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 Experience

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

Indiana University Bloomington — Bloomington, IN, US
Research Assistant — Aug. 2021 –Jul. 2025
Advisor: Prof. 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: Prof. Sujun Li
Area: MHC (Major Histocompatibility Complex) binding prediction

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

Teaching Experience

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

Scholarships and Awards

- **UW Data Science Fellow at the eScience Institute** — 2025
  University of Washington
- **Luddy Outstanding Research Award** — 2025
  Indiana University Bloomington
- **Special Academic Scholarship** — 2019
  (Top 20%) Xi'an Jiao Tong University

- **Second-tier Scholarship** 2018
  (Top 10%) Xidian University
- **Meritorious Winner of MCM (Mathematical Contest In Modeling)** 2018
  (Top 10% in the 8085 teams) Consortium for Mathematics and Its Application (COMAP)

Publications

The deep learning models, 3DMolMS for retention time and collision-cross section [7] and 3DMolCSP for enantioselectivity [5], have been evaluated on internal data and positively considered for application by biotech, pharmaceutical, and agricultural leaders, including **Agilent**, **Merck**, **AbbVie**, 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**, Yuzhen Ye & Haixu Tang (2025). "Machine Learning in Small-Molecule Mass Spectrometry." *Annual Review of Analytical Chemistry*, 18. [Paper]

4 **Yuhui Hong**, Sujun Li, Yuzhen Ye, & Haixu Tang (2024). "FIDDLE: a deep learning method for chemical formulas prediction from tandem mass spectra." *bioRxiv*, 2024-11. *accepted by Nature Communications*.
[Preprint] [Code] [PyPI package]

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 Mahsa Monshizadeh*, **Yuhui Hong***, & 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 (2024). "Koina: Democratizing machine learning for proteomics research." *Nature Communications*, 16(1), 9933. [Website] [Code]

9 Yifan Zhang, **Yuhui Hong**, & Luyi Xing (2024). "Resurfacing Vulnerabilities: An Empirical Study on the Reemergence of Previously Patched Security Issues in App-in-App Ecosystems." In *Proceedings of the ACM Workshop on Secure and Trustworthy Superapps*, pp. 23-26. 2024.

10 Yifan Zhang, Zhaojie Hu, Xueqiang Wang, **Yuhui Hong**, Yuhong Nan, XiaoFeng Wang, Jiatao Cheng & Luyi Xing (2024). "Navigating the Privacy Compliance Maze: Understanding Risks with Privacy-Configurable Mobile SDKs." In *33rd USENIX Security Symposium*, pp. 6543-6560. [Paper]

11 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]

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

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.

Professional Services

- **Reviewer**: (conferences) 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, ISMB/ECCB 2025, RECOMB 2025, ACM BCB 2024, ISMB/ECCB 2023, RECOMB 2023, RECOMB 2022; (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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