Nmr Spectroscopy In Pharmaceutical Analysis

On-line LC-NMR and Related Techniques

This book gives a comprehensive overview of the basis and the current applications of LC-NMR and related techniques. It deals with the practical aspects of the hardware and software set-up for a successful performance of on-line coupling experiments. It covers the solution of real-word problems from the fields of biomedical, pharmaceutical and environmental studies as

well as the analysis of natural products and polymeric compounds. Thus guidelines for an efficient application of the powerful hyphenated technique LC-NMR in combination with LC-MS are presented. Besides LC-NMR, important techniques such as the on-line coupling of gel permeation chromatography and supercritical fluid chromatography, together with 1H NMR spectroscopy, are described in detail. Fascinating further aspects, such as the application of capillary separation techniques either in the single or parallel detection mode, together with the possibilities of direct 13C monitoring of chromatographic events, are also discussed. Key features include: * Up-to-date information on the theoretical and experimental methodology * Coverage of applications in biomedical, pharmaceutical and natural product analysis, as well as environmental polymer and related hyphenated techniques * Information appropriate for researchers in organic, pharmaceutical and medical chemistry Overall, this book is a requirement for all researchers and staff members dealing with structure elucidation problems in separation science.

Modern Magnetic Resonance

A comprehensive collection of the applications of Nuclear Magnetic Resonance (NMR), Magnetic Resonance Imaging (MRI) and Electron-Spin Resonance (ESR). Covers the wide ranging disciplines in which these techniques are used: * Chemistry; * Biological Sciences; * Pharmaceutical Sciences; * Medical uses; * Marine Science; * Materials Science; * Food Science. Illustrates many techniques through the applications described, e.g.: * High resolution solid and liquid state NMR; * Low resolution NMR, especially important in food science; * Solution State NMR, especially important in pharmaceutical sciences; * Magnetic Resonance Imaging, especially important for medical uses; * Electron Spin Resonance, especially important for spin-labelling in food, marine and medical studies.

Structure-activity Relationship Studies in Drug Development by NMR Spectroscopy

\"NMR (Nuclear Magnetic Resonance) Spectroscopy has found significant applications in drug discovery based on its capacity to map molecular interactions at the atomic level. Chemical shifts, cross relaxation, and exchange of protons are among the NMR parame\"

Applications of NMR Spectroscopy

Applications of NMR Spectroscopy is a book series devoted to publishing the latest advances in the applications of nuclear magnetic resonance (NMR) spectroscopy in various fields of organic chemistry, biochemistry, health and agriculture. The fifth volume of the series features several reviews focusing on NMR spectroscopic techniques for identifying natural and synthetic compounds (polymer and peptide characterization, GABA in tinnitus affected mice), medical diagnosis and therapy (gliomas) and food analysis. The spectroscopic methods highlighted in this volume include high resolution proton magnetic resonance spectroscopy and solid state NMR.

NMR Spectroscopy in Organic Chemistry

In recent years high-resolution nuclear magnetic resonance spec troscopy has found very wide application in organie chemistry in structural and physicochemical investigations and. also in the study of the characteristics of organic compounds which are re lated to the distribution of the electron cloud in the molecules. The vigorous development of this method, which may really be re garded as an independent branch of science, is the result of ex tensive progress in NMR technology, the refinement of its theory, and the accumulation of large amounts of experimental material, which has been correlated by empiricallaws and principles. The literature directly concerned with the NMR method and its applica tion has now grown to such an extent that a complete review of it is practically impossible. Therefore the authors have limited themselves to an examination of only the most important, funda mental, and general investigations. The book consists of six chapters. In the first chapter we have attempted to present the fundamentals of the NMR method in such a way that the reader with little knowledge of the subject will be able to use the method in practical work for investigating simple compounds and solving simple problems. The three subsequent chapters give a deeper

analysis of the method, while the last two chapters and the appendix illustrate the various applications of NMR spectroscopy in organic chemistry.

Spectroscopic Analyses

The book presents developments and applications of these methods, such as NMR, mass, and others, including their applications in pharmaceutical and biomedical analyses. The book is divided into two sections. The first section covers spectroscopic methods, their applications, and their significance as characterization tools; the second section is dedicated to the applications of spectrophotometric methods in pharmaceutical and biomedical analyses. This book would be useful for students, scholars, and scientists engaged in synthesis, analyses, and applications of materials/polymers.

Pharmaceutical Excipients

Meeting the need for a hands-on guide elucidating the role of molecular spectroscopy in the physical characterization of pharmaceutical solids, two experts from the industry gather theoretical discussions of infrared, Raman, and nuclear magnetic resonance spectroscopy. They provide recommendations on spectral data acquisition techniques and include 600 spectra for 300 of the most commonly used excipients. Complete with references, equations, tables, and a CAS registry number index, the book covers the drug development process, including chemical identification of substances, investigative studies, competitor analysis, problem solving activities, reproduction of spectral data, and more.

