Curriculum Vitae

HUAXU YU

Postdoctoral Research Fellow, Prof. Oliver Fiehn's Lab, Genome Center, University of California, Davis
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EDUCATION

2023-present **Postdoctoral Scholar**
Genome Center, University of California Davis, Davis, CA, United States
Research Supervisor: Prof. Oliver Fiehn

2019-2023 **Ph.D., Chemistry**
Department of Chemistry, The University of British Columbia, Vancouver, BC, Canada
Research Supervisor: Prof. Tao Huan

2014-2018 **B.S., Chemistry**
Department of Chemistry, Zhejiang University, Hangzhou, Zhejiang, China

RESEARCH INTEREST

- Development of analytical and bioinformatic methods for mass spectrometry-based nontargeted metabolomics.
- Large-scale mass spectrometry data processing and data mining using deep learning and Bayesian statistics.
- Integration of metabolomics with other 'omics' (genomics, transcriptomics, and proteomics) data for the systems-level interrogation of biological questions.
- Application of state-of-art metabolomics technologies on brain research, neural science, and cancer research.

FIRST AUTHOR PUBLICATIONS

1 **Yu, H.,** Low, B., Zhang, Z., Guo, J., Huan, T. Quantitative challenges and their bioinformatic solutions in mass spectrometry-based metabolomics.

Trends in Analytical Chemistry, **2023**.

2 **Yu, H.**, Huan, T. MAFFIN: metabolomics sample normalization using maximal density fold change with high-quality metabolic features and corrected signal intensities.

Bioinformatics, **2022**.

3 **Yu, H.**, Sang, P., Huan, T. Adaptive Box-Cox transformation: a highly flexible feature-specific data transformation to improve metabolomics data normality for better statistical analysis.

Analytical Chemistry, **2022**.

4 **Yu, H.**, Huan, T. Comprehensive assessment of the diminished statistical power caused by nonlinear electrospray ionization responses in mass spectrometry-based metabolomics.

Analytica Chimica Acta, **2022**.

5 **Yu, H.**, Huan, T. Patterned signal ratio biases in mass spectrometry-based quantitative metabolomics.

Analytical Chemistry, **2021**.

6 **Yu, H.**, Chen, Y., Huan, T. Computational variation: An under-investigated quantitative variability caused by automated data processing in untargeted metabolomics.

Analytical Chemistry, **2021**.

7 **Yu, H.**, …, Huan, T. Fold-Change compression: An unexplored but correctable quantitative bias caused by nonlinear electrospray ionization responses in untargeted metabolomics.

Analytical Chemistry, **2020**.

8 **Yu, H.**, …, Huan, T. Parallel metabolomics and lipidomics enables the comprehensive study of mouse brain regional metabolite and lipid patterns.

Analytica Chimica Acta, **2020**.

COLLABORATIVE PUBLICATIONS

9 Zhao, L., Qiu, Z., Yang, Z., Xu, L., Pearce, T.M., Wu, Q., Yang, K., Li, F., Saulnier, O., Fei, F., **Yu, H.**, …, Rich, J. Lymphatic endothelial-like cells promote glioblastoma stem cell growth through cytokine-driven cholesterol metabolism.

Nature Cancer, **2024**.

10 Low, B., Wang, Y., Zhao, T., **Yu, H.**, Huan, T. Closing the Knowledge Gap of Post-Acquisition Sample Normalization in Untargeted Metabolomics.

ACS Measurement Science Au., **2024**.

11 Chen, Y., Wang, Y., Delgado, D. H., **Yu, H.**, Zhao, T., Fang, M., Huan, T. Constructing HairDB to facilitate exposome research using human hair.

Environment International, **2024**.

12 Zhang, Z., **Yu, H.**, …, Huan, T. Reducing Quantitative Uncertainty Caused by Data Processing in Untargeted Metabolomics.

Analytical Chemistry, **2024**.

13 Zhao, T., Xing, S., **Yu, H.**, Huan, Tao. De novo cleaning of chimeric MS/MS spectra for LC-MS/MS-based metabolomics.

Analytical Chemistry, **2024**.

14 Zhao, T., Wawryk, N.J., Xing, S., Low, B., Li, G., **Yu, H.**, …, Huan, T. ChloroDBPFinder: machine learning-guided recognition of chlorinated disinfection byproducts from nontargeted LC-HRMS analysis.

Analytical Chemistry, **2024**.

