

Yuhui Hong

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 Yuhui Hong
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Education

Indiana University Bloomington

Ph.D. in Computer Science

Bloomington, IN, US
Sep. 2020 –Jul. 2025

Xidian University

B.S. in Computer Science and Technology

Xi'an, Shaanxi, China
Sep. 2015–Jul. 2019

Research Experience

University of Washington

Postdoc Scholar

Seattle, WA, US
Aug. 2025 –Present

Advisor: Professor William Stafford Noble

Area: Computational biology, Deep Learning, Proteomics mass spectrometry

Indiana University Bloomington

Research Assistant

Bloomington, IN, US
Aug. 2021 –Jul. 2025

Advisor: Professor Haixu Tang

Area: Computational biology, Deep Learning, Small molecular mass spectrometry

The First Affiliated Hospital of Nanchang University

Research Intern

Nanchang, Jiangxi, China
May 2021 –Jul. 2021

Advisor: Professor Sujun Li

Area: MHC (Major Histocompatibility Complex) binding prediction

Xi'an Jiaotong University

Research Assistant

Xi'an, Shaanxi, China
Sep. 2019 –Jul. 2020

Advisor: Associate Professor Yaochen Li

Area: Computer vision, Object tracking and segmentation in traffic scene

Teaching Experience

Course Designer

DSCI-D590, AI on Ramp

Indiana University Bloomington
From Fall 2025 onward

Instructor

DSCI-D590, Topics in Data Science

Indiana University Bloomington
Spring 2025

Instructor

INFO-1529, Machine Learning Bioinformatics

Indiana University Bloomington
Fall 2024

Assistant Instructor

DSCI-D351, Big Data Analytics

Instructor: Prof. Haixu Tang

Indiana University Bloomington
Aug.-Sep. 2024

Scholarships and Awards

- **UW Data Science Fellow at the eScience Institute**

University of Washington

2025

• Luddy Outstanding Research Award Indiana University Bloomington	2025
• Special Academic Scholarship (Top 20%) Xi'an Jiao Tong University	2019
• Second-tier Scholarship (Top 10%) Xidian University	2018
• Meritorious Winner of MCM (Mathematical Contest In Modeling) (Top 10% in the 8085 teams) Consortium for Mathematics and Its Application (COMAP)	2018

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**, 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 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

- 13 **Yuhui Hong**, & Haixu Tang (2025). "A Task-Specific Transfer Learning Approach to Enhancing Small Molecule Retention Time Prediction with Limited Data." (Under review). [\[Preprint\]](#) [\[Code\]](#)
- 14 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 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

Last updated: December 28, 2025