Proceedings '94

Proceedings of the conference held in Atlantic City, New Jersey, June 1994. Eleven sessions are devoted to NDA/ANDA requirements and international harmonization for analytical development; mass spectrometry in drug discovery and development; FDA issues affecting analytical development and testing; capillary electrophoresis in the pharmaceutical laboratory;

separation of chiral pharmaceutical compounds; solid-state NMR spectroscopy in pharmaceutical analysis; data handling, management, and automation; chiroptical spectroscopy; advances in liquid chromatography; HPLC method development; and on- line analysis. The print is often exaggeratedly large, providing far less material than one would expect out of 411 pages. No index. The publisher is at 7500 Old Oak Blvd., Cleveland, OH 44130. Annotation copyright by Book News, Inc., Portland, OR

Analytical NMR

Reviews the state of the art in analytical NMR, including many specialist applications in NMR spectroscopy. Emphasizing actual practice with modern instruments, the text presents the fundamentals of NMR, experimental procedures for various applications, and NMR automation. Considers a wide range of applications of NMR, from the simplest uses in quality control to advanced pulsed experiments for examination of complex mixtures and biological specimens.

LC-NMR and Other Hyphenated NMR Techniques

This practical guide provides a basic overview of the pros and cons of NMR spectroscopy as both a hyphenated and non-hyphenated technique. The book begins with a description of basic NMR concepts for the structural elucidation of organic compounds and then details the historical development of NMR and hyphenated NMR in the structural elucidation world, followed by applications of hyphenated NMR as LC-NMR and LC-MS-NMR in industry and academia. It also contains updated information on the latest advancements and applications of LC-NMR in such areas as degradation products, drug metabolism, food analysis, and drug discovery. An essential resource for scientists in industry and academia who work in the areas of organic chemistry, medicinal chemistry, process chemistry, and analytical chemistry.

NMR Crystallography

The content of this volume has been added toeMagRes (formerly Encyclopedia of MagneticResonance) - the ahref=\"http://onlinelibrary.wiley.com/book/10.1002/9780470034590/homepage/rf_coils_virtual_issue.htm?c chem&cs=chem-analytic&cu=sitename-ln&cd=sitename-In-MRIgroup-VI\" target=\"_blank\"ultimate online resource for NMR and MRI/a. The term \"NMR Crystallography\" has only recently come intocommon usage, and even now causes raised eyebrows within some partsof the diffraction community. The power of solid-state NMR to givecrystallographic information has considerably increased since theCPMAS suite of techniques was introduced in 1976. In the firstyears of the 21st century, the ability of NMR to provideinformation to support and facilitate the analysis ofsingle-crystal and powder diffraction patterns has become widelyaccepted. Indeed, NMR can now be used to refine diffraction resultsand, in favorable cases, to solve crystal structures with minimal(or even no) diffraction data. The increasing ability to relatechemical shifts (including the tensor components) to thecrystallographic location of relevant atoms in the unit cell viacomputational methods has added significantly to the practice ofNMR crystallography. Diffraction experts will increasingly welcomeNMR as an allied technique in their structural analyses. Indeed,

itmay be that in the future crystal structures will be determined bysimultaneously fitting diffraction patterns and NMR spectra. This Handbook is organised into six sections. The first containsan overview and some articles on fundamental NMR topics, followedby a section concentrating on chemical shifts, and one on couplinginteractions. The fourth section contains articles describing howNMR results relate to fundamental crystallography concepts and todiffraction methods. The fifth section concerns specific aspects ofstructure, such as hydrogen bonding. Finally, four articles in thesixth section give applications of NMR crystallography tostructural biology, organic & pharmaceutical chemistry,inorganic & materials chemistry, and geochemistry. About EMR Handbooks / eMagResHandbooks The Encyclopedia of Magnetic Resonance (up to 2012) andeMagRes (from 2013 onward) publish a wide range of onlinearticles on all aspects of magnetic resonance in physics,chemistry, biology and medicine. The existence of this large numberof articles, written by experts in various fields, is enabling thepublication of a series of EMR Handbooks / eMagResHandbooks on specific areas of NMR and MRI. Thechapters of each of these handbooks will comprise a carefullychosen selection of articles from eMagRes. In consultationwith the eMagRes Editorial Board, the EMRHandbooks / eMagRes Handbooks are coherentlyplanned in advance by specially-selected Editors, and

new articlesare written (together with updates of some already existingarticles) to give appropriate complete coverage. The handbooks areintended to be of value and interest to research students,postdoctoral fellows and other researchers learning about thescientific area in question and undertaking relevant experiments,whether in academia or industry. Have the content of this Handbook and the complete content ofeMagRes at your fingertips! Visit: ahref=\"http://www.wileyonlinelibrary.com/ref/eMagRes\"www.wileyonlinelibrary.com/ref/eMagRes/a View other eMagRes publications ahref=\"http://onlinelibrary.wiley.com/book/10.1002/9780470034590/homepage/emagres_publications.htm\" target=\"_blank\"here/a

