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Research Training

2023-present **Postdoctoral Researcher**

Genome Center, University of California Davis, Davis, CA, United States

Research Supervisor: Prof. Oliver Fiehn

2019-2023 **Ph.D. in Chemistry**

Department of Chemistry, The University of British Columbia, Vancouver, BC, Canada

Research Supervisor: Prof. Tao Huan

2014-2018 **B.S. in Chemistry**

Department of Chemistry, Zhejiang University, Hangzhou, Zhejiang, China

Research Interests

- **Software development:** breaking through conventional limitations in accuracy and efficiency for ultra-large-scale (>10,000 samples) untargeted metabolomics data processing.
- **AI-driven metabolomics:** integrating human-knowledge-based molecular representations with neural network architectures to enhance biological interpretation and discovery from large population studies.
- **Cancer metabolomics:** developing predictive models of treatment response and metabolic reprogramming using tumor microenvironment-derived metabolomics data to support precision oncology and clinical decision-making.

Publications

- 1 **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, **2025**, 16(1), 5487. <https://doi.org/10.1038/s41467-025-60640-5>
- 2 **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**, 161, 117009. <https://doi.org/10.1016/j.trac.2023.117009>
- 3 **Yu, H.**, Huan, T. MAFFIN: metabolomics sample normalization using maximal density fold change with high-quality metabolic features and corrected signal intensities.
Bioinformatics, **2022**, 38(13), 3429-3437. <https://doi.org/10.1093/bioinformatics/btac355>
- 4 **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**, 94(23), 8267–8276. <https://doi.org/10.1021/acs.analchem.2c00503>
- 5 **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**, 1200, 339614. <https://doi.org/10.1016/j.aca.2022.339614>
- 6 **Yu, H.**, Huan, T. Patterned signal ratio biases in mass spectrometry-based quantitative metabolomics.
Analytical Chemistry, **2021**, 93(4), 2254–2262. <https://doi.org/10.1021/acs.analchem.0c04113>
- 7 **Yu, H.**, Chen, Y., Huan, T. Computational variation: An under-investigated quantitative variability caused by automated data processing in untargeted metabolomics.
Analytical Chemistry, **2021**, 93(25), 8719–8728. <https://doi.org/10.1021/acs.analchem.0c03381>
- 8 **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**, 92(10), 7011–7019. <https://doi.org/10.1021/acs.analchem.0c00246>
- 9 **Yu, H.**, ..., Huan, T. Parallel metabolomics and lipidomics enables the comprehensive study of mouse brain regional metabolite and lipid patterns.
Analytica Chimica Acta, **2020**, 1136, 168-177. <https://doi.org/10.1016/j.aca.2020.09.051>
- 10 **Yu, H.**, Biswas, P., Rideout, E., Cao, Y., Huan, T. Bayesian optimization of separation gradients to maximize the performance of untargeted LC-MS.
bioRxiv. **2023**. <https://doi.org/10.1101/2023.09.08.556930>
- 11 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**, 5(1), 147-166. <https://doi.org/10.1038/s43018-023-00658-0>
- 12 Biswas, P., Bako, J. A., Liston, J. B., **Yu, H.**, ..., Rideout, E. J. Insulin/insulin-like growth factor signaling pathway promotes higher fat storage in *Drosophila* females.
Cell Reports, **2024**. Accepted. <https://doi.org/10.1101/2024.11.18.623936>
- 13 Low, B., Wang, Y., Zhao, T., **Yu, H.**, Huan, T. Closing the Knowledge Gap of Post-Acquisition Sample Normalization in Untargeted Metabolomics.
ACS Meas. Sci. Au, **2024**, 4(6), 702-711. <https://doi.org/10.1021/acsmeasuresciau.4c00047>
- 14 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**, 193, 109077. <https://doi.org/10.1016/j.envint.2024.109077>
- 15 Zhang, Z., **Yu, H.**, ..., Huan, T. Reducing Quantitative Uncertainty Caused by Data Processing in Untargeted Metabolomics.
Analytical Chemistry, **2024**, 96(9), 3727-3732. <https://doi.org/10.1021/acs.analchem.3c04046>
- 16 Zhao, T., Xing, S., **Yu, H.**, Huan, T. De novo cleaning of chimeric MS/MS spectra for LC-MS/MS-based metabolomics.
Analytical Chemistry, **2024**, 95(35), 13018-13028. <https://doi.org/10.1021/acs.analchem.3c00736>
- 17 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**, 96(6), 2590-2598. <https://doi.org/10.1021/acs.analchem.3c05124>
- 18 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**, 27(4), 109382. <https://doi.org/10.1016/j.isci.2024.109382>
- 19 Chao, C. F., Pesch, Y. Y., **Yu, H.**, ..., Rideout, E. An important role for triglyceride in regulating spermatogenesis.
eLife, **2024**, 12, RP87523. <https://doi.org/10.7554/eLife.87523.4>
- 20 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**, 12(3), 212. <https://doi.org/10.3390/metabo12030212>
- 21 Guo, J., **Yu, H.**, Xing, S., Huan, T. Addressing big data challenges in mass spectrometry-based metabolomics.
Chemical Communications, **2022**, 58(72), 9979-9990. <https://doi.org/10.1039/D2CC03598G>
- 22 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.

