Jiaming Hu

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Miami, FL - 33155, United States

Reseach Interests

AI-driven Drug Discovery • Computational Chemistry • Machine Learning • Deep Learning • Generative AI • Multimodal and Multi-omics Studies • Precision Oncology • Cheminformatics • Bioinformatics • Molecular Modeling

Research Experience

University of Miami Miller School of Medicine *Aug 2020 - Dec 2025*
Graduate Researcher | *Advisor: Stephan C. Schürer, Ph.D.* Miami, FL

- Develop machine learning and deep learning models for predictive and generative modeling in drug discovery and precision oncology
- Conduct large-scale multi-omics and multimodal biomedical data to study drug-target interactions and cellular responses
- Support the development of cloud-based research data platform for large-scale data management and analysis
- Collaborate with cross-functional teams to validate computational predictions and present findings through peer-reviewed publications and scientific conferences

Nucleate FL *Oct 2024 - Jun 2025*
Computational Scientist Miami, FL

- Developed machine learning models and applied molecular modeling tools in a collaborative biotech research environment
- Led large-scale data-driven projects, integrating computational methods and cross-disciplinary efforts to drive innovation and translational research

University of Miami *Jan 2019 - Jan 2021*
Undergraduate Researcher | *Advisor: Grace R. Zhai, Ph.D.* Miami, FL

- Conducted laboratory experiments using *Drosophila melanogaster* to assess toxin-induced changes in brain health and neurological function
- Collaborated with cross-functional teams to investigate the biological effects of environmental toxins and their potential link to neurodegenrative diseases.

Education

University of Miami *Dec 2025*
Ph.D. in Human Genetics and Genomics | *Advisor: Stephan C. Schürer, Ph.D.* Miami, FL

- Dissertation: Multimodal Data-Driven Computational Models for Kinase Inhibitor Discovery and Cellular Drug Response Prediction

University of Miami *May 2020*
B.S. in Marine Biology Miami, FL

Projects

- **Project A: Sylvester Data Portal - Cloud-based Multi-Omics Research Platform** *2024-Ongoing*
  Tools: Python, R, KNIME, Pipeline Pilot, RDKit, TileDB
  - Co-develope a cloud-based platform for secure storing, managing, and analyzing large-scale multi-omics data, accelerating cross-team collaboration and data accessibility.
  - Enable integration of diverse transcriptomic, proteomic, and drug response datasets to support real-time computational modeling and discovery workflows.
  - Facilitated reproducible data management practices and transparent research dissemination across internal and external collaborators.
- **Project B: AI-Powered Platform for Kinome-Wide Virtual Screening in Precision Oncology** *2024-2025*
  Tools: Python, Docker, Azure, GCP, Schrödinger Maestro, AlphaFold, ChemAxon, InfiniSee, RDKit
  - Developed the KNet platform for kinome-wide virtual screening and prediction of kinase binding affinities, enabling rapid prioritization of active compounds.
  - Applied structure-based modeling and molecular simulations to uncover binding modes and conformational dynamics of understudied kinases.

- Collaborated with experimental teams to design and implement *in vitro* binding assays, establishing an iterative computational-experimental loop that improved prediction accuracy and accelerated hit-to-lead optimization.
- Github Repository:
  KNet: A Web-Based Deep Learning Platform for Kinome-Wide Virtual Screening

- **Project C: Pan-Cancer Multimodal Models for Drug Sensitivity Prediction** *2023-2024*
  Tools: Python, R, Tensorflow, KNIME, Machine Learning, Deep Learning, RDKit
  - Constructed multimodal models integrating molecular fingerprints, transciptional consensus signatures, and multi-omics features to predict cellular drug sensitivity across cancer-types.
  - Developed scalable, automated pipelines for high-throughput model training, evaluation, and reproducibility.
  - Generated pan-cancer predictive insights linking compound response patterns to transcriptomic and proteomic profiles, advancing precision oncology research
  - Github Repository:
    Pan-Cancer Drug SensitivitySeq