NMR Spectroscopy in Pharmaceutical Analysis

For almost a decade, quantitative NMR spectroscopy (qNMR) has been established as valuable tool in drug analysis. In all disciplines, i. e. drug identification, impurity profiling and assay, qNMR can be utilized. Separation techniques such as high performance liquid chromatography,

gas chromatography, super fluid chromatography and capillary electrophoresis techniques, govern the purity evaluation of drugs. However, these techniques are not always able to solve the analytical problems often resulting in insufficient methods. Nevertheless such methods find their way into international pharmacopoeias. Thus, the aim of the book is to describe the possibilities of qNMR in pharmaceutical analysis. Beside the introduction to the physical fundamentals and techniques the principles of the application in drug analysis are described: quality evaluation of drugs, polymer characterization, natural products and corresponding reference compounds, metabolism, and solid phase NMR spectroscopy for the characterization drug substances, e.g. the water content, polymorphism, and drug formulations, e.g. tablets, powders. This part is accompanied by more special chapters dealing with representative examples. They give more detailed information by means of concrete examples. Combines theory, techniques, and concrete applications—all of which closely resemble the laboratory experience Considers international pharmacopoeias, addressing the concern for licensing Features the work of academics and researchers, appealing to a broad readership

NMR in Drug Design

NMR in Drug Design discusses the use of nuclear magnetic resonance (NMR) in studies of the design, structure, mechanism, and actions of pharmaceutical agents. Topics include rational drug design, NMR techniques in drug design, conformational analysis by NMR, macromolecular structure determination, protein-ligand interactions, drug-DNA interactions, and studies of enzyme mechanisms by NMR. This reference book provides invaluable practical information to the scientist working in drug design or NMR research.

Coupling of Capillary Electrophoresis with Nuclear Magnetic Resonance Spectroscopy for the Analysis of Pharmaceutical and Environmental Relevant Compounds

Master's Thesis from the year 2009 in the subject Chemistry - Analytical Chemistry, grade: 1,0, University of Hannover (Anorganische Chemie), language: English, abstract: Separation and

identification of mass-limited chemical samples is the key to understand the complex nature of pharmaceutical and environmental systems. High efficiency separation techniques, such as capillary electrophoresis (CE), coupled to a non-destructive, information-rich detection, such as nuclear magnetic resonance (NMR) spectroscopy, have revolutionized the ability to separate and identify components in small sample volumes. Using this hyphenated system, structure elucidation of analytes separated during an electrophoretic process can be performed using NMR as an on-line detector. Although sensitivity remains an issue for on-line NMR detection, capillary NMR spectroscopy using microcoils has emerged as a major breakthrough for increasing the mass-sensitivity of NMR spectroscopy, because the limit of detection is proportional to the coil diameter. A further development is the miniaturization of the magnet enabling the possibility of a truly portable NMR system. This portable, low-cost NMR sensor, coupled to the rapid CE separation system could enable high-throughput and on-site identification of nanoliter amounts of solution. Furthermore, CE can provide on-line pre-concentration via electrokinetic injection or other stacking techniques to increase the sample concentration. In this research, coupling CE to a laboratory-scale NMR and to a portable NMR system are investigated, with the emphasis on the development of the miniaturized system. For

the experiments with the large-scale 1H NMR system, a group of selected uric acids and xanthines are studied since those compounds are representative of various classes of therapeutical drugs. The portable NMR instrument incorporates lithographically patterned microcoils and a small 1.8 T permanent magnet to measure 19F NMR spectra for the analysis of trifluoroacetic acid (TFA) and longer chain perfluorinated carboxylic acids (PFCAs). Our results demonstrate that coupling CE to a portable NMR system is feasible and can provide a low cost method to obtain structural information about the samples of interest. The results confirm that it was possible to acquire congruent sample data using the ultraviolet/visible (UV/VIS) detector of the CE and the 19F NMR detector. To obtain data, CE and NMR conditions were optimized and different modes of data acquisition were investigated.

Multidimensional Solid-State NMR and Polymers

NMR spectroscopy is the most valuable and versatile analytical tool in chemistry. While excellent monographs exist on high-resolution NMR in liquids and solids, this is the first book

to address multidimensional solid-state NMR. Multidimensional techniques enable researchers to obtain detailed information about the structure, dynamics, orientation, and phase separation of solids, which provides the basis of a better understanding of materials properties on the molecular level.Dramatic progress-much of it pioneered by the authors-has been achieved in this area, especially in synthetic polymers. Solid-state NMR now favorably competes with well-established techniques, such as light, x-ray, or neutron scattering, electron microscopy, and dielectric and mechanical relaxation. The application of multidimensional solid-state NMR inevitably involves use of concepts from different fields of science. This book also provides the first comprehensive treatment of both the new experimental techniques and the theoretical concepts needed in more complex data analysis. The text addresses spectroscopists and polymer scientists by treating the subject on different levels; descriptive, technical, and mathematical approaches are used when appropriate. It presents an overview of new developments with numerous experimental examples and illustrations, which will appeal to readers interested in both the information content as well as the potential of solid-state NMR. The book also contains many previously unpublished details that will be appreciated by those who want to perform the experiments. The techniques described are applicable not only to the

study of synthetic polymers but to numerous problems in solid-state physics, chemistry, materials science, and biophysics. Key Features * Presents original theories and new perspectives on scattering techniques * Provides a systematic treatment of the whole subject * Gives readers access to previously unpublished material * Includes extensive illustrations