15 Jandu, R. S., **Yu, H.**, Zhao, Z., Le, H. T., Kim, S., Huan, T., van Hoa, F. D., Capture of endogenous lipids in peptidiscs and effect on protein stability and activity.

iScience, **2024**.

16 Chao, C. F., Pesch, Y. Y., **Yu, H.**, …, Rideout, E. An important role for triglyceride in regulating spermatogenesis.

eLife, **2024**.

17 Guo, J., Shen, S., Liu, M., Wang, C., Low, B., Chen, Y., Hu, Y., Xing, S., **Yu, H.**, Gao, Y., Fang, M., Huan, T. JPA: Joint metabolic feature extraction increases the depth of chemical coverage for LC-MS-based metabolomics and exposomics.

Metabolites, **2022**.

18 Guo, J., **Yu, H.**, Xing, S., Huan, T. Addressing big data challenges in mass spectrometry-based metabolomics.

Chemical Communications, **2022**.

19 Xing, S., **Yu, H.**, Liu, M., Jian, Q., Sun, Z., Fang, M., Huan, T. Recognizing contamination fragment ions in liquid chromatography-tandem mass spectrometry data.

Journal of the American Society for Mass Spectrometry, **2021**.

20 Chen, Y., Guo, J., Xing, S., **Yu, H.**, Huan, T. Global-scale metabolomic profiling of Human Hair for simultaneous monitoring of endogenous metabolome, short–and long-term exposome.

Frontiers in chemistry, **2021**.

21 Guo, J., Shen, S., Xing, S., **Yu, H.**, Huan, T. ISFrag: De novo recognition of in-source fragments for liquid chromatography–mass spectrometry data.

Analytical Chemistry, **2021**.

22 Guo, J., Shen, S., Xing, S., Chen, Y., Chen, F., Porter, E.M., **Yu, H.**, Huan, T. EVA: Evaluation of Metabolic Feature Fidelity Using a Deep Learning Model Trained with Over 25000 Extracted Ion Chromatograms.

Analytical Chemistry, **2021**.

23 Sun, Y., Yao, Y., Wang, H., Fu, W., Chen, C., Saha, M. L., Zhang, M., Datta, S., Zhou, Z., **Yu, H.**, Li, X., Stang, P. J. Self-assembly of metallacages into multidimensional suprastructures with tunable emissions.

Journal of the American Chemical Society, **2018**.

24 Yao, Y., Sun, Y., **Yu, H.**, Chen, W., Dai, H., Shi, Y. A pillar[5]arene based gel from a low-molecular-weight gelator for sustained dye release in water.

Dalton Transactions, **2017**.

SUBMITTED WORK

25 **Yu, H.**, Biswas, P., Rideout, E., Cao, Y., Huan, T. Bayesian optimization of separation gradients to maximize the performance of untargeted LC-MS.

Nature Communications, **2024**.

Preprint: https://www.researchsquare.com/article/rs-3338667/v1

26 **Yu, H.**, Ding, J., Shen, T., Liu, M., Li, Y., Fiehn, O. MassCube: a Python framework for end-to-end metabolomics data processing from raw files to phenotype classifiers.

Nature Communications, **2024**.

Preprint: https://www.researchsquare.com/article/rs-5530740/v1

HONORS AND AWARDS

2023.8	ASMS Asilomar Conference Travel Award, American Society for Mass Spectrometry
2022.9	President's Academic Excellence Initiative PhD Award, The University of British Columbia
2021.9	Pei-Huang Tung and Tan-Wen Tung Graduate Fellowship, The University of British Columbia
2021.9	Gladys Estella Laird Research Fellowship, The University of British Columbia
2021.9	President's Academic Excellence Initiative PhD Award, The University of British Columbia
2019.5	Chemistry Graduate Fellowship, The University of British Columbia
2018.6	Award of Graduation with Distinction of Zhejiang Province (Provincial level, **top 1%**), Zhejiang University
2017.12	First-Class Scholarship for Distinguished Students in Basic Science (top 5%), Zhejiang University
2017.12	Outstanding Undergraduate, Department of Chemistry, Zhejiang University
2016.12	First-Class Scholarship for Distinguished Students in Basic Science (top 5%), Zhejiang University
2016.12	Outstanding Undergraduate, Department of Chemistry, Zhejiang University