- **Project D: Kinome-Wide Deep Learning Framework for Biochemical Activity Prediction** *2022 - 2024*
  Tools: Python, Pytorch, Tensorflow, SQL, Machine Learning, Deep Learning, DeepChem, Scikit-learn
  - Developed a multi-task deep learning framework to predict ligand-target biochemical activity across the kinome, enabling large-scale virtual screening and mechanism-of-action analysis
  - Integrated diverse chemical and structural data sources to build a unified foundation for structure-based drug discovery and model generalization across novel chemotypes.
  - Enhanced biomedical ontologies (BAO, DTO) to support standarized data integration and interoperable modeling pipelines for predictive toxicology and pharmacology.
  - Github Repository:
    Kinome-wide-Virtual-Screening-by-Multi-task-Deep-Learning

Publications and Preprints

P=Published, S=In Submission, C=Conference, T=Thesis

[T.1] **Hu J.** (2025). Multimodal Data-Driven Computational Models for Kinase Inhibitor Discovery and Cellular Drug Response Prediction. PhD Thesis, University of Miami.

[S.1] **Hu, J.**, Rupprecht, L., Schürer, S.C. (2025). KNet: A Web Application for Kinome-Wide Small Molecules Drug Discovery in Cancer. Manuscript under review for publication in *iScience*. Preprint available at SSRN eLibrary

[S.2] Glenny-Pescov, J., Chung, C., Ross, N., **Hu, J.**, Sinclair, M., Khurshid, R., Karlsson, A., Schürer, S.C. (2025). Advancing the BioAssay Ontology through Integrated PK/PD and Safety Pharmacology Representation. Manuscript under review for publication in *Journal of Biomedical Semantics*.

[S.3] Ocasio, B.A., **Hu, J.**, Stathias, V., Martinez, M.J., Burnstein, K.L., Schürer S.C. (2024). Pan-Cancer Drug Sensitivity Prediction from Gene Expression using Deep Learning. Prepare for submission. Preprint available at bioRxiv

[C.1] Ocasio, B.A., **Hu, J.**, Stathias, V., Martinez, M.J., Burnstein, K.L., Schürer S.C. (2024). Pre-clinical pan-cancer drug repurposing via deep learning. Abstract presented at the European Society for Medical Oncology (ESMO) Congress, published in ESMO Open. [Impact Factor: 8.3]

[P.1] **Hu, J.**, Allen, B.K., Stathias, V., Ayad, N.G., Schürer, S.C. (2024). **Kinome-Wide Virtual Screening by Multi-Task Deep Learning.** International Journal of Molecular Sciences. 25(5):2538. https://doi.org/10.3390/ijms25052538 [Impact Factor: 4.9]

[P.2] Khurshid, R., Schulz, J. M., **Hu, J.**, Snowden, T. S., Reynolds, R. C., Schürer, S. C. (2024). **Targeted degrader technologies as prospective SARS-CoV-2 therapies.** Drug discovery today, 29(1), 103847. https://doi.org/10.1016/j.drudis.2023.103847 [Impact Factor: 7.5]

[P.3] **Hu, J.**, Liu, J., Zhu, Y., Diaz-Perez, Z., Sheridan, M., Royer, H., Leibensperger, R., 3rd, Maizel, D., Brand, L., Popendorf, K. J., Gaston, C. J., Zhai, R. G. (2020). **Exposure to Aerosolized Algal Toxins in South Florida Increases Short- and Long-Term Health Risk in Drosophila Model of Aging.** Toxins, 12(12), 787. https://doi.org/10.3390/toxins12120787 [Impact Factor: 4.0]

Presentations and Posters

O=Oral, P=Poster

[P.1] Kinome-Wide Virtual Screening by Multi-task Deep Learning for Small Molecule Drug Discovery in Cancer. 24th Annual Zubrod Memorial Lecture and Cancer Research. May 2025. Poster

[P.2] Kinome-Wide Virtual Screening by Multi-task Deep Learning for Small Molecule Drug Discovery in Cancer. Drug Discovery Chemistry. Apr 2025. Poster

[O.1] Pre-clinical pan-cancer drug repurposing via deep learning. Molecular Analysis for Precision Oncology Congress (MAP). Oct 2024. Oral Presentation.

