

Preface

This ACS Symposium Series Book was evolved from the ACS symposium "Instrumental Methods for Analysis of Bioactive Molecules", sponsored by the Division of Agricultural and Food Chemistry at the 246th American Chemical Society National Meeting & Exposition in Indianapolis, Indiana, September 8-12, 2013. Researchers in this field with common interests in the analysis of natural bioactive compounds were successfully brought together from all over the world to attend this exciting symposium to exchange ideas and results focusing on sample preparation, method development, validation, and application to real samples. A total of 33 scientists from 12 countries participated in this symposium. A World-class group of academic researchers and industrial scientists wrote the chapters published in this book to provide a state-of-the-art review and global perspective on this rapidly changing field.

The main purpose of this book is to discuss cutting-edge research techniques in the field of biologically active compounds derived from plants and foods, and in particular to describe advanced instrumental methods for the identification and quantification of these important compounds. Natural products are used worldwide to prevent and treat various diseases. The efficacy and safety of natural products require the development and application of reliable analytical methods to regulate and control usage. Because of their complex chemical compositions, natural products often require separation techniques for reliable analysis of their constituents. This book provides an integrated approach to address the separation, identification, quantification and chemistry of natural products for their analysis through various instrumental analyses.

Based on the symposium themes, this book contains nineteen chapters and is divided into four sections: 1) Sample Preparation, Separation and Identification 2) Identification by LC-MS and LC-NMR 3) Identification by GC, GC-MS, LC-GC and Spectroscopic Methods and 4). Metabolomic Fingerprinting. The first section covers sample preparation, extraction and rapid flash separation techniques, rapid LC analysis with bioassays and hyphenations to identify active constituents. The second section covers chromatographic separation by LC for active constituents, identification by mass spectra, and LC-NMR for the characterization of specific constituents from species such as *Melia azedarach*, *Sambucus nigra*, Citrus and Pomegranate. The third section covers separation of volatile constituents by GC and GC-MS. In recent years, analysis of volatiles using headspace has become more sensitive and popular, as it does not alter the original composition of volatile chemicals. This section also describes an approach based on solid-phase extraction and on-line LC-GC for the determination of naturally occurring free sterols, stanols and their esters. In addition, non-destructive

methods for the determination of chemical fingerprints and metabolomics profiles of natural products are also described; these methods allow reliable analysis of samples through the rapid acquisition of complex samples using nuclear magnetic resonance spectra. Moreover, Fourier Transform Infrared Photoacoustic Spectroscopy (FTIR-PAS) provides a method to measure resistant starch without separating it from the biological matrix is described. The fourth section includes two chapters on metabolic fingerprinting techniques. Metabolomics involves the study of small molecules from cells, plants, foods, tissues, organisms, or other biological tissues. These small molecules include primary and intermediary metabolites, as well as exogenous compounds, such as secondary metabolites, drugs and other compounds. Metabolic fingerprinting compares patterns, also called signatures or fingerprints of metabolites; these patterns change in response to external stimuli either in different plant varieties or species, or in response to adulteration, toxins, drug exposure, environmental or genetic alterations.

Thus, this book comprehensively describes the basic information presented at the symposium, providing a current review that will be useful for scientists, researchers, teachers, and engineers in general, and is particularly useful for chemists, biochemists, chemical engineers, biochemical engineers, and others in chemistry-related fields.

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