

USING MASS SPECTROMETRY FOR DRUG METABOLISM STUDIES



EDITED BY

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Using Mass Spectrometry For Drug Metabolism Studies

Marco Cascella



Using Mass Spectrometry For Drug Metabolism Studies:

Using Mass Spectrometry for Drug Metabolism Studies Walter A. Korfmacher, 2009-11-03 The first edition of this now classic work helped to establish mass spectrometry as the premier tool for drug metabolism studies Completely rewritten from start to finish *Using Mass Spectrometry for Drug Metabolism Studies* Second Edition brings medicinal chemists and mass spectrometry professionals up to speed with the rapid advances in the field *Using Mass Spectrometry for Drug Metabolism Studies, Second Edition* Walter A. Korfmacher, 2009-11-03 The first edition of this now classic work helped to establish mass spectrometry as the premier tool for drug metabolism studies Completely rewritten from start to finish *Using Mass Spectrometry for Drug Metabolism Studies* Second Edition brings medicinal chemists and mass spectrometry professionals up to speed with the rapid advances in the field the emergence of cutting edge approaches and ways to meet steadily increasing vendor demands Written by international scientists who are experts in their respective disciplines this state of the art reference effectively encapsulates current mass spectrometry best practices The stand alone chapters cover various topics from metabolite identification to fast chromatography with UPLC and in a style that is understandable to experts and field newcomers alike The second edition of this bestseller includes coverage of new instrumentation and software as well as a wealth of updated information on the latest findings surrounding biomarkers and metabolomics and new chapters on both UPLC and DESI DART With more than 180 illustrations and an eight page color insert this valuable reference explores multiple modern mass spectrometry techniques and strategies It includes an excellent overview of the entire drug discovery process plus the latest developments on how mass spectrometry is used to support this endeavor *Using Mass Spectrometry for Drug Metabolism Studies* Walter A. Korfmacher, 2009-11-03 The first edition of this now classic work helped to establish mass spectrometry as the premier tool for drug metabolism studies Completely rewritten from start to finish *Using Mass Spectrometry for Drug Metabolism Studies* Second Edition brings medicinal chemists and mass spectrometry professionals up to speed with the rapid advances in the field *Mass Spectrometry in Drug Metabolism and Pharmacokinetics* Ragu Ramanathan, 2011-09-20 This timely reference discusses mass spectrometry in drug metabolism and pharmacokinetic studies With contributions by professionals from the pharmaceutical industry this book begins with a review of current mass spectrometry techniques and applications followed by discussions of various methods for using MS in drug metabolism studies and pharmacokinetics Highlighting the critical importance of ADME studies for understanding how a drug is absorbed distributed metabolized and excreted by the body the book s focuses on the use of LC MS and MALDI MS This is a valuable reference for scientists in the pharmaceutical industry medicine academia and even those working in homeland defense *Mass Spectrometry in Drug Metabolism and Disposition* Mike S. Lee, Mingshe Zhu, 2011-03-16 This book examines the background industrial context process analytical methodology and technology of metabolite identification It emphasizes the applications of metabolite identification in drug research While primarily a

textbook the book also functions as a comprehensive reference to those in the industry The authors have worked closely together and combine complementary backgrounds to bring technical and cultural awareness to this very important endeavor while serving to address needs within academia and industry It also contains a variety of problem sets following specific sections in the text

Mass Spectrometry in Drug Metabolism Frigerio,2012-12-06 When a dose of drug is administered three main phases of drug action may be distinguished In the pharmaceutical phase the dosage form disintegrates the active substance dissolves and becomes available for absorption The second phase pharmacokinetic phase includes absorption distribution metabolism and excretion That fraction of the dose which finally reaches the circulation after absorption will be available for biological action in the third or pharmacodynamic phase when the drug reaches the target tissues and a drug receptor interaction takes place The objectives in studies of drug metabolism are a to identify the pathways by which drugs are transformed in the body b to ascertain quantitatively the importance of each pathway and intermediate c to identify and quantify endogenous constituents influenced by the drug or its metabolites which may interfere with common metabolic processes Since metabolites usually differ from their precursors by only a single chemical group the resulting metabolic pathways generally consist of a series of closely related compounds Mass spectrometry is uniquely suited for the analysis of drugs and metabolites for several reasons only a minimal amount of sample preparation is needed closely related compounds can be analyzed in a single step structures can often be deduced directly from the mass spectra without the need for pure reference spectra and constituents can be quantified with relative ease even when present in fractional nanogram quantity

