

Cheng Wang

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RESEARCH INTEREST

Systems biology (*omics* study), metabolomics, lipidomics, computational drug discovery, machine learning, cancer/chronic disease prevention.

SELECTED RESEARCH PROJECTS

“Multi-omics integration for biomarker discovery in cardiovascular disease”

- Performed metagenomic sequencing (feces) and untargeted metabolomics analysis (feces, plasma, and urine) from ischemic stroke patients and healthy volunteers.
- Conducted differential analysis to find key differential microbiota and metabolites for ischemic stroke.
- Spearman's rank correlation and linear regression analyses were used to study the association between microbiota and metabolites of different metabolic mixtures.
- The systematic association analysis between gut microbiome and metabolomics reveals that fecal metabolites show the strongest association with the gut microbiome, followed by urine and plasma.

“Enzymatic reaction link learning by variational graph autoencoders”

- Developed a Variational Graph Autoencoders (VGAE) based framework to predict metabolite-protein interaction (MPI) in genome-scale heterogeneous enzymatic reaction networks across ten organisms.
- Incorporated molecular features of metabolites and proteins as well as neighboring information in the MPI networks, the MPI-VAGE predictor achieved the best predictive performance compared to other machine learning methods
- Applied the MPI-VGAE framework to reconstruct hundreds of metabolic pathways, functional enzymatic reaction networks, and a metabolite-metabolite interaction network and obtained the most robust performance among all scenarios.
- Implemented the MPI-VGAE framework to reconstruct the disease-specific MPI network based on the disrupted metabolites and proteins in Alzheimer's disease and colorectal cancer, respectively. A substantial number of novel enzymatic reaction links were identified.

“Accurate identification of lipids by combining NMR and MS”

- Designed a new two-dimensional (2D) NMR metabolite database “COLMAR Lipids” that was specifically curated for hydrophobic metabolites presently containing 501 compounds with accurate experimental 2D ^{13}C - ^1H chemical shift data measured in CDCl_3 .
- Nonuniform sampling in combination with pure shift spectroscopy was applied To obtain 2D HSQC spectra with the necessary high spectral resolution along both ^{13}C and ^1H dimensions.

- The integration of the new 2D ^{13}C - ^1H HSQC lipid database into COLMAR enabled the unique identification of many lipids present in complex lipidomics mixtures such as Caco-2 cell and lung tissue cell extracts.

“Accurate and efficient determination of unknown metabolites in metabolomics by NMR-based cheminformatics approaches”

- Developed the SUMMIT method for the untargeted identification of metabolites by combining ultrahigh-resolution Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) and 3D nuclear magnetic resonance (NMR)
- Extracted the individual compound information from NMR spectrum by maximal clique algorithm and derived the all possible metabolite candidates from FT-ICR MS data.
- Demonstrated the performance for untargeted analysis of both a model mixture and *E. coli* cell lysate based on 2D/3D NMR experiments in combination with Fourier transform ion cyclotron resonance MS and MS/MS data.

PROFESSIONAL EXPERIENCE

Department of Biostatistics, Shandong University , Shandong, China Assistant Professor	06/2021-Present
School of Medicine, Washington University in St. Louis , St. Louis, MO Postdoctoral Researcher	06/2020-06/2021
Insight Data Science , San Francisco, CA Health Data Science Fellow	01/2020-05/2020
The Ohio State University , Columbus, OH Graduate Research Assistant	05/2016-12/2019

EDUCATION

The Ohio State University , Columbus, OH, USA Ph.D. Chemistry (Bioinformatics) Advisor: Prof. Rafael Brühweiler	2014-2019
Indiana University , Bloomington, IN, USA M.S. Data Science (Machine learning)	2017-2019
China University of Petroleum , Qingdao, China B.S. Applied Chemistry (Cheminformatics)	2009-2013

RESEARCH FUNDING AND GRANTS

PI, 300,000 RMB, National Natural Science Foundation of China	2024-2026
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“Research on Metabolomic Pseudo-mass Spectrometry Imaging Feature Screening Method Based on Variational Self-coding Nonlinear Dimensionality Reduction”

PI, 150,000 RMB, Natural Science Foundation of Shandong Province 2023-2025
“Research on Structural Identification of Metabolites Based on Density Functional Theory and Deep Learning”

PI, 500,000 RMB, Future Young Scholar of Shandong University 2022-2026
“Integrative Multi-omics Analysis by Deep Learning”

Co-PI, 200,000 RMB, "2030 Science and Technology Innovation - 'Brain Science and Neuromimetic Research' Major Project" 2022-2026
"Alzheimer's Disease and Other Dementia Clinical Cohort Study"

PI, 150,000 RMB, Shandong First-Medical University 2022-2024
“Investigation of Gastric Biomarkers by Mass Spectrometry Imaging”

PUBLICATIONS

Google scholar:

<https://scholar.google.com/citations?user=UAZhchQAAAAJ&hl=en>

First/Corresponding author papers (5 in total, under review/in revision)

