



U. Holzgrabe, I. Wawer,
B. Diehl (editors)

NMR

SPECTROSCOPY IN PHARMACEUTICAL ANALYSIS

Nmr Spectroscopy In Pharmaceutical Analysis

Atta-ur-Rahman,M. Iqbal Choudhary

Nmr Spectroscopy In Pharmaceutical Analysis:

NMR Spectroscopy in Pharmaceutical Analysis Iwona Wawer,Bernd Diehl,2008-08-22 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 Spectroscopy in Drug Development and Analysis Ulrike Holzgrabe,