Mass Spectrometry in Drug Metabolism 3Island Press,1977-03-01 *Identification and Quantification of Drugs, Metabolites and Metabolizing Enzymes by LC-MS* Swapna Chowdhury,2005-11-04 As new techniques of transferring from liquid to gas phase and measuring masses of drug molecules and metabolites become more prevalent so do the technical challenges of putting these techniques into proper use as well as the task of consolidating emerging applications Identification and Quantification of Drugs Metabolites and Metabolizing Enzymes by LC MS Volume 6 fills the gap in the lack of presently available literature by providing a critical review in the current use of liquid chromatography mass spectrometry LC MS in drug discovery and development With chapters written by experts with a wide range of practical experience from the pharmaceutical industry emphasis is placed on techniques and applications The book also includes chapters on how to utilize LC MS instrumentation for current drug metabolism problems This book is intended for those beginning to use LC MS for drug metabolism studies as well as for those considered advanced practitioners Introduces readers to the practical applications of modern liquid chromatography mass spectrometry LC MS in a wide range of drug metabolism studies Provides a comprehensive description of different forms of metabolites with detailed discussion on the wide range of methodologies used to identify them Highlights problems associated with drug quantification and offers practical solutions

Mass Spectrometry in Drug Metabolism Alberto Frigerio,Emilio L. Ghisalberti,1976

High-Throughput Analysis in the Pharmaceutical Industry Perry G. Wang, 2008-08-20 The introduction of combinatorial chemistry technology has increased the amount of compounds generated in a year from 50 to 2000 Conventional analytical approaches simply cannot keep up These circumstances have caused drug discovery to take on the shape of a bottleneck like traffic through a toll booth In order to break the bottleneck a corres *Handbook of Drug Metabolism, Third Edition* Paul G. Pearson, Larry C. Wienkers, 2019-05-20 This book continues to be the definitive reference on drug metabolism with an emphasis on new scientific and regulatory developments It has been updated based on developments that have occurred in the last 5 years with new chapters on large molecules disposition stereo selectivity in drug metabolism drug transporters and metabolic activation of drugs Some chapters have been prepared by new authors who have emerged as subject area experts in the decade that has passed since publication of the first edition **Handbook of LC-MS Bioanalysis** Wenkui Li, Jie Zhang, Francis L. S. Tse, 2013-10-21 Consolidates the information LC MS bioanalytical scientists need to analyze small molecules and macromolecules The field of bioanalysis has advanced rapidly propelled by new approaches for developing bioanalytical methods new liquid chromatographic LC techniques and new mass spectrometric MS instruments Moreover there are a host of guidelines and regulations designed to ensure the quality of bioanalytical results Presenting the best practices experimental protocols and the latest understanding of regulations this book offers a comprehensive review of LC MS bioanalysis of small molecules and macromolecules It not only addresses the needs of bioanalytical scientists working on routine projects but also explores advanced and emerging technologies such as high resolution mass spectrometry and dried blood spot microsampling *Handbook of LC MS Bioanalysis* features contributions from an international team of leading bioanalytical scientists Their contributions reflect a review of the latest findings practices and regulations as well as their own firsthand analytical laboratory experience The book thoroughly examines Fundamentals of LC MS bioanalysis in drug discovery drug development and therapeutic drug monitoring The current understanding of regulations governing LC MS bioanalysis Best practices and detailed technical instructions for LC MS bioanalysis method development validation and stability assessment of analyte s of interest Experimental guidelines and protocols for quantitative LC MS bioanalysis of challenging molecules including pro drugs acyl glucuronides N oxides reactive compounds and photosensitive and autooxidative compounds With its focus on current bioanalytical practice *Handbook of LC MS Bioanalysis* enables bioanalytical scientists to develop and validate robust LC MS assay methods all in compliance with current regulations and standards **Mass Spectrometry in Medicinal Chemistry** Klaus Wanner, Georg Höfner, 2007-04-09 This first overview of mass spectrometry based pharmaceutical analysis is the key to improved high throughput drug screening rational drug design and analysis of multiple ligand target interactions The ready reference opens with a general introduction to the use of mass spectrometry in pharmaceutical screening followed by a detailed description of recently developed analytical systems for use in the pharmaceutical laboratory Applications range from simple binding assays to complex screens of biological

