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This book comprehensively describes the development and practice of DNA-encoded library synthesis technology. Together, the chapters detail an approach to drug discovery that offers an attractive addition to the portfolio of existing hit generation technologies such as high-throughput screening, structure-based drug discovery and fragment-based screening. The book: Provides a valuable guide for understanding and applying DNA-encoded combinatorial chemistry Helps chemists generate and screen novel chemical libraries of large size and quality Bridges interdisciplinary areas of DNA-encoded combinatorial chemistry synthetic and analytical chemistry, molecular biology, informatics, and biochemistry Shows medicinal and pharmaceutical chemists how to efficiently broaden available "chemical space" for drug discovery Provides expert and up-to-date summary of reported literature for DNA-encoded and DNA-directed chemistry technology and methods

This is the first book to examine organelle proteomics in depth. It begins by introducing the different analytical strategies developed and successfully utilized to study organelle proteomes, and detailing the use of multidimensional liquid chromatography coupled to tandem mass spectrometry for peptide sample analysis. Detailed protocols are provided and a section is devoted to methods enabling a global estimate of the reliability of the protein list assigned to an organelle.

A definitive reference, completely updated Published in 1989, the First Edition of this book, originally entitled Quadrupole Storage Mass Spectrometry, quickly became the definitive reference in analytical laboratories worldwide. Revised to reflect scientific and technological advances and new applications in the field, the Second Edition includes new chapters covering: * New ion trap instruments of high sensitivity * Peptide analysis by liquid chromatography/ion trap tandem mass spectrometry * Analytical aspects of ion trap mass spectrometry combined with gas chromatography * Simulation of ion trajectories in the ion trap One additional chapter discusses the Rosetta mission, a "cometchaser" that was sent on a ten-year journey in 2004 to study the comet Churyumov-Gerasimenko using, among other instruments, a GC/MS system incorporating a specially designed ion trap mass spectrometer. This comprehensive reference also includes discussions of the history of the quadrupole ion trap, the theory of quadrupole mass spectrometry, the dynamics of ion-trapping chemistry in the quadrupole ion trap, the cylindrical ion trap, miniature traps, and linear ion traps. Complete with conclusions and references, this primer effectively encapsulates the body of knowledge on quadrupole ion trap mass spectrometry. With its concise descriptions of the theory of ion motion and the principles of operation, Quadrupole Ion Trap Mass Spectrometry, Second Edition is ideal for new users of quadrupole devices, as well as for scientists, researchers, and graduate and post-doctoral students working in analytical laboratories.

Over the last decade, scientific and engineering interests have been shifting from conventional ion mobility spectrometry (IMS) to field asymmetric waveform ion mobility spectrometry (FAIMS). Differential Ion Mobility Spectrometry: Nonlinear Ion Transport and Fundamentals of FAIMS explores this new analytical technology that separates and characterizes ions by the difference between their mobility in gases at high and low electric fields. It also covers the novel topics of higher-order differential IMS and IMS with alignment of dipole direction. The book relates the fundamentals of FAIMS and other nonlinear IMS methods to the physics of gas-phase ion transport. It begins with the basics of ion diffusion and mobility in gases, covering the main attributes of conventional IMS that are relevant to all IMS approaches. Building on this foundation, the author reviews diverse high-field transport phenomena that underlie differential IMS. He discusses the conceptual implementation and first-principles optimization of FAIMS as a filtering technique, emphasizing the dependence of FAIMS performance metrics on instrumental parameters and properties of ion species. He also explores ion reactions in FAIMS caused by field heating and the effects of inhomogeneous electric field in curved FAIMS gaps. Written by an accomplished scientist in the field, this state-of-the-art book supplies the foundation to understand the new technology of nonlinear IMS methods.

Ambient ionization has emerged as one of the hottest and fastest growing topics in mass spectrometry enabling sample analysis with minimal sample preparation. Introducing the subject and explaining the basic concepts and terminology, this book will provide a comprehensive, unique treatise devoted to the subject. Written by acknowledged experts, there are full descriptions on how new ionization techniques work, with an overview of their strengths, weaknesses and applications. This title will bring the reader right up to date, with both applications and theory, and will be suitable as a tutorial text for those starting in the field from a variety of disciplines.