2015.12 First-Class Scholarship for Distinguished Students in Basic Science (top 5%), Zhejiang University

2015.12 Scholarship for Distinguished Students in Chemistry, Zhejiang University

ORAL PRESENTATIONS

2024.1 Confident structural identification of small molecule using retention time standardization. University of California, Davis, USA

2023.10 Data alignment of untargeted LC-MS/MS experiments using internal standards. ASMS Asilomar Conference, USA

2023.10 Accurate annotation of metabolite mass spectra using deep learning. Virtual Metabolomics Journal Club

2023.6 Development of analytical and bioinformatic solutions for quantitative metabolomics. University of California, Davis, USA

2023.3 Development of analytical workflows and bioinformatic programs for mass spectrometry-based metabolomics. University of British Columbia, Canada

2023.1 Integrated method development of quantitative metabolomics using conventional analytical chemistry and machine learning. Princeton University, USA

2022.10 MAFFIN: metabolomics sample normalization using maximal density fold change with high-quality metabolic features and corrected signal intensities. The 2nd CASMS Virtual Conference

2021.10 Patterned signal ratio biases in mass spectrometry-based quantitative metabolomics. The 1st CASMS Virtual Conference

POSTER PRESENTATIONS

2024. 6 Standardizing retention times to reduce ambiguity of small molecule identification. 72nd ASMS Conference on Mass Spectrometry and Allied Topics, US

2023. 6 Sexual dimorphism of rewarding system in mouse brain revealed by parallel metabolomics and lipidomics. 71st ASMS Conference on Mass Spectrometry and Allied Topics, US

2022.10 MAFFIN: metabolomics sample normalization using maximal density fold change with high-quality metabolic features and corrected signal intensities. The 2nd CASMS Virtual Conference

2022.6 Fold change bases in mass spectrometry-based quantitative metabolomics: causes and solutions. 70th ASMS Conference on Mass Spectrometry and Allied Topics, US

2022.4 Fold change biases in untargeted metabolomics: causes and solutiuons. Chemistry Graduate Research Symposium, University of British Columbia, Canada

2021.8 Patterned signal ratio biases in mass spectrometry-based quantitative metabolomics. The 1st CASMS Virtual Conference

2020.6 Calibrating nonlinear ESI responses using quality control samples to overcome quantitative errors in mass spectrometry-based metabolomics. 68th ASMS Conference on Mass Spectrometry and Allied Topics, US

TEACHING

2023. 8 Introduction: Demo on MassCube software. International Sessions in Metabolomics and Exposome Studies 2024

2023. 8 Quantification in untargeted analysis: using serial dilutions. International Sessions in Metabolomics and Exposome Studies 2024

2023. 8 Quantification in targeted analyses: using internal standards, NIST reference materials, MRMs and kits. International Sessions in Metabolomics and Exposome Studies 2024

2023. 8 Data processing on Compound Discoverer, MassCube, Skyline. International Sessions in Metabolomics and Exposome Studies 2024

2023. 8 mz-rt peak grouping in MS-based untargeted small molecule analysis. International Sessions in Metabolomics and Exposome Studies 2024

2024. 5 Quantification in Metabolomics: Tools for Robustness. WCMC Bits & Bites #4, 2024

2023. 8 Recent advances of discovering feature relations in MS-based untargeted small molecule analysis. WCMC metabolomics summer course 2023

2023. 8 Improving quantitative accuracy in untargeted small molecule analysis using serial diluted QC samples and computational tools. WCMC metabolomics summer course 2023

VOLUNTEERING

2023. 6 Conference assistant. 71th ASMS Conference on Mass Spectrometry and Allied Topics, USA

2023. 2 Conference assistant. 2023 BC Proteomics & Metabolomics Network Symposium, University of British Columbia, Canada

SKILLS

Metabolomics experiment

Metabolomics and lipidomics sample preparation, sample analysis using high-performance liquid chromatography, Q-TOF mass spectrometry, orbitrap mass spectrometry, triple-quadrupole mass spectrometry and MALDI imaging mass spectrometry.

Mass spectrometry data processing

Python programming (developer and maintainer of three Python packages and one Windows software), R programming (developer and maintainer of two R packages), MS-DIAL, XCMS and MZmine

Machine learning and artificial intelligence

Tensorflow, Pytorch and scikit-learn (expertise: neural network, Gaussian process regression and Bayesian optimization)

REFERRERS

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Ph.D. Research Supervisor

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