activity and systems containing multiple targets or ligands all highly relevant techniques in the early stages in drug discovery from target characterization to hit and lead finding

Drug Metabolism Handbook Ala F. Nassar, 2009-01-28 A valuable reference tool for professionals involved in the industry Drug Metabolism in Pharmaceuticals covers new tools such as LC MS and LC MS NMR along with experimental aspects of drug metabolism This work fills a gap in the literature by covering the concepts and applications of pharmaceutical research development and assessment from the point of view of drug metabolism By providing both a solid conceptual understanding of the drug metabolism system and a well illustrated detailed demonstration and explanation of cutting edge tools and techniques this book serves as a valuable reference tool for bench scientists medical students and students of general health sciences

Encyclopedia of Spectroscopy and Spectrometry, 2016-09-22 This third edition of the Encyclopedia of Spectroscopy and Spectrometry Three Volume Set provides authoritative and comprehensive coverage of all aspects of spectroscopy and closely related subjects that use the same fundamental principles including mass spectrometry imaging techniques and applications It includes the history theoretical background details of instrumentation and technology and current applications of the key areas of spectroscopy The new edition will include over 80 new articles across the field These will complement those from the previous edition which have been brought up to date to reflect the latest trends in the field Coverage in the third edition includes Atomic spectroscopy Electronic spectroscopy Fundamentals in spectroscopy High Energy spectroscopy Magnetic resonance Mass spectrometry Spatially resolved spectroscopic analysis Vibrational rotational and Raman spectroscopies The new edition is aimed at professional scientists seeking to familiarize themselves with particular topics quickly and easily This major reference work continues to be clear and accessible and focus on the fundamental principles techniques and applications of spectroscopy and spectrometry Incorporates more than 150 color figures 5 000 references and 300 articles for a thorough examination of the field Highlights new research and promotes innovation in applied areas ranging from food science and forensics to biomedicine and health Presents a one stop resource for quick access to answers and an in depth examination of topics in the spectroscopy and spectrometry arenas

Topics on Drug Metabolism James Paxton, 2012-02-22 In order to avoid late stage drug failure due to factors such as undesirable metabolic instability toxic metabolites drug drug interactions and polymorphic metabolism an enormous amount of effort has been expended by both the pharmaceutical industry and academia towards developing more powerful techniques and screening assays to identify the metabolic profiles and enzymes involved in drug metabolism This book presents some in depth reviews of selected topics in drug metabolism Among the key topics covered are the interplay between drug transport and metabolism in oral bioavailability the influence of genetic and epigenetic factors on drug metabolism impact of disease on transport and metabolism and the use of novel microdosing techniques and novel LC MS and genomic technologies to predict the metabolic parameters and profiles of potential new drug candidates

Mass Spectrometry in Food Analysis Leo Nollet, Robert Winkler, 2022-03-21 The quality and safety of food are crucial

