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Teaching Modules: Phytochemistry of Chinese Medicines (BP12209, Coordinator), Unique Processing Methods of Chinese Medicines (BP12307, Coordinator), Phytochemistry of Chinese Medicines－Laboratory (BP12210), Instrumental Analysis (DPPE04/ME1002), Experimental Technology in Chemistry of Chinese Materia Medica (ME1008), Advances in Research into Chinese Materia Medica (ME1005), Current Topics in Research of Chinese Medicines (DCMSZ01)

Research areas: LC-MS-based Chemical Proteomics and Application, Quality Standards of Traditional Chinese Medicines, Natural Product Chemistry

Professor and PhD supervisor of the State Key Laboratory of Quality Research in Chinese Medicines, Macau University of Science and Technology. She has rich experience in the research of Chinese medicines, especially in the use of advanced technologies such as mass spectrometry, nuclear magnetic resonance and their hyphenated technology, databases and molecular networking to identify the bioactive and/or toxic components, elucidate the mechanism of action, and improve quality standards for traditional Chinese medicines (TCMs). In recent years, research interests have focused on the following three directions. The first is the development of methods for chemical proteomics and their applications. A series of LC–MS-based chemical proteomics approaches were established and successfully applied to determine the mechanism of action of drugs and screen for covalent antidepressant drugs. The second category includes quality standards for TCMs and

classic famous prescriptions as well as product development. Using our developed metabolomics approaches, the components of TCMs, especially those with medicinal and food origins, were fully revealed. The third is the methods for the rapid discovery of bioactive components of TCMs and their application. By integrating LC–MS/NMR, molecular networking, virtual screening, and other advanced technologies, the rapid screening, identification and structure–activity relationships can be achieved. Moreover, some original approaches were developed for the identification of macromolecules, some bioactive polysaccharides were obtained, and some of them have been applied to 3D printing. Seven Science and Technology Development Fund projects, Macau SAR (FDCT) projects, including 1 Key R&D Project (AKP) and 1 Joint Scientific Research Project with the National Natural Science Foundation of China (FDCT-NSFC), were hosted, and 1 FDCT project was cohosted. She has published more than 120 SCI papers in a number of international journals, including *Environ Sci Technol, Food Hydrocolloid, Int J Biol Macromol, TRAC-Trend Anal Chem, Med Res Rev, Anal Chem, Food Chem*, etc. She has applied for and granted 9 international patents and 13 Chinese patents. One ISO standard has been approved.

Academic Qualifications

1999.7 Ph. D. China Pharmaceutical University, Nanjing, Jiangsu Province, China

1994.7 B. Sc. West China University of Medical Sciences, Chengdu, Sichuan Province, China

Working Experiences

2011.9 – Present Assistant Professor, Associate Professor, Professor, State Key Laboratory of Quality Research in Chinese Medicine, Macau University of Science and Technology

2007.11 – 2011.8 Research Associate, The Chinese University of Hong Kong, Hong Kong

2003.12 – 2007.10 Associate Professor, The National Center for Drug Screening, Shanghai Institute of Materia Medica, CAS

2001.11 – 2003.11 Postdoctoral Fellow, Niigata University, Japan

1999.9 – 2001.10 Postdoctoral Fellow, Institute of Mataria Medica, CAMS & PUMC

Representative publications in recent 3 years (*Corresponding author)

1) YH Ge, LL Zhang, SL Gong, W Miao, L Zhang, WB Bai, JL Wu*, **N Li***. FPS_P/N: A two-dimensional mass spectrometry utilization program with precursor ion determination

for accurately distinguishing anthocyanin from other flavonoids. *J Pharm Anal* published online 10.1016/j.jpha.2025.101385.

2) XL Hu, JW Liu, JL Wu*, ZQ Xiong, **N Li***. Chemical Proteomics Unraveling the Contribution of Covalent Protein Modifications to Antidepressant Effects of Ketamine. *J Anal Test* published online https://doi.org/10.1007/s41664-025-00369-8.

