-driven Auto-Trading** [[Paper](#)] *2022*
#Reinforcement Learning #Hidden Markov Model #Time Series Data #Financial Index
- **Evolution of Key Themes in Learning Sciences** [[Web](#)] *2020*
#Text Mining #LDA-Topic Model #TF-IDF #Data Visualization

HONORS AND AWARDS

- **Kellogg Fellowship**, The Scripps Research Institute *Aug 2025 – Aug 2028*
- **National Innovation and Entrepreneurship Training Award (1%)**, Ministry of Education *2021*
- **Outstanding Teaching Practice (1%)**, Beijing Normal University *2021*
- **Jianghaiziqiang Fellowship (1%)**, Beijing Normal University *2020*
- **First-class Scholarship for Competition Excellence (1%)**, Beijing Normal University *2019*
- **First-class Scholarship for Academic Excellence (10%)**, Beijing Normal University *2017 - 2021*

SKILL SET

Machine Learning & NLP	TensorFlow, PyTorch, LangGraph, LangChain, sklearn, NLTK
Programming Language	Python, Java, C, JavaScript, HTML, Stata
Framework & Database	React, Node.js, RESTful API, MySQL, MongoDB, Neo4j
Cloud	AWS, EC2, API Gateway
Code Management & Others	Git/Github, Docker, Tableau, Unit Testing, L ^A T _E X