for human nutrition However evaluating the chemical composition of food is challenging for the analyst and requires powerful methods Chromatography and mass spectrometry MS is the gold standard for analyzing complex food samples including raw materials and intermediate and finished products Mass Spectrometry in Food Analysis covers the MS based analysis of different aspects of food quality which include nutritional value profile of macronutrients proteins lipids and carbohydrates micronutrients vitamins and nutraceutical active compounds Additionally sensory quality flavor food pigments safety and detection of pesticides contact materials veterinary drugs and pharmaceuticals organic pollutants and pathogens are covered Key Features Contains the basics of mass spectrometry and experimental strategies Explores determination of macro and micronutrients Analyzes sensory and nutraceutical food quality Discusses detection of contaminants and proof of authenticity Presents emerging methods for food analysis This book contains an introductory section that explains the basics of MS and the difference between targeted and untargeted strategies for beginners Further it points out new analytical challenges such as monitoring contaminants of emerging concern and presents innovative techniques e g ambient ionization MS and data mining Also available in the Food Analysis Properties Series Nanoemulsions in Food Technology Development Characterization and Applications edited by Javed Ahmad and Leo M L Nollet ISBN 978 0 367 61492 8 Sequencing Technologies in Microbial Food Safety and Quality edited by Devarajan Thangadurai Leo M L Nollet Saher Islam and Jeyabalan Sangeetha ISBN 978 0 367 35118 2 Chiral Organic Pollutants Monitoring and Characterization in Food and the Environment edited by Edmond Sanganyado Basil K Munjanja and Leo M L Nollet ISBN 978 0 367 42923 2 For a complete list of books in this series please visit our website at www.crcpress.com Food Analysis Properties book series CRCFOODANPRO

ADME-Enabling Technologies in Drug Design and Development Donglu Zhang, Sekhar Surapaneni, 2012-04-13 A comprehensive guide to cutting edge tools in ADME research The last decade has seen tremendous progress in the development of analytical techniques such as mass spectrometry and molecular biology tools resulting in important advances in drug discovery particularly in the area of absorption distribution metabolism and excretion ADME ADME Enabling Technologies in Drug Design and Development focuses on the current state of the art in the field presenting a comprehensive review of the latest tools for generating ADME data in drug discovery It examines the broadest possible range of available technologies giving readers the information they need to choose the right tool for a given application a key requisite for obtaining favorable results in a timely fashion for regulatory filings With over thirty contributed chapters by an international team of experts the book provides A thorough examination of current tools covering both electronic mechanical technologies and biologically based ones Coverage of applications for each technology including key parameters optimal conditions for intended results protocols and case studies Detailed discussion of emerging tools and techniques from stem cells and genetically modified animal models to imaging technologies Numerous figures and diagrams throughout the text Scientists and researchers in drug metabolism pharmacology medicinal chemistry pharmaceuticals toxicology and bioanalytical

science will find ADME Enabling Technologies in Drug Design and Development an invaluable guide to the entire drug development process from discovery to regulatory issues ADMET for Medicinal Chemists Katya Tsaoun,Steven A. Kates,2011-02-15 This book guides medicinal chemists in how to implement early ADMET testing in their workflow in order to improve both the speed and efficiency of their efforts Although many pharmaceutical companies have dedicated groups directly interfacing with drug discovery the scientific principles and strategies are practiced in a variety of different ways This book answers the need to regularize the drug discovery interface it defines and reviews the field of ADME for medicinal chemists In addition the scientific principles and the tools utilized by ADME scientists in a discovery setting as applied to medicinal chemistry and structure modification to improve drug like properties of drug candidates are examined **ADME and Translational Pharmacokinetics / Pharmacodynamics of Therapeutic Proteins** Honghui Zhou, Frank-Peter Theil,2015-10-26 With an emphasis on the fundamental and practical aspects of ADME for therapeutic proteins this book helps readers strategize plan and implement translational research for biologic drugs Details cutting edge ADME absorption distribution metabolism and excretion and PKPD pharmacokinetic pharmacodynamics modeling for biologic drugs Combines theoretical with practical aspects of ADME in biologic drug discovery and development and compares innovator biologics with biosimilar biologics and small molecules with biologics giving a lessons learned perspective Includes case studies about leveraging ADME to improve biologics drug development for monoclonal antibodies fusion proteins pegylated proteins ADCs bispecifics and vaccines Presents regulatory expectations and industry perspectives for developing biologic drugs in USA EU and Japan Provides mechanistic insight into biodistribution and target driven pharmacokinetics in important sites of action such as tumors and the brain

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