1. **Wang, C.**,* Yuan, C.,* Wang, Y.,* Shi, Y., Zhang, T. and Patti, G.J.,* 2024. Prediction of Collision Cross-Section Values by Multimodal Graph Attention Network for Accurate Identification of Small Molecules. *Journal of Chemical Information and Modeling*, (Manuscript under revision)
2. Fan, Z.,* Lv, J.,* Zhang, S., Gu, B., **Wang, C.**,* and Tao, Z.,* 2024. Benchmarking statistical correlation methods for zero-inflated microbiome-metabolome association analysis, *Briefings in Bioinformatics*, (Manuscript under review)
3. Ma, X.,* **Wang, C.**,* and Wang, Z.,* 2024. VisRNA: interactive visualization tool for scRNA-seq data analysis to discover therapeutic targets for non-small cell lung cancer, *BMC Genomics*, (Manuscript under review)

First/Corresponding author papers (9 in total, published)

1. **Wang, C.**, Yuan, C., Wang, Y., Chen, R., Shi, Y., Zhang, T., Xue, F., Patti, G.J.,* Wei, L.* and Hou, Q.,* 2023. MPI-VGAE: protein-metabolite enzymatic reaction link learning by variational graph autoencoders. *Briefings in Bioinformatics*, p.bbaf189.
2. **Wang, C.**, Timári, I., Zhang, B., Li, D.W., Leggett, A., Amer, A.O., Bruschweiler-Li, L., Kopec, R.E. and Bruschweiler, R.,* 2020. COLMAR Lipids Web Server and Ultrahigh-Resolution Methods for Two-Dimensional Nuclear Magnetic Resonance-and Mass Spectrometry-Based Lipidomics. *Journal of proteome research*, 19(4), pp.1674-1683.
3. **Wang, C.**, Zhang, B., Timári, I., Somogyi, Á., Li, D.W., Adcox, H.E., Gunn, J.S., Bruschweiler-Li, L. and Bruschweiler, R.,* 2019. Accurate and efficient determination of unknown metabolites in metabolomics by NMR-based molecular motif identification. *Analytical chemistry*, 91(24), pp.15686-15693.

4. **Wang, C.**,⁺ He, L.,⁺ Li, D.W.,⁺ Bruschweiler-Li, L., Marshall, A.G. * and Brüscheiler, R.,* 2017. Accurate identification of unknown and known metabolic mixture components by combining 3D NMR with fourier transform ion cyclotron resonance tandem mass spectrometry. *Journal of proteome research*, 16(10), pp.3774-3786.
5. Zhao, L.,⁺ **Wang, C.**,⁺ Peng, S., Zhu, X., Zhang, Z., Zhao, Y., Zhang, J., Zhao, G., Zhang, T.,* Heng, X.* and Zhang, L.,* 2022. Pivotal interplays between fecal metabolome and gut microbiome reveal functional signatures in cerebral ischemic stroke. *Journal of Translational Medicine*, 20(1), pp.1-15.
6. Wang, B.,⁺ **Wang, C.**,⁺ and Hanks, A.,* 2024. Where Are They and How Do They Perform? Measuring Long-term Career Outcomes of Public Health Doctoral Recipients, *Journal of Public Health*, fdae031.
7. Che J, Zhao Y, Gu B, Li S, Li Y, Pan K, Sun T, Han X, Lv J, Zhang S, Fan B., Li, C., **Wang, C.**, * Wang, J. * and Zhang, T., * 2023. Untargeted serum metabolomics reveals potential biomarkers and metabolic pathways associated with the progression of gastroesophageal cancer. *BMC cancer*. Dec 15;23(1):1238.
8. Chen, R., Li, X., Yang, Y., Song, X., **Wang, C.*** and Qiao, D.,* 2022. Prediction of protein-protein interaction sites in intrinsically disordered proteins. *Frontiers in Molecular Biosciences*, 9.
9. Leggett, A.,⁺ **Wang, C.**,⁺ Li, D.W., Somogyi, A., Bruschweiler-Li, L. and Brüscheiler, R.,* 2019. Identification of unknown metabolomics mixture compounds by combining NMR, MS, and cheminformatics. *Methods in enzymology* (Vol. 615, pp. 407-422). Academic Press.

