Yuhui Hong

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Yuhui Hong
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Education

Indiana University Bloomington — Bloomington, IN, US
Ph.D. in Computer Science — Sep. 2020 –Jul. 2025

Xidian University — Xi'an, Shaanxi, China
B.S. in Computer Science and Technology — Sep. 2015–Jul. 2019

Research Interests

My research develops deep learning methods for computational biology and chemistry, focusing on mass spectrometry and chromatography applications in metabolomics and proteomics. I create both high-performance predictive models and interpretable AI approaches that provide mechanistic insights for scientific discovery.

Research Experience

University of Washington — Seattle, WA, US
Postdoc Scholar — Aug. 2025 –Present
Advisor: Professor William Stafford Noble
Area: Computational biology, Deep Learning, Proteomics mass spectrometry

Indiana University Bloomington — Bloomington, IN, US
Research Assistant — Aug. 2021 –Jul. 2025
Advisor: Professor Haixu Tang
Area: Computational biology, Deep Learning, Small molecular mass spectrometry

The First Affiliated Hospital of Nanchang University — Nanchang, Jiangxi, China
Research Intern — May 2021 –Jul. 2021
Advisor: Professor Sujun Li
Area: MHC (Major Histocompatibility Complex) binding prediction

Xi'an Jiaotong University — Xi'an, Shaanxi, China
Research Assistant — Sep. 2019 –Jul. 2020
Advisor: Associate Professor Yaochen Li
Area: Computer vision, Object tracking and segmentation in traffic scene

Publications

The deep learning models, 3DMolMS for retention time and collision-cross section [7], 3DMolCSP for enantioselectivity [5], and FIDDLE for chemical formula identification [3] have been evaluated on internal data and positively considered for application by biotech, pharmaceutical, and agricultural leaders, including **AbbVie**, **Agilent**, **Amgen**, **Merck**, and **Corteva**.

Books & Patents

1 Qingyang Xiao, Kaiyuan Liu, **Yuhui Hong** & Haixu Tang (2024). "Neural Networks for Chemists." *American Chemical Society*, DOI:10.1021/acsinfocus.7e8012. [Primer]

2 Haixu Tang, **Yuhui Hong**, & Sujun Li. "Method of predicting ms/ms spectra and properties of chemical compounds." US Patent No. WO2023239720A1, June 6, 2023.

Peer-Reviewed Articles (First Author)

**equal contribution as co-first authors*

3 **Yuhui Hong**, Sujun Li, Yuzhen Ye, & Haixu Tang (2025). "FIDDLE: a deep learning method for chemical formulas prediction from tandem mass spectra." *Nature Communications*, 16(1), 11102. [Paper] [Code] [PyPI package]

4 **Yuhui Hong**, Yuzhen Ye & Haixu Tang (2025). "Machine Learning in Small-Molecule Mass Spectrometry." *Annual Review of Analytical Chemistry*, 18. [Paper]

5 **Yuhui Hong**, Christopher J Welch, Patrick Piras, & Haixu Tang (2024). "Enhanced Structure-Based Prediction of Chiral Stationary Phases for Chromatographic Enantioseparation from 3D Molecular Conformations." *Analytical Chemistry*, 96(6), 2351-2359. [Paper] [Code]

6 **Yuhui Hong***, Mahsa Monshizadeh*, & Yuzhen Ye (2024). "Multitask Knowledge-primed Neural Network for Predicting Missing Metadata and Host Phenotype based on Human Microbiome." *Bioinformatics Advances*, vbae203. [Paper] [Code]

7 **Yuhui Hong**, Sujun Li, Christopher J Welch, Shane Tichy, Yuzhen Ye, & Haixu Tang (2023). "3DMolMS: Prediction of Tandem Mass Spectra from Three Dimensional Molecular Conformations." *Bioinformatics*, btad354. [Paper] [Code] [PyPI package] [Service on Konia]

Peer-Reviewed Articles (Collaborative Author)

8 Ludwig Lautenbacher, Kevin L. Yang, Tobias Kockmann, Christian Panse, Wassim Gabriel, Dulguun Bold, Elias Kahl, Matthew Chambers, Brendan X. MacLean, Kai Li, Fengchao Yu, Brian C. Searle, Wilburn, Damien, Mohammad Reza Zare Shahneh, **Yuhui Hong**, Haixu Tang, Mingxun Wang, Ralf Gabriels, Robbin Bouwmeester, Robbe Devreese, Tobias K. Schmidt, Alexey I. Nesvizhskii, & Mathias Wilhelm (2025). "Koina: Democratizing machine learning for proteomics research." *Nature Communications*, 16(1), 9933. [Paper] [Website] [Code]

