



Editorial

Guowang Xu¹

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Warmly invited by the JOAT, as a guest editor, I organized this special issue on metabolomics: state of art in method development and applications. Nine manuscripts are included in this issue including 5 reviews and 4 research articles.

Metabolomics is a science to study the endogenous metabolites in a biological system. It has been used to discover new potential biomarkers for disease diagnosis and typing, and help pharmaceutical R. & D., and it is also playing an important role in plant and microbe fields.

To perform metabolomics, analytical methods are very important. In this issue, focusing on challenges of liquid chromatography–mass spectrometry (LC–MS) in analysis of hydrophilic metabolomics analysis, Wang et al. summarized the nonderivatization and derivatization strategies, with the intention of providing multiple choices for analysis of hydrophilic metabolites. Zhu et al. demonstrated applications of ion mobility–mass spectrometry in untargeted metabolomics from separation to identification, and discussed the future developments of this technology for improving analytical ability of untargeted metabolomics. Xu et al. summarized the workflow and design of chemoselective probes and applications in natural product enrichment and metabolite derivatization. Lipidomics is a sub-field of metabolomics focusing on lipids. Kown et al. primarily discussed the recent advances in untargeted LC–MS-based lipidomics and highlighted the importance of data treatment in metabolic phenotyping studies. Metabolomics at the single-cell level is attracting more and more attention. Shi et al. reviewed the

recent new advances of single-cell metabolomics based on microfluidics and mass spectrometry. These reviews show the new progresses of metabolomics-related fields.

Besides reviews, we have several research articles to report the brand-new results. Xia et al. characterized detailed structures of different classes of phospholipids in human platelets. Based on the acetone Paternò–Büchi reaction multi-level structural identification of phospholipids can be realized including head group, chain composition, and C=C locations in the fatty acyl/alkyl chains. Zhang et al. presented the results on global profiling of acidic glycosphingolipids in C6 glioma rats treated with temozolomide using UPLC–Q-TOF MS. Lu et al. sought to explore the regulatory role of manganese (Mn²⁺) on small-molecule metabolism of biofilm formation in *Escherichia coli* using structural imaging assay combined with precision-targeted metabolomics method. To enable accurate quantification of total protein bound tryptophan in soybean seeds, Lei et al. compared four common protein precipitation methods to determine the best method to separate soy proteins from carbohydrates. These articles reflect the requirement for detailed structure characterization and precision determination for defined metabolites.

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✉ Guowang Xu
xugw@dicp.ac.cn

¹ CAS Key Laboratory of Separation Science for Analytical Chemistry, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, China