Yuanyue Li, Ph.D.

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PERSONAL STATEMENT

Metabolites are fundamental components in biological processes, yet their large-scale detection remains a big challenge, limiting our understanding of metabolomics. My research aims to bridge this gap by integrating mass spectrometry with computational strategies to enhance metabolite identification techniques. I am interested in the development of innovative computational tools and the integration of machine learning strategies for large-scale metabolite structure identification. In tandem with this, I am interested in integrating metabolomics with other 'omics' like proteomics and genomics to better understand the function of metabolomics, thereby enhancing our knowledge of life science and human health.

EDUCATION EXPERIENCE

Ph.D. in Biochemistry and Molecular Biology 2008.9-2014.6

Xiamen University, Xiamen, China

Thesis title: A novel analysis method for data-independent acquisition MS data

B.Sc. in Life Science 2004.9-2008.7

Xiamen University, Xiamen, China

RESEARCH EXPERIENCE

University of California, Davis Davis, United States

Postdoctoral Fellow / Assistant Project Scientist, advisor: Dr. Oliver Fiehn 2020.1-now

Focus: Mass Spectrometry-based Metabolomics

- Designed and implemented Flash entropy search algorithm, magnifying the speed of library searching by five orders of magnitude.
- Introduced the concept of spectral entropy and entropy similarity to the mass spectrometry field, reducing the false positive rate in metabolite identification by up to 40%.

European Molecular Biology Laboratory Heidelberg, Germany

Postdoctoral Fellow, advisor: Dr. Peer Bork 2015.12-2019.3

Focus: Proteomics and Metabolomics

- Invented SF-Matching, a machine learning-driven approach to improve metabolite identification.

- Established a strategy coupling proteomics and metabolomics techniques to unsupervised identify protein-metabolite interactions.

Xiamen University Xiamen, China

Graduate Student, advisor: Dr. Jiahuai Han 2008.9-2015.6

Focus: Mass Spectrometry-based Proteomics

- Developed Group-DIA, an approach that enhances protein identification notably by grouping multiple mass spectrometry datasets.

PUBLICATIONS AND AWARDS

Main author publications:

6. **Yuanyue Li** & Oliver Fiehn. Flash entropy search to query all mass spectral libraries in real time. ***Accepted by Nature Methods*** (2023) doi:10.21203/rs.3.rs-2693233/v1.

5. **Yuanyue Li**, Tobias Kind, Jacob Folz, Arpana Vaniya, Sajjan Singh Mehta & Oliver Fiehn. Spectral entropy outperforms MS/MS dot product similarity for small-molecule compound identification. ***Nature Methods*** *18*, 1524–1531 (2021).

4. **Yuanyue Li**, Michael Kuhn, Joanna Zukowska-Kasprzyk, Marco L. Hennrich, Panagiotis L. Kastritis, Francis J. O'Reilly, Prasad Phapale, Martin Beck, Anne-Claude Gavin & Peer Bork. Coupling proteomics and metabolomics for the unsupervised identification of protein–metabolite interactions in Chaetomium thermophilum. ***PLOS ONE*** *16*, e0254429 (2021).

3. **Yuanyue Li**, Michael Kuhn, Anne-Claude Gavin & Peer Bork. Identification of metabolites from tandem mass spectra with a machine learning approach utilizing structural features. ***Bioinformatics*** *36*, 1213–1218 (2020).

2. **Yuanyue Li**, Chuan-Qi Zhong, Xiaozheng Xu, Shaowei Cai, Xiurong Wu, Yingying Zhang, Jinan Chen, Jianghong Shi, Shengcai Lin & Jiahuai Han. Group-DIA: analyzing multiple data-independent acquisition mass spectrometry data files. ***Nature Methods*** *12*, 1105–1106 (2015).