9 Yaochen Li, **Yuhui Hong**, Yonghong Song, Chao Zhu, Ying Zhang, & Ruihao Wang (2022). "SiamPolar: Semi-supervised Realtime Video Object Segmentation with Polar Representation." *Neurocomputing*, 467, 491-503. [Paper] [Code]

10 Yaochen Li, Chao Zhu, Yuehu Liu, **Yuhui Hong**, & Jianji Wang (2021). "Geometric and Semantic Analysis of Road Image Sequences for Traffic Scene Construction." *Neurocomputing*, 465, 336-349. [Paper] [Code]

Ongoing Articles

11 **Yuhui Hong**, & Haixu Tang (2025). "A Task-Specific Transfer Learning Approach to Enhancing Small Molecule Retention Time Prediction with Limited Data." (Under review). [Preprint] [Code]

12 **Yuhui Hong***, Mahsa Monshizadeh*, & Yuzhen Ye (2025). "Confounder Free Predictive Models for Microbiome-based Host Phenotype Prediction." (Under review). [Preprint] [Code]

Teaching Experience

Course Designer — Indiana University Bloomington
DSCI-D590, AI on Ramp — From Fall 2025 onward

Instructor — Indiana University Bloomington
DSCI-D590, Topics in Data Science — Spring 2025

Instructor — Indiana University Bloomington
INFO-I529, Machine Learning Bioinformatics — Fall 2024

Assistant Instructor — Indiana University Bloomington
DSCI-D351, Big Data Analytics — Aug.-Sep. 2024
Instructor: Prof. Haixu Tang

Conference Presentations

1 **Oral Presentation** "A Task-Specific Transfer Learning Approach to Enhancing Small Molecule Retention Time Prediction with Limited Data" [Slides]
73rd Conference on Mass Spectrometry and Allied Topics. Jun. 1 - 5, 2025. Baltimore, MD.

2 **Poster presentation.** "Predicting Compositional Fragments of Compounds from Their Tandem Mass Spectra Using Deep Neural Networks" [Poster]
72nd Conference on Mass Spectrometry and Allied Topics. Jun. 2 - 6, 2024. Anaheim, CA.

3 **Poster presentation.** "3DMolMS: Prediction of Tandem Mass Spectra from 3D Molecular Conformations"
Turkey Run Analytical Chemistry Conference 2023. Sep. 29 - 30, 2023. Marshall, IN.

4 **Oral Presentation** "A Machine Learning Model for Chemical Formula Prediction Using Tandem Mass Spectra of Compounds" [Slides]
71st Conference on Mass Spectrometry and Allied Topics. Jun. 4 - 8, 2023. Houston, TX.

5 **Poster Presentation** "Prediction of Molecular Tandem Mass Spectra Using 3-Dimensional Conformers" [Poster]
70th Conference on Mass Spectrometry and Allied Topics. Jun. 5 - 9, 2022. Minneapolis, MN.

Scholarships and Awards

- **UW Data Science Fellow at the eScience Institute** 2025
  University of Washington
  Awarded $1,000 fellowship for mass spectra data analysis
- **Luddy Outstanding Research Award** 2025
  Indiana University Bloomington
  Sole recipient university-wide for outstanding research contributions
- **Special Academic Scholarship** 2019
  Xi'an Jiao Tong University
- **Meritorious Winner of MCM (Mathematical Contest In Modeling)** 2018
  Consortium for Mathematics and Its Application (COMAP)
  Top 10% internationally (ranked among 8,085 participating teams)

Professional Services

- **Reviewer**: (conferences) KDD AI4Science Track 2026, ACM BCB 2025; (journals) Journal of Chromatography A, BMC Genomics, BMC Bioinformatics, IEEE Transactions on Computational Biology and Bioinformatics, PeerJ Computer Science, Pharmaceutical Research, Beilstein Journal of Organic Chemistry, Chemical Physics Letters.
- **Sub-reviewer**: (conferences) RECOMB 2026 2025 2023 2022, ISMB/ECCB 2025 2023, ACM BCB 2024; (journals) Analytical Chemistry, International Journal of Mass Spectrometry.
  assisted in reviewing papers under the guidance of Professor William Noble and Professor Haixu Tang

Professional Affiliations

- American Society for Mass Spectrometry (ASMS), Member. 2022 - Present
- NSF Center for Bioanalytic Metrology (CBM), Student. 2022 - 2025

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