Analysis of Drug Impurities

A key component of the overall quality of a pharmaceutical is control of impurities, as their presence, even in small amounts, may affect drug safety and efficacy. The identification and quantification of impurities to acceptable standards presents a significant challenge to the analytical chemist. Analytical science is developing rapidly and provides increasing opportunity to identify the structure, and therefore the origin and safety implications of these impurities, and the challenges of their measurement drives the development of modern quantitative methods. Written for both practicing and student analytical chemists, Analysis of Drug Impurities provides a detailed overview of the challenges and the techniques available to

permit accurate identification and quantification of drug impurities.

Advanced Instrumentation Technology for Pharmaceutical Analysis

This book helps to know the basic Instrumentation techniques in related to Pharmaceutical analysis for the graduate and post graduate scholars in the field of Pharmacy and Pharm D students mainly based on the syllabus prescribed by Pharmacy Council of India. In the important quality control screening of Pharmaceutical components like raw materials, bulk components and finished products, Analytical validation and Product and process development, Thermal analytical methods and X Ray diffraction studies and to know about the modern analytical methods in the Characterisation of interpretation of spectral analytical methods and Chromatographic techniques for the research and development in the field of Pharmaceutical science.

Solid State Characterization of Pharmaceuticals

The field of solid state characterization is central to the pharmaceutical industry, as drug products are, in an overwhelming number of cases, produced as solid materials. Selection of the optimum solid form is a critical aspect of the development of pharmaceutical compounds, due to their ability to exist in more than one form or crystal structure (polymorphism). These polymorphs exhibit different physical properties which can affect their biopharmaceutical properties. This book provides an up-to-date review of the current techniques used to characterize pharmaceutical solids. Ensuring balanced, practical coverage with industrial relevance, it covers a range of key applications in the field. The following topics are included: Physical properties and processes Thermodynamics Intellectual guidance X-ray diffraction Spectroscopy Microscopy Particle sizing Mechanical properties Vapour sorption Thermal analysis & Calorimetry Polymorph prediction Form selection

Applications of NMR Spectroscopy: Volume 9

Applications of NMR Spectroscopy is a book series devoted to publishing the latest advances in the applications of nuclear magnetic resonance (NMR) spectroscopy in various fields of organic chemistry, biochemistry, health and agriculture. The ninth volume of the series features reviews that highlight NMR spectroscopic techniques in microbiology, food science, pharmaceutical analysis and cancer diagnosis. The reviews in this volume are: - NMR spectroscopy for the characterization of photoprotective compounds in cyanobacteria - Coffee assessment using 1H NMR spectroscopy and multivariate data analysis: a review - Evaluation of structure-property relationship of coconut shell lignins by NMR spectroscopy: from biorefinery to high-added value products - Application of NMR spectroscopy in chiral recognition of drugs - NMR-based metabolomics: general aspects and applications in cancer diagnosis

NMR in Pharmaceutical Science

NMR in Pharmaceutical Sciences is intended to be a comprehensive source of information for the many individuals that utilize MR in studies of relevance to the pharmaceutical sector. The book is intended to educate and inform those who develop and apply MR approaches within the wider pharmaceutical environment, emphasizing the toolbox that is available to spectroscopists and radiologists. This book is structured on the key processes in drug discovery, development and manufacture, but underpinned by an understanding of fundamental NMR principles and the unique contribution that NMR (including MRI) can provide. After an introductory chapter, which constitutes an overview, the content is organised into five sections. The first section is on the basics of NMR theory and relevant experimental methods. The rest follow a sequence based on the chronology of drug discovery and development, firstly 'Idea to Lead' then 'Lead to Drug Candidate', followed by 'Clinical Development', and finally 'Drug Manufacture'. The thirty one chapters cover a vast range of topics from analytical chemistry, including aspects involved in regulatory matters and in the prevention of fraud, to clinical imaging studies. Whilst this comprehensive volume will be essential reading for many

scientists based in pharmaceutical and related industries, it should also be of considerable value to a much wider range of academic scientists whose research is related to the various aspects of pharmaceutical R&D; for them it will supply vital understanding of pharmaceutical industrial concerns and the basis of key decision making processes. About eMagRes Handbooks eMagRes (formerly the Encyclopedia of Magnetic Resonance) publishes a wide range of online articles on all aspects of magnetic resonance in physics, chemistry, biology and medicine. The existence of this large number of articles, written by experts in various fields, is enabling the publication of a series of eMagRes Handbooks on specific areas of NMR and MRI. The chapters of each of these handbooks will comprise a carefully chosen selection of eMagRes articles. In consultation with the eMagRes Editorial Board, the eMagRes handbooks are coherently planned in advance by specially-selected Editors, and new articles are written to give appropriate complete coverage. The handbooks are intended to be of value and interest to research students, postdoctoral fellows and other researchers learning about the scientific area in question and undertaking relevant experiments, whether in academia or industry. Have the content of this handbook and the complete content of eMagRes at your fingertips! Visit: www.wileyonlinelibrary.com/ref/eMagRes