1. Chuan-Qi Zhong*, **Yuanyue Li***, Daowei Yang, Na Zhang, Xiaozheng Xu, Yaying Wu, Jinan Chen & Jiahuai Han. Quantitative phosphoproteomic analysis of RIP3-dependent protein phosphorylation in the course of TNF-induced necroptosis. ***Proteomics*** *14*, 713–724 (2014). (* equal contributions)

Contributing author publications:

7. Elys P. Rodríguez, **Yuanyue Li**, Arpana Vaniya, Patrick M. Shih & Oliver Fiehn. Alternative Identification of Glycosides Using MS/MS Matching with an In Silico-Modified Aglycone Mass Spectra Library. ***Analytical Chemistry*** (2023) doi:10.1021/acs.analchem.3c00957.

6. Panagiotis L. Kastritis, Francis J. O'Reilly, Thomas Bock, **Yuanyue Li**, Matt Z. Rogon, Katarzyna Buczak, Natalie Romanov, Matthew J. Betts, Khanh Huy Bui, Wim J. Hagen, Marco L. Hennrich, Marie-Therese Mackmull, Juri Rappsilber, Robert B. Russell, Peer Bork, Martin Beck & Anne-Claude Gavin. Capturing protein communities by structural proteomics in a thermophilic eukaryote. ***Molecular Systems Biology*** *13*, 936 (2017).

5. Xiurong Wu, Wan-Ting He, Shuye Tian, Dan Meng, **Yuanyue Li**, Wanze Chen, Lisheng Li, Lili Tian, Chuan-Qi Zhong, Felicia Han, Jianming Chen & Jiahuai Han. pelo Is Required for High Efficiency Viral Replication. ***PLOS Pathogens*** *10*, e1004034 (2014).

4. Ting Wu, **Yuanyue Li**, Deli Huang, Felicia Han, Ying-Ying Zhang, Duan-Wu Zhang & Jiahuai Han. Regulator of G-Protein Signaling 19 (RGS19) and Its Partner Gα-Inhibiting Activity Polypeptide 3 (GNAI3) Are Required for zVAD-Induced Autophagy and Cell Death in L929 Cells. ***PLOS ONE*** *9*, e94634 (2014).

3. Xiurong Wu, Lili Tian, Jie Li, Yingying Zhang, Victor Han, **Yuanyue Li**, Xiaozheng Xu, Hanjie Li, Xi Chen, Jinan Chen, Wenhai Jin, Yongming Xie, Jiahuai Han & Chuan-Qi Zhong. Investigation of receptor interacting protein (RIP3)-dependent protein phosphorylation by quantitative phosphoproteomics. ***Molecular & cellular proteomics*** *11*, 1640–1651 (2012).

2. Hanjie Li, Congting Ye, Guoli Ji, Xiaohui Wu, Zhe Xiang, **Yuanyue Li**, Yonghao Cao, Xiaolong Liu, Daniel C. Douek, David A. Price & Jiahuai Han. Recombinatorial Biases and Convergent Recombination Determine Interindividual TCRβ Sharing in Murine Thymocytes. ***The Journal of Immunology*** *189*, 2404–2413 (2012).

1. Duan-Wu Zhang, Min Zheng, Jing Zhao, **Yuan-Yue Li**, Zhe Huang, Zhu Li & Jiahuai Han. Multiple death pathways in TNF-treated fibroblasts: RIP3- and RIP1-dependent and independent routes. ***Cell Research*** *21*, 368–371 (2011).

PRESENTATIONS

Invited oral talk:

2023.08	(Upcoming) Chinese American Society for Mass Spectrometry Conference
2023.02	University of Ottawa
2022.06	JRNLclub.org
2022.03	National Center of Protein Sciences, China
2022.02	Metabolomics Association of North America SODAMeets

Oral talk:

2022.10	Chinese American Society for Mass Spectrometry Conference
2021.10	Metabolomics Association of North America Annual Conference
2020.09	NIH Common Fund Metabolomics Consortium Meeting

Poster:

2022.06	American Society for Mass Spectrometry Annual Conference
2021.09	NIH Common Fund Metabolomics Consortium Meeting
2020.09	Metabolomics Association of North America Annual Conference
2020.05	American Society for Mass Spectrometry Annual Conference