Natural Products Isolation: Second Edition presents a practical overview of just how natural products can be extracted, prepared, and isolated from the source material. Maintaining the main theme and philosophy of the first edition, this second edition incorporates all the new significant developments in this field of research. The chapters are divided into four distinct sections: introduction, extraction, chromatography, and special topics. This second edition provides substantial background information for natural product researchers and will prove a useful reference guide to all of the available techniques.

A multidisciplinary approach to understanding the fundamentals of mass spectrometry for bacterial analysis From chemotaxonomy to characterization of targeted proteins, Identification of Microorganisms by Mass Spectrometry provides an overview of both well-established and cutting-edge mass spectrometry techniques for identifying microorganisms. A vital tool for microbiologists, health professionals, and analytical chemists, the text is designed to help scientists select the most effective techniques for use in biomedical, biochemical, pharmaceutical, and bioterror defense applications. Since microbiological applications of mass spectrometry require a basic understanding of both microbiology and analytical chemistry, the editors have incorporated material from both disciplines so that readers from either field will come to understand the necessary principles of the other. Featuring contributions from some of the most recognized experts in both fields, this volume provides specific examples of fundamental methods as well as approaches developed in the last decade, including: * Metastable atom bombardment pyrolysis mass spectrometry * Matrix-assisted laser desorption/ionization mass spectrometry (MALDI) * MALDI time-of-flight mass spectrometry (MALDI-TOF MS) of intact bacteria * High-resolution Fourier transform mass spectrometry (FTMS) * Electrospray ionization (ESI) mass spectrometry Identification of Microorganisms by Mass Spectrometry represents the most comprehensive and up-to-date work on the topic currently available. It is liberally illustrated with figures and tables and covers every aspect of spectrometric identification of microorganisms, including experimental procedures, various means of sample preparation, data analysis, and interpretation of complex mass spectral data.

Hands-on experts from academia and industry comprehensively describe how to successfully perform all the critical HPLC techniques needed for the analysis of peptides and proteins. The methods range from commonly used techniques to those for capillary to large-scale preparative isolation. The authors have also presented a number of specific applications as case studies to illustrate the analytical approaches to a particular separation or assay challenge, with examples drawn from contemporary fields in biochemistry and biotechnology. Follow step-by-step instructions that ensure experimental success Develop your own separation and analytical protocols for peptide and protein analysis.

Classical natural product chemistry is transitioning to modern day metabolomics as a result of the advent of comprehensive analytical platforms and sensitive analytical instrumentation. Therefore, it is worthwhile to summarize recent developments with current analytical platforms and highlight how metabolomics is being integrated into this classical field to dereplicate and profile natural product extracts. Metabolomics Tools for Natural Product Discoveries: Methods and Protocols aims to unite diverse and recently developed methodologies and protocols in order to identify bioactive secondary metabolites for

the purpose of drug discovery. Some topics covered in this volume include applications for the extraction of selected natural products from less common sources such as bryophytes and hard corals, various biological assays, comprehensive applications and strategies for GC-MS, LC-MS, and NMR, as well as protocols and strategies for the structure elucidation of isolated natural products. Written in the successful Methods in Molecular Biology series format, chapters include introductions to their respective topics, lists of the necessary materials and reagents, step-by-step, readily reproducible protocols, and notes on troubleshooting and avoiding known pitfalls. Authoritative and easily accessible Metabolomics Tools for Natural Product Discoveries: Methods and Protocols seeks to serve both professionals and research students with its well-honed methodologies for natural product isolation, biomarker discovery, dereplication, biological assays, and comprehensive metabolomic platforms available for high-throughput analyses.

This volume explores the latest techniques and workflow for the analysis of single cells metabolism. The chapters in this book cover topics such as the development of mass spectrometry-based single cell approaches, Pico-ESI-MS for single-cell metabolomics analysis; laser capture microdissection; ambient single cell metabolite profile (DESI and LAESI); and MALDI-MS methodology, quantum dots for quantitative cytology to study metabolic heterogeneity of single cells. Written in the highly successful Methods in Molecular Biology series format, the chapters consist of introductions to the topic, lists of the necessary materials and reagents, step-by-step guidelines, readily reproducible laboratory protocols, and tips on troubleshooting and avoiding known pitfalls. Comprehensive and authoritative, Single Cell Metabolism: Methods and Protocols is a valuable resource for any researcher and scientist interested in learning more about this field.

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