Quantitative NMR Spectroscopy in Pharmaceuticals

Over the past fifty years nuclear magnetic resonance spectroscopy, commonly referred to as NMR, has become the preeminent technique for structure determination of organic compounds. With developments in both methodology and instrumentation in the past two decades, NMR has become one of the most powerful and versatile spectroscopic techniques for characterization and quantification. An increasing concern with the well being of individuals and life in general has led to initiatives for improvements in medicine and the world environment, and in these areas analytical chemistry has particularly vital roles to play. Where new drugs or materials with potential commercial value are synthesized, a complete chemical characterization may be required involving considerable analytical work. More than any other analytical method the NMR spectroscopy provides information about the chemical structure and the dynamics of organic molecules. NMR spectroscopy is by definition a quantitative spectroscopic tool because the intensity of a resonance line is directly proportional to the number of resonant nuclei (spins). This fact enables accurate and precise determinations of the

amount of substance.

High-Resolution NMR Techniques in Organic Chemistry

From the initial observation of proton magnetic resonance in water and in paraffin, the discipline of nuclear magnetic resonance has seen unparalleled growth as an analytical method. Modern NMR spectroscopy is a highly developed, yet still evolving, subject which finds application in chemistry, biology, medicine, materials science and geology. In this book, emphasis is on the more recently developed methods of solution-state NMR applicable to chemical research, which are chosen for their wide applicability and robustness. These have, in many cases, already become established techniques in NMR laboratories, in both academic and industrial establishments. A considerable amount of information and guidance is given on the implementation and execution of the techniques described in this book.

New Applications of NMR in Drug Discovery and Development

This book presents a review of new developments in NMR for applications in medicinal chemistry and drug discovery. The contents will focus on consolidated and emerging techniques and methods that are at present not widely applied, however it is considered that they could contribute to the advancement of drug discovery and drug development.

Handbook of Modern Pharmaceutical Analysis

Handbook of Modern Pharmaceutical Analysis, Second Edition, synthesizes the complex research and recent changes in the field, while covering the techniques and technology required for today's laboratories. The work integrates strategy, case studies, methodologies, and implications of new regulatory structures, providing complete coverage of quality assurance from the point of discovery to the point of use. Treats pharmaceutical analysis (PA) as an integral partner to the drug development process rather than as a service to it Covers method

development, validation, selection, testing, modeling, and simulation studies combined with advanced exploration of assays, impurity testing, biomolecules, and chiral separations Features detailed coverage of QA, ethics, and regulatory guidance (quality by design, good manufacturing practice), as well as high-tech methodologies and technologies from \"lab-on-a-chip\" to LC-MS, LC-NMR, and LC-NMR-MS

BioNMR in Drug Research

The vast progress made in the investigation of biomolecules using NMR has only recently been rewarded with the Nobel Prize for Kurt Wüthrich. Edited by a former coworker of Wüthrich, this book presents the theoretical background on NMR of biomolecules, plus the use of NMR techniques in determining the structures of proteins and nucleic acids. BioNMR spectroscopy offers a universal tool for examining the binding of an active substance to its target protein. Its use thereby benefits the rational development of drugs. This interaction can now be investigated in a hitherto unparalleled precision and displayed in 3D - an important prerequisite

for the targeted development of new active substances. The latest methods for characterizing substance-receptor complexes are demonstrated backed by many case studies from pharmaceutical research. Thus it comes as no surprise that a large number of the authors are working for leading pharmaceutical companies. With its successful mixture of basic information and application strategies, coupled with many real-life examples, this is an invaluable guide for both NMR spectroscopists and pharmaceutical researchers.

Essentials of Pharmaceutical Analysis

Recent advances in the pharmaceutical sciences and biotechnology have facilitated the production, design, formulation and use of various types of pharmaceuticals and biopharmaceuticals. This book provides detailed information on the background, basic principles, and components of techniques used for the analysis of pharmaceuticals and biopharmaceuticals. Focusing on those analytical techniques that are most frequently used for pharmaceuticals, it classifies them into three major sections and 19 chapters, each of which

discusses a respective technique in detail. Chiefly intended for graduate students in the pharmaceutical sciences, the book will familiarize them with the components, working principles and practical applications of these indispensable analytical techniques.