3) X Wang, T Tian, **N Li***, LL Zheng, YY Wu, W Bian, JL Wu*, TT Zhou*. Characterization and gelling properties of pectin extracted from Gardenia fruit. *Food Hydrocolloids* **2025**, *163*, 111055.

4) JQ Chen, WY Yuan, W Miao, SL Gong, J Zhou, Y Liu, JL Wu*, **N Li***. *In vitro* and *in vivo* immune-enhancing effects of polysaccharides with different molecular weights and structural characteristics from *Gastrodia elata* Blume. *Int J Biol Macromol* **2025**, *295*, 139526.

5) XL Hu, JL Wu*, Q He, ZQ Xiong, **N Li***. Strategy for cysteine-targeting covalent inhibitors screening using in-house database based LC-MS/MS and drug repurposing. *J Pharm Anal* **2025**, *15*, 101045.

6) SL Gong, GY Bai, YJ Ban, MX Liu, Y Liu, YY Wu, **N Li***, JL Wu*. The underappreciated diversity of furanocoumarins in grapefruits revealed by MassQL filtered molecular networking. *Food Chem X* **2025**, *25*, 102233.

7) W Miao, **N Li***, JQ Chen, JL Wu*. Composition-dependent MRM transitions and structure-indicative elution segments (CMTSES)-based LC-MS strategy for disaccharide profiling and isomer differentiation. *Anal Chim Acta* **2025**, *1337*, 343562.

8) J Han, QY Yang, Z Zheng, **N Li***, JL Wu*. Bromine signature coded derivatization LC-MS for specific profiling of carboxyl or carbonyl-containing metabolites in Mycoplasma pneumoniae infection. *Talanta* **2025**, *285*, 127345.

9) L Zhang, SL Gong, YL Zuo, LL Zhang, JQ Chen, YQ Xu, YY Wu, YH Zhao, JL Wu*, **N Li***. Soybean fermentation drives the production of native neuroprotective peptides based on a peptidomics strategy. *Curr Res Food Sci* **2025**, *10*, 101082.

10) MX Liu, ZY Ning, Y Cheng, ZY Zheng, XX Yang, T Zheng, **N Li***, JL Wu*. The key to 2,6-dichloro-1,4-benzoquinone reproductive toxicity and green tea detoxification: Covalent binding and competitive binding. *Ecotox Environ Safe* **2024**, *286*, 117239.

11) S Zhang, F Yan, F Luan, Y Chai, **N Li***. YW Wang, ZL Chen, DQ Xu, YP Tang*. The pathological mechanisms and potential therapeutic drugs for myocardial ischemia reperfusion injury. *Phytomedicine* **2024**, *129*, 155649.

12) XC Wang, XQ Bian, PP Dong, L Zhang, LL Zhang, CF Gao, HY Zeng, **N Li***, JL Wu*. Food processing drives the toxic lectin reduction and bioactive peptide enhancement in *Pinellia ternate*. *Curr Res Food Sci* **2024**, *9*, 100895.

13) YL Zuo, SL Gong, L Zhang, J Zhou, JL Wu*, **N Li***. A Deep Mining Strategy for Peptide Rapid Identification in *Lactobacillus reuteri* Based on LC–MS/MS Integrated with FBMN and De Novo Sequencing. *Metabolites* **2024**, *14(9)*, 467.

14) J Zhou, JQ Chen, SL Gong, YJ Ban, L Zhang, Y Liu, JL Wu*, **N Li***. Isolation, bioactivity, and molecular docking of a rare gastrodin isocitrate and diverse parishin derivatives from *Gastrodia elata* Blume. *ACS Omega* **2024**, *9*, 14520.

15) JQ Chen, W Miao, Y Liu, J Zhou, J Han, L Zhang, XQ Bian, T Zhong, JL Wu*, **N Li***. Structural characterization, molecular dynamic simulation, and conformational visualization of a water-soluble glucan with high molecular weight from *Gastrodia elata* Blume. *Int J Biol Macromol* **2024**, *263*, 130207.

