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Jun Han obtained his MS (1993) and PhD (1999) degrees, both in Pharmaceutical Analysis, from China Pharmaceutical University. He worked as a Research Scientist at Guangzhou Institute for Drug Control (Guangdong Province, China) and completed his postdoctoral training at the University of North Carolina-Chapel Hill (USA) and the Medical University of South Carolina (SC, USA). Since 2007, he has been a Research Assistant Professor at the University of Victoria-Genome British Columbia Proteomics Centre, where he leads the Metabolomics Subgroup which develops MS-based techniques for metabolomics and tissue imaging.

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Carol Parker received her BA degree from Cornell University (1969), and her MS (1973) and PhD (1977) from the Department of Chemistry at UNC-Chapel Hill. She was a member of the MS group at NIEHS (RTP, North Carolina, USA), for nearly 25 years, where she worked on projects which included the interfacing of MS with GC, LC, and CZE. She has worked for Christoph Borchers in MS-based proteomics since 2001, first at UNC and now at the University of Victoria-Genome British Columbia Proteomics Centre, Victoria, Canada.

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Foreword

Jun Han, Carol E Parker &
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Since the concept was formally introduced in the late 1990s, metabolomics has evolved as an integral member of the functional genomics family to complement transcriptomics and proteomics. The goal of metabolomics is to detect and quantitate all the low molecular mass (typically <1500 Da) compounds (i.e., the metabolome) that define the metabolic status of a given biological system, either animal or plant cells, tissues, body fluids or microorganisms. Because of the diverse chemical structures and the wide concentration range of different metabolites in biological samples, multiple analytical techniques are often employed in a concert to achieve a high coverage of the metabolome, and these techniques are often used to measure the changes of metabolite profiles in relation to genetic modifications or environmental interventions. LC/MS stands out from other analytical techniques and has become the most commonly used analytical technique in metabolomics, in part because of the compatibility of liquid phase separation with the aquatic cell environment in which the metabolites are synthesized and metabolized.

LC/MS – the online coupling of a liquid-phase separation method to a gas-phase detection method – was intrinsically more difficult to accomplish than the coupling of gas chromatography with MS, both of which are gas phase techniques. This was particularly true at the time LC/MS was developed because the only available ionization techniques were electron impact and chemical ionization. Not surprisingly, the first two approaches developed

were the moving belt (where the liquid was removed) and the Direct Liquid Introduction technique, where the LC mobile phase became the CI reagent gas. Later LC/MS techniques, such as thermospray and the now widely used electrospray ionization, were also designed to volatilize the solvent, and all result in protonated molecular ions in the positive ion mode. Adding MS/MS provides a fragmentation ‘fingerprint’ that helps to identify the analyte. LC/MS/MS is now the ‘gold standard’ technique in metabolomics. This is in most part due to the high degree of flexibility in selecting the most appropriate chromatographic separation methods, the high sensitivity and high specificity of state-of-the-art mass spectrometers, as well as its high-throughput capability.

This book provides several minireviews on the current status of various LC/MS techniques for metabolomics research. A mini-review on the current status of chemical derivatization for improved LC/MS-based quantitative metabolomics is reported in this book (Chapter 1). Other chapters in this book reflect the variety of aspects of the application of modern electrospray-based LC/MS to metabolomics. These applications range from the detection of inborn errors of metabolism in infants (Chapter 2), to Alzheimer’s Disease (Chapter 3) and plant metabolomics using untargeted LC/MS techniques (Chapter 4). Several chapters describe the applications for metabolomics to biomarker discovery – specifically, the possibility of using metabolomics to determine early biomarkers for Alzheimer’s Disease (Chapter 3), and for early detection of hepatotoxicity and nephrotoxicity (Chapter 5). The challenges of metabolite identification and quantitation are described in Chapter 6, a new approach for rapid and segmented flow injection analysis is described in Chapter 2 and ion mobility applications are described in Chapter 7.

Taken together, these chapters show the wide range of metabolomic applications of the LC/MS technique.

Financial & competing interests disclosure

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No writing assistance was utilized in the production of this manuscript.