Co-author papers (9 in total)

10. Gu, B., Zhang, S., Fan, Z., Che, J., Li, S., Li, Y., Pan, K., Lv, J., **Wang, C.**, Zhang, T. and Wang, J., 2023. Prognostic model construction and immune microenvironment analysis of esophageal cancer based on gene expression data and microRNA target genes. *Translational Cancer Research*, 12(5), p.1165.
11. Yuan, C.,* **Wang, C.**, Zhu, K., Li, S. and Miao, Z.,* 2022. Measles epidemiology and viral nucleoprotein gene evolution in Shandong Province, China. *Journal of Medical Virology*, 94(10), pp.4926-4933.
12. Wang, Y., Stancliffe, E., Fowle-Grider, R., Wang, R., **Wang, C.**, Schwaiger-Haber, M., Shriver, L.P. and Patti, G.J.,* 2022. Saturation of the mitochondrial NADH shuttles drives aerobic glycolysis in proliferating cells. *Molecular cell*, 82(17), pp.3270-3283.
13. Hansen, A.L., Kupče, E., Li, D.W., Bruschweiler-Li, L., **Wang, C.** and Brüscheiler, R.,* 2021. 2D NMR-based metabolomics with HSQC/TOCSY NOAH supersequences. *Analytical Chemistry*, 93(15), pp.6112-6119.
14. Knobloch, T.J., Ryan, N.M., Bruschweiler-Li, L., **Wang, C.**, Bernier, M.C., Somogyi, A., Yan, P.S., Cooperstone, J.L., Mo, X., Brüscheiler, R.P. and Weghorst, C.M.,* 2019. Metabolic regulation of glycolysis and AMP activated protein kinase pathways during black raspberry-mediated oral cancer chemoprevention. *Metabolites*, 9(7), p.140.
15. Timári, I., **Wang, C.**, Hansen, A.L., Costa dos Santos, G., Yoon, S.O., Bruschweiler-Li, L. and Brüscheiler, R.,* 2019. Real-time pure shift HSQC NMR for untargeted metabolomics. *Analytical chemistry*, 91(3), pp.2304-2311.
16. Yuan, J., Zhang, B., **Wang, C.** and Brüscheiler, R.,* 2018. Carbohydrate background removal in metabolomics samples. *Analytical chemistry*, 90(24), pp.14100-14104.

17. Hansen, A.L., Li, D., **Wang, C.** and Brüschweiler, R.,* 2017. Absolute Minimal Sampling of Homonuclear 2D NMR TOCSY Spectra for High-Throughput Applications of Complex Mixtures. *Angewandte Chemie*, 129(28), pp.8261-8264.
18. Li, D.W., **Wang, C.** and Brüschweiler, R.,* 2017. Maximal clique method for the automated analysis of NMR TOCSY spectra of complex mixtures. *Journal of biomolecular NMR*, 68(3), pp.195-202.

CONFERENCES AND PRESENTATIONS

1. 18th Annual Conference of the Metabolomics Society
 Oral presentation, Online 06/2021
 “Protein–metabolite Enzymatic Reaction Link Learning by Graph Neural Network”

2. 2nd Annual MANA Conference
 Oral presentation, Seattle, WA 09/2020
 “COLMAR Lipids Web Server and Ultrahigh-Resolution Methods for Two-Dimensional Nuclear Magnetic Resonance-and Mass Spectrometry-Based Lipidomics”

3. 3rd Gateway NMR Conference
 Oral presentation, Pittsburgh, PA 11/2018
 “Accurate Identification of Known and Unknown Metabolites by Multidimensional NMR and Customized Metabolite Database”

4. 14th Annual Conference of the Metabolomics Society
 Oral presentation, Seattle, WA 06/2018
 “Accurate Identification of Known and Unknown Metabolites by Multidimensional NMR and Customized Metabolite Database”

5. 2nd Annual Ohio Mass Spectrometry and Metabolomics Symposium
 Oral presentation, Columbus, OH 05/2018
 “Accurate Identification of Known and Unknown Metabolites in Gallbladder Bile by Multidimensional NMR and Customized Metabolite Database”

6. Inaugural Conference on Food and Nutritional Metabolomics and 14th Annual Ohio Mass Spectrometry Symposium
 Poster presentation, Columbus, OH 05/2017
 “Facilitating Accurate Identification and Quantitation of Metabolites by Non-uniformly Sampled (NUS) Multi-dimensional NMR”

ACADEMIC SERVICE AND TEACHING EXPERIENCE

Guest editor: *Metabolites* (IF:5.581), *Journal of Personalized Medicine* (IF:3.508)
Reviewer of journals: *eLife*, *Metabolites*, *Nutrients*, *IJMS*, *Applied Sciences*, *Journal of personalized medicine*, etc.

Shandong University, Shandong, China

06/2021-present

Assistant Professor, Department of Biostatistics

- Teaching undergraduate courses, big data mining, machine learning, intro to biostatistics, data structure

The Ohio State University, Columbus, OH

Graduate Teaching Assistant, Physical Chemistry

08/2015-05/2016

- Instructor of recitation to 35 chemistry and chemical engineering majors.
- Taught basics of quantum mechanics, calculus, linear algebra and fundamentals of probability.

Language: Proficient in English, oral, writing and reading, native speaker of Chinese.

HONORS AND AWARDS

- **Food for Health Graduate Student Fellowship**, The Ohio State University 2017-2018
- **Graduate Student Fellowship for Data Science Program**, Indiana University 2017-2019
- **Student Travel Award**, 14th International Conference of Metabolomics Society 06/2018