Handbook of Pharmaceutical Analysis

Exploring the analysis of pharmaceuticals, including polymorphic forms, this book discusses regulatory requirements in pharmaceutical product development and pharmaceutical testing. It covers methods of drug separation and procedures such as capillary electrophoresis for chromatographic separation of molecules. Additional topics include drug formulation analysis using vibrational and magnetic resonance spectroscopy and identification of drug metabolites and decomposition products using such techniques as mass spectrometry. The book provides more than 300 tables, equations, drawings, and photographs, and convenient, easy-to-use indices, facilitating quick access to each topic.

Coupling of Capillary Electrophoresis with Nuclear Magnetic Resonance Spectroscopy for the Analysis of Pharmaceutical and Environmental Relevant Compo

Master's Thesis from the year 2009 in the subject Chemistry - Analytical Chemistry, grade: 1,0, University of Hannover (Anorganische Chemie), language: English, abstract: Separation and identification of mass-limited chemical samples is the key to understand the complex nature of pharmaceutical and environmental systems. High efficiency separation techniques, such as capillary electrophoresis (CE), coupled to a non-destructive, information-rich detection, such as nuclear magnetic resonance (NMR) spectroscopy, have revolutionized the ability to separate and identify components in small sample volumes. Using this hyphenated system, structure elucidation of analytes separated during an electrophoretic process can be performed using NMR as an on-line detector. Although sensitivity remains an issue for on-line NMR detection, capillary NMR spectroscopy using microcoils has emerged as a major breakthrough for increasing the mass-sensitivity of NMR spectroscopy, because the limit of detection is

proportional to the coil diameter. A further development is the miniaturization of the magnet enabling the possibility of a truly portable NMR system. This portable, low-cost NMR sensor, coupled to the rapid CE separation system could enable high-throughput and on-site identification of nanoliter amounts of solution. Furthermore, CE can provide on-line pre-concentration via electrokinetic injection or other stacking techniques to increase the sample concentration. In this research, coupling CE to a laboratory-scale NMR and to a portable NMR system are investigated, with the emphasis on the development of the miniaturized system. For the experiments with the large-scale 1H NMR system, a group of selected uric acids and xanthines are studied since those compounds are representative of various classes of therapeutical drugs. The portable NMR instrument incorporates lithographically patterned microcoils and a small 1.8 T permanent magnet to measure 19F NMR spectra for the analysis of

Annual Reports on NMR Spectroscopy

Nuclear magnetic resonance (NMR) is an analytical tool used by chemists and physicists to

study the structure and dynamics of molecules. In recent years, no other technique has gained such significance as NMR spectroscopy. It is used in all branches of science in which precise structural determination is required and in which the nature of interactions and reactions in solution is being studied. Annual Reports on NMR Spectroscopy has established itself as a premier means for the specialist and non-specialist alike to become familiar with new techniques and applications of NMR spectroscopy. This volume of Annual Reports on NMR Spectroscopy focuses on the analytical tools used by chemists and physicists, taken together with other volumes of this series, an excellent account of progress in NMR and its many applications is provided and anyone using NMR will find interest in this Serial

Discrimination of Chiral Compounds Using NMR Spectroscopy

A comprehensive overview of the use of NMR spectroscopy for chiral discrimination Discrimination of Chiral Compounds Using NMR Spectroscopy concisely covers the broad array of reagents that make it possible to determine the optical purity and assign the absolute

configuration of many classes of compounds. It describes chiral NMR derivatizing agents, solvating agents, metal-based reagents, and liquid crystals and discusses the range and types of compounds for which they can be used for analysis. After an overview of chiral reagents and methodologies, this reference: * Includes comprehensive coverage of the chiral reagents that have been reported * Catalogs the range of compounds for which different reagents have been shown to be effective * Includes specialty categories such as liquid crystals, ionic liquids, and the formation of chiral aggregates from achiral building blocks that do not fit into the broader categories * Offers experimental strategies for using the reagents that are likely to improve the quality of the results This guide describes the various systems and their overall utility, but goes further to show the full scope of the field as a way of guiding investigations into the optimal chiral reagents for use in NMR spectroscopy. It's a practical reference for organic chemists in the pharmaceutical industry, academia, and other areas, NMR spectroscopists, and researchers involved in the isolation and structure determination of natural products.

NMR Applications in Biopolymers

Elucidating the structures of biopolymers as they exist in nature has long been a goal of biochemists and biologists. Understanding how these substances interact with themselves, other solutes, and solvents can provide useful insights into many areas of biochemistry, agriculture, food science and medicine. Knowledge of the structure of a protein or complex carbohydrate in its native form provides guidelines for the chemical or genetic modifications often desired to optimize these compounds to specific needs and applications. For example, in the pharmaceutical industry, structure-function relationships involving biopolymers are studied rou tinely as a means to design new drugs and improve their efficacies. The tools to conduct structure investigations of biopolymers at the molecular level are limited in number. Historically X-ray crystallography has been the most attractive method to conduct studies of this type. How ever, X-ray methods can only be applied to highly ordered, crystalline materials, thus obviating studies of solution dynamics that are often critical to attaining a global understanding of biopolymer behavior. In recent years, nuclear magnetic resonance (NMR) spectroscopy has evolved to become a powerful tool to probe the structures of biopolymers in

solution and in the solid state. NMR provides a means to study the dynamics of polymers in solution, and to examine the effects of solute, solvent and' other factors~n polymer behavior. With the development of 2D and 3D forms of NMR spectroscopy, it is now possible to assess the solution conforma tions of small proteins, oligonucleotides and oligosaccharides.

