
Preface

Metabolomics, also commonly known as metabolic profiling or metabonomics, is a fast growing field in systems biology and offers a powerful and promising approach for a broad range of applications. Metabolomics focuses on deriving the concentrations and fluxes of low molecular weight metabolites ($< \sim 1$ kDa) in bio-fluids, cells or tissue, plants, foods, and related samples, and this information provides enormous detail on biological systems and their current status. Mass spectrometry (MS) is one of most powerful and commonly used analytical methods in metabolomics. The high sensitivity of MS makes possible the routine analysis of many hundreds of metabolites in a typical sample. A variety of MS-based methods is now available for global or targeted metabolic profiling using GC-MS, LC-MS, CE-MS, as well as direct infusion methods, providing an exciting set of capabilities for advanced investigations.

A broad coverage of the major MS-based metabolomics methods, along with detailed step-by-step procedures, is provided in *Mass Spectrometry in Metabolomics: Methods and Protocols*. Each chapter provides a brief introduction of the methodology, sample type, and application followed by a detailed protocol designed to allow others familiar with MS to duplicate the results or at least learn from the provided expertise. We have purposely left out in-depth discussions of the MS fundamental principles, as there are many excellent books and review articles available for the interested reader. However, because so many different MS systems are used in metabolomics, we have strived to include a wide variety, including triple quads, time of flight, Fourier transform ion cyclotron resonance, and even simple quadrupole systems. Front end chromatography used in metabolomics spans the range from liquid to gas, and includes capillary electrophoresis. Infusion and several atmospheric sample introduction methods are also represented.

The analyses also span a wide range of samples from bio-fluids to cell and tissue extracts as well as plants. An important issue covered in several chapters is standardization, including the isotope-labeled compounds used for quantitation by several approaches. Imaging methods are described in two chapters, and tracer analysis, which provides important mechanistic information and can be adapted to many if not most of the MS methods, is also described in this volume. Because of their importance in metabolomics, we also have included a chapter on the more popular statistical methods used by researchers in the field.

A growing number of metabolomics studies have been reported for detecting various diseases including numerous cancers, diabetes, heart disease, and neurological diseases. In addition, a variety of nutritional, environmental, and plant studies are the focus of current research. Studies of cells under a variety of conditions have identified a number of novel metabolic findings in the complex systems biology, while animal studies have been used to develop toxicology markers, therapy prediction methods, and for mechanistic studies in support of human biomarker discovery efforts. We have therefore included several chapters that are representative of the many and growing number of applications in metabolomics.

We thank our colleagues who have provided their detailed methodologies to help others learn from their expertise. We hope that readers can benefit from the wealth of information compiled in these chapters to further the dynamic field of metabolomics.

Seattle, WA, USA

Daniel Raftery

Mass Spectrometry in Metabolomics

Methods and Protocols

Raftery, D. (Ed.)

2014, XVI, 360 p. 71 illus., 52 illus. in color., Hardcover

ISBN: 978-1-4939-1257-5

A product of Humana Press