- J. Am. Soc. Mass Spectrom.*, **2021**, 32(9), 2296-2305. <https://doi.org/10.1021/jasms.0c00478>
- 23 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**, 9, 674265. <https://doi.org/10.3389/fchem.2021.674265>
- 24 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**, 93(29), 10243-10250. <https://doi.org/10.1021/acs.analchem.1c01644>
- 25 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**, 93(36), 12181-12186. <https://doi.org/10.1021/acs.analchem.1c01309>
- 26 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. *J. Am. Chem. Soc.*, **2018**, 140(40), 12819-12828. <https://doi.org/10.1021/jacs.8b05809>
- 27 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**, 46(48), 16802-16806. <https://doi.org/10.1039/C7DT04001F>
- 28 Xing, S., Charron-Lamoureux, V., Ekelöf, M., El Abiead, Y., **Yu, H.**, ..., Dorrestein, P. C. Structural annotation of full-scan MS data: A unified solution for LC-MS and MS imaging analyses. *Nature Communications*, **2025**. In revision. <https://doi.org/10.1101/2024.10.14.618269>

Talks

- Jun. 2025 MassCube: a Python framework for end-to-end metabolomics data processing from raw files to phenotype classifiers. *73rd ASMS Conference on Mass Spectrometry and Allied Topics*. Baltimore Convention Center, Baltimore, Maryland, USA
- May 2025 Uncovering dietary biomarkers through human postprandial metabolic responses. *West Coast Metabolomics Center Seminar*. University of California, Davis, Davis, USA
- Apr. 2025 MassCube: a Python framework for end-to-end metabolomics data processing from raw files to phenotype classifiers. *The Software Data Exchange (SODA) Meetup*. Online meeting (recording: <https://www.youtube.com/watch?v=oxQAnanqbT8>).
- Oct 2024 Analytical and bioinformatic solutions for mass spectrometry-based untargeted metabolomics. *Invited talk by Prof. Feng Zhu*, College of Pharmaceutical Sciences, Zhejiang University, Hangzhou, China.

Curriculum Vitae

- Jan 2024 Confident structural identification of small molecule using retention time standardization. *West Coast Metabolomics Center Seminar*. University of California, Davis, Davis, USA
- Oct 2023 Data alignment of untargeted LC-MS/MS experiments using internal standards. *37th Asilomar Conference on Mass Spectrometry Security and Forensic Applications of Mass Spectrometry*, Asilomar Conference Center, Asilomar, CA, USA
- Oct 2023 Accurate annotation of metabolite mass spectra using deep learning. *Virtual Metabolomics Journal Club*. Online meeting.
- Jun 2023 Development of analytical and bioinformatic solutions for quantitative metabolomics. *West Coast Metabolomics Center Seminar*. University of California, Davis, Davis, USA
- Mar 2023 Development of analytical workflows and bioinformatic programs for mass spectrometry-based metabolomics. *Ph.D. defense*. Department of Chemistry, University of British Columbia, Canada
- Jan 2023 Integrated method development of quantitative metabolomics using conventional analytical chemistry and machine learning. *Invited talk by Prof. Joshua Rabinowitz*. Princeton University, Princeton, NJ, USA
- Oct 2022 MAFFIN: metabolomics sample normalization using maximal density fold change with high-quality metabolic features and corrected signal intensities. *The 2nd CASMS Virtual Conference*. Online meeting.
- Oct 2021 Patterned signal ratio biases in mass spectrometry-based quantitative metabolomics. *The 1st CASMS Virtual Conference*. Online meeting.

Posters

- Jun 2024 Standardizing retention times to reduce ambiguity of small molecule identification. *72nd ASMS Conference on Mass Spectrometry and Allied Topics*. Anaheim Convention Center, Anaheim, CA, USA
- Jun 2023 Sexual dimorphism of rewarding system in mouse brain revealed by parallel metabolomics and lipidomics. *71st ASMS Conference on Mass Spectrometry and Allied Topics*. George R. Brown Convention Center, Houston, TX, USA
- Jun 2022 Fold change bases in mass spectrometry-based quantitative metabolomics: causes and solutions. *70th ASMS Conference on Mass Spectrometry and Allied Topics*.
- Jun 2020 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*. Online meeting.

Expertise

Mass spectrometry (MS)

Extensive hands-on experience with Bruker Impact II Q-TOF MS, ThermoFisher Q Exactive Orbitrap MS, Orbitrap Exploris™ 240 MS, TSQ Plus Triple Quadrupole MS, Bruker timsTOF Pro 2 MS and SCIEX TripleTOF 6600+ MS.

Software development

Sole developer and maintainer of [MassCube](#) Python package, [BAGO](#) Python package, [BAGO](#) Windows software, [ABCstats](#) R package and [MAFFIN](#) R package.

Machine learning and artificial intelligence

Gaussian processing regression-guided Bayesian optimization workflow for liquid chromatography configuration design (developed the BAGO software). Deep learning-based chromatographic peak recognition (contributed to the EVA software). Phenotype classifier tool based on random forest model (developed and implemented in MassCube).

Teaching

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| 2024. 8 | Introduction: Demo on MassCube software. International Sessions in Metabolomics and Exposome Studies 2024 |
| 2024. 8 | Quantification in untargeted analysis: using serial dilutions. International Sessions in Metabolomics and Exposome Studies 2024 |
| 2024. 8 | Quantification in targeted analyses: using internal standards, NIST reference materials, MRMs and kits. International Sessions in Metabolomics and Exposome Studies 2024 |
| 2024. 8 | Data processing on Compound Discoverer, MassCube, Skyline. International Sessions in Metabolomics and Exposome Studies 2024 |
| 2024. 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 |

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