Applications of NMR Spectroscopy: Volume 9

Applications of NMR Spectroscopy is a book series devoted to publishing the latest advances in the applications of nuclear magnetic resonance (NMR) spectroscopy in various fields of organic chemistry, biochemistry, health and agriculture. The ninth volume of the series features reviews that highlight NMR spectroscopic techniques in microbiology, food science, pharmaceutical analysis and cancer diagnosis. The reviews in this volume are: - NMR spectroscopy for the characterization of photoprotective compounds in cyanobacteria - Coffee assessment using 1H NMR spectroscopy and multivariate data analysis: a review - Evaluation of structure-property relationship of coconut shell lignins by NMR spectroscopy: from

biorefinery to high-added value products - Application of NMR spectroscopy in chiral recognition of drugs - NMR-based metabolomics: general aspects and applications in cancer diagnosis

LC-NMR

The isolation and structural characterization of substances present at very low concentrations, as is necessary to satisfy regulatory requirements for pharmaceutical drug degradants and impurities, can present scientific challenges. The coupling of HPLC with NMR spectroscopy has been at the forefront of cutting-edge technologies to address these issues. LC-NMR: Expanding the Limits of Structure Elucidation presents a comprehensive overview of key concepts in HPLC and NMR that are required to achieve definitive structure elucidation with very low levels of analytes. Because skill sets from both of these highly established disciplines are involved in LC-NMR, the author provides introductory background to facilitate readers' proficiency in both areas, including an entire chapter on NMR theory. The much-anticipated

second edition provides guidance in setting up LC-NMR systems, discussion of LC methods that are compatible with NMR, and an update on recent hardware and software advances for system performance, such as improvements in magnet design, probe technology, and solvent suppression techniques that enable unprecedented mass sensitivity in NMR. This edition features methods to quantify concentration and assess purity of isolated metabolites on the micro scale and incorporates computational approaches to accelerate the structure elucidation process. The author also includes implementation and application of qNMR and automated and practical use of computational chemistry combined with QM and DFT to predict highly accurate NMR chemical shifts. The text focuses on current developments in chromatographic-NMR integration, with particular emphasis on utility in the pharmaceutical industry. Applications include trace analysis, analysis of mixtures, and structural characterization of degradation products, impurities, metabolites, peptides, and more. The text discusses novel uses and emerging technologies that challenge detection limits as well future directions for this important technique. This book is a practical primary resource for NMR structure determination—including theory and application—that guides the reader through the steps required for isolation and NMR structure elucidation on the micro scale.

NMR Spectroscopy in Drug Development and Analysis

Since the development of the NMR spectrometer in the 1950s, NMR spectra have been widely used for the elucidation of the 2D structure of newly synthesized and natural compounds. In the 1980s, the high-resolution NMR spectrometer (\u003e 300 Mhz) and 2D experiments were introduced, which opens up the possibility to determine the 3D structure of large molecules, especially biomolecules. However, NMR spectroscopy has been rarely applied to drug analysis. This book illustrates the power and versatility of NMR spectroscopy in the determination of impurities in and the content of drugs, the composition of polymer excipients, the characterization of isomeric drug mixtures, the complexity of drugs with small-size components or ions, and the behavior of drugs in acid and basic solution. In addition, NMR spectroscopy and especially the hyphenated technique with HPLC is shown to be a powerful tool to measure a drug and its metabolites in various body fluids. The solid state NMR technique can give information on the structure, especially the conformation of drugs and excipients in drug formulations. Recently, SAR by NMR, introduced by Fesik, impressively

demonstrated the potential of NMR spectroscopy in drug development and in the characterization of the interaction between large molecules and ligands. The complexation between proteins, lipids and cyclodextrins with drugs is described. Finally, NMR imaging (MRI and MRS) can be used to characterize the liberation of drugs from a drug formulation. Furthermore, the distribution of substances in plants, in animals, in tissues and in humans can be visualized by imaging. In short, this book covers all aspects of drug analysis.