[P.3] Predict and Prioritize Small Molecule Inhibitors against PNCK using Kinome-wide Multi-task Deep Neural Network Classifiers. Inaugural Computing Day Poster Presentation. Apr 2023. Poster

[O.2] Structural-based Molecular Simulation and Machine Learning Studies to Identify Inhibitors Against SARS-CoV-2 Papain-like Protease (PLpro). 22nd Annual Zubrod Memorial Lecture and 3-minute Virtual Cancer Research Trainee Talks. Oral Presentation.

[P.4] Exposure to Aerosolized Microcystin of Harmful Algal Blooms in Lake Okeechobee Poses Negative Impact on Health in a Drosophila Model of Aging. Summer Undergraduate Research Fellowship (SURF) Symposium. Aug 2019. Poster.

Teaching Experience

Teaching Assistant – HGG630 Variation and Disease *Spring 2024*
University of Miami Miller School of Medicine | Professor: Holly N. Cukier, Ph.D. Miami, FL

Tutor – Camner Center for Academic Resources *Sep 2019 – Mar 2020*
University of Miami Coral Gables, FL

Clinical Training

Human Genetics Clinical Rotation *Fall 2023*
University of Miami Miller School of Medicine Miami, FL

Skills

- **Programming:** Python, R, SQL, Git, Bash, Docker
- **Computing Environments:** Linux/Unix systems, HPC clusters, shell scripting, command-line tools
- **ML/DL:** Machine learning, Deep learning, Generative AI, Tensorflow, PyTorch, DeepChem, Scikit-learn
- **Computational Biology/Chemistry Tools** Schrödinger Maestro Suite - Molecular Docking, Molecular Dynamics Simulation, AlphaFold, PyMOL, ChemAxon, InstantJchem, BioSolveIT InfiniSee, RDKit
- **Data Analysis:** KNIME, Pipeline Pilot, Statistical Analysis
- **Data Visualization:** Tableau, Spotfire, Matplotlib, Seaborn
- **Cloud Computing:** Microsoft Azure, Google Cloud Platform

Honors and Awards

- **Award of Academic Merit** *Dec 2025*
  University of Miami
- **Graduate Student Travel Award** *April 2025*
  University of Miami
- **U-LINK fellowship** *2019-2021*
  University of Miami
- **Provost's Honor Roll** *Spring 2018, Fall 2019*
  University of Miami
- **Dean's List** *Spring 2018, Spring 2019, Fall 2019*
  University of Miami
- **National Honor Society** *2016*

Professional Memberships

- **American Association for Cancer Research (AACR)**
- **Sylvester Comprehensive Cancer Center Trainee Member (SCCC)**

Certifications

Academy Accreditation – Generative AI Fundamentals *Issued Jan 2025 · Expires Jan 2027*
Databricks
Azure Certification *Issued Jul 2024*
Great Learning

Additional Information

Languages: English (Full professional proficiency), Mandarin (Native)
Soft Skills: Teamwork, Collaboration, Problem-solving, Time-management, Multi-tasking, Communication, and Presentation skills
Interests: Hiking, Tennis, Art museums, Films, Travel

REFERENCES

1. **Stephan C. Schürer**
   Professor of Molecular and Cellular Pharmacology
   Director of Digital Drug Discovery, Institute for Data Science & Computing
   Associate Director of Data Science, Sylvester Comprehensive Cancer Center
   University of Miami Miller School of Medicine
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2. **Vasileios Stathias**
   Assistant Director of Data Science, Sylvester Comprehensive Cancer Center
   University of Miami
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