16) XL Hu, SL Gong, Q He, JL Wu*, **N Li***. Less is more: A new perspective for toxicity of emerging contaminants by structures, protein adducts and proteomics. *TrAC-Trends in Analytical Chemistry* **2023**, *167*, 117289.

17) J Han, SL Gong, XQ Bian, Y Qian, GL Wang, **N Li***, JL Wu*. Polarity-regulated derivatization-assisted LC-MS method for amino-containing metabolites profiling in gastric cancer. *J Pharm Anal* **2023**, *13*, 1353.

18) YH Ge, X Li, MZ Huang, ZX Huang, MM Wu, BQ Sun, LS Wang, JL Wu*, **N Li***. Aroma correlation assisted volatilome coupled network analysis strategy to unveil main aroma-active volatiles of *Rosa roxburghii*. *Food Res Int* **2023**, *169*, 112819.

19) YQ Zhang, XQ Bian, GY Yan, BQ Sun, W Miao, MZ Huang, **N Li***, JL Wu*. Discovery of novel ascorbic acid derivatives and other metabolites in fruit of *Rosa Roxburghii* Tratt through untargeted metabolomics and feature-based molecular networking. *Food Chem* **2023**, *405*, 134807.

20) WS Li, XX Pan, LR Chen, HS Cui, SC Mo, YD Pan, YR Shen, ML Shi, JL Wu, FF Luo*, J Liu*, **N Li***. Cell metabolism-based optimization strategy of CAR-T cell function in cancer therapy. *Front Immunol* **2023**, 1186383.

21) LL Zhang, **N Li***, SS Chen, XQ Bian, MA Farag, YH Ge, JB Xiao, JL Wu*. Carboxyl-containing compounds in food: category, functions, and analysis with chemical derivatization-based LC-MS. *TrAC-Trends in Analytical Chemistry* **2022**, *157*, 116818.

22) SL Gong, XL Hu, SS Chen, BQ Sun, **N Li***, JL Wu*. Dual roles of drug or its metabolite-protein conjugate: cutting-edge strategy of drug discovery using shotgun proteomics. *Med*

Res Rev **2022**, *42*, 1704.

23) XL Hu, JL Wu*, W Miao, F Long, HD Pan, T Peng, XJ Yao, **N Li***. Covalent protein modification: an unignorable factor for bisphenol A induced hepatotoxicity. *Environ Sci Technol* **2022**, *56*, 9536.

24) LL Zhang, JL Wu*, P Xu, S Guo, TT Zhou, **N Li***. Soy protein degradation drives diversity of amino-containing compounds via *Bacillus subtilis* natto fermentation. *Food Chem* **2022**, *388*, 133034.

25) XQ Bian, W Miao, M Zhao, YR Zhao, Y Xiao, **N Li***, JL Wu*. Microbiota drive insoluble polysaccharides utilization via microbiome-metabolome interplay during Pu-erh tea fermentation. *Food Chem* **2022**, *377*, 132007.

26) XQ Bian, XY Xie, JL Cai, YR Zhao, W Miao, XL Chen, Y Xiao, **N Li***, JL Wu*. Dynamic changes of phenolic acids and antioxidant activity of Citri Reticulatae Pericarpium during aging processes. *Food Chem* **2022**, *373*, 131399.

27) SS Chen, Y Fu, XQ Bian, M Zhao, YL Zuo, YH Ge, Y Xiao, JB Xiao, **N Li***, JL Wu*. Investigation and dynamic profiling of oligopeptides, free amino acids and derivatives during Pu-erh tea fermentation by ultra-high performance liquid chromatography tandem mass spectrometry. *Food Chem* **2022**, *371*, 131176.

28) X Wang, **N Li***, SS Chen, YH Ge, Y Xiao, M Zhao, JL Wu*. MS-FINDER Assisted Understanding the Flavonoids Profile in Temporal Dimension during Fermentation of Pu-erh Tea. *J Agric Food Chem* **2022**, *70*, 7085.