Natural Products Analysis

This book highlights analytical chemistry instrumentation and practices applied to the analysis of natural products and their complex mixtures, describing techniques for isolating and characterizing natural products. • Applies analytical techniques to natural products research – an area of critical importance to drug discovery • Offers a one-stop shop for most analytical methods: x-ray diffraction, NMR analysis, mass spectrometry, and chemical genetics • Includes coverage of natural products basics and highlights antibacterial research, particularly important

as efforts to combat drug resistance gain prominence • Covers instrumental techniques with enough detail for both current practitioners and beginning researchers

Proceedings of 4th World Congress on Mass Spectrometry 2017

June 19-21, 2017 London, UK Key Topics : Applications of Mass Spectrometry, New Approaches in Mass Spectrometry, Recent Advances and Development in Mass Spectrometry, Mass spectrometry Imaging, Fundamentals of Mass Spectrometry, Ionization Techniques, Mass Spectrometry Configurations and Separation Techniques, Chromatography and High Performance Liquid Chromatography (HPLC), Maintenance, Troubleshooting, Data Analysis and Experimentation in Mass Spectrometry, Mass Spectrometry in Proteome Research, Proteomics and its applications, Mass Spectrometry in Metabolomics and Lipidomics, Hyphenated Techniques (LC-NMR-MS, HPLC-ESI-MS, MC-ICP-MS, HPLC-ICP-MS, UPLC-Q-TOF/MS), Mass spectrometry in environmental analysis, Spectroscopy, Clinical application of mass spectrometry, UV, IR and Ion Spectroscopy, Nuclear Magnetic

Resonance(NMR) Spectroscopy, Mass Spectrometry in Toxicology, Mass spectrometry in Analytical Science, Mass Spectrometry in Pharmaceutical Analysis,

Pharmaceutical Analysis

The use of analytical sciences in the discovery, development andmanufacture of pharmaceuticals is wide-ranging. From the analysisof minute amounts of complex biological materials to the qualitycontrol of the final dosage form, the use of analytical technologycovers an immense range of techniques and disciplines. This book concentrates on the analytical aspects of drugdevelopment and manufacture, focusing on the analysis of the activeingredient or drug substance. It provides those joining theindustry or other areas of pharmaceutical research with a source ofreference to a broad range of techniques and their applications,allowing them to choose the most appropriate analytical techniquefor a particular purpose. The volume is directed at analytical chemists, industrialpharmacists, organic chemists, pharmaceutical chemists andbiochemists.

Annual Reports on NMR Spectroscopy

Nuclear magnetic resonance (NMR) is an analytical tool used by chemists and physicists to study the structure and dynamics of molecules. In recent years, no other technique has gained such significance as NMR spectroscopy. It is used in all branches of science in which precise structural determination is required and in which the nature of interactions and reactions in solution is being studied. Annual Reports on NMR Spectroscopy has established itself as a premier means for the specialist and non-specialist alike to become familiar with new techniques and applications of NMR spectroscopy. This volume of Annual Reports on NMR Spectroscopy focuses on the analytical tool used by chemists and physicists and inlcudes topics such as Profiling of Food Samples, Recent Advances in Solution NMR Studies and Magic Angle Spinning NMR Studies of Protein Assemblies

Peptide Therapeutics

Peptide therapy has become a key strategy in innovative drug development, however, one of the potential barriers for the development of novel peptide drugs in the clinic is their deficiencies in clearly defined chemistry, manufacturing and controls (CMC) strategy from clinical development to commercialization. CMC can often become a rate-limiting step due to lack of knowledge and lack of a formal policy or guidelines on CMC for peptide-based drugs. Regulators use a risk-based approach, reviewing applications on a case-by-case basis. Peptide Therapeutics: Strategy and Tactics for Chemistry, Manufacturing, and Controls covers efficient manufacturing of peptide drug substances, a review of the process for submitting applications to the regulatory authority for drug approval, a holistic approach for quality attributes and quality control from a regulatory perspective, emerging analytical tools for the characterisation of impurities, and the assessment of stability. This book is an essential reference work for students and researchers, in both academia and industry, with an interest in learning about CMC, and facilitating development and manufacture of peptide-based drugs.

Process Analytical Technology

Process Analytical Technology explores the concepts of PAT and its application in the chemical and pharmaceutical industry from the point of view of the analytical chemist. In this new edition all of the original chapters have been updated and revised, and new chapters covering the important topics of sampling, NMR, fluorescence, and acoustic chemometrics have been added. Coverage includes: Implementation of Process Analytical Technologies UV-Visible Spectroscopy for On-line Analysis Infrared Spectroscopy for Process Analytical Applications Process Raman Spectroscopy Process NMR Spectrscopy: Technology and On-line Applications Fluorescent Sensing and Process Analytical Applications Chemometrics in Process Analytical Technology (PAT) On-Line PAT Applications of Spectroscopy in the Pharmaceutical Industry Future Trends for PAT for Increased Process Understanding and Growing Applications in Biomanufacturing NIR Chemical Imaging This volume is an important starting point for anyone wanting to implement PAT and is intended not only to assist a newcomer to the field but also to provide up-to-date information for those who practice process analytical chemistry and PAT. It is relevant for chemists, chemical and process

engineers, and analytical chemists working on process development, scale-up and production in the pharmaceutical, fine and specialty chemicals industries, as well as for academic chemistry, chemical engineering, chemometrics and pharmaceutical science research groups focussing on PAT. Review from the First Edition “The book provides an excellent first port of call for anyone seeking material and discussions to understand the area better. It deserves to be found in every library that serves those who are active in the field of Process Analytical Technology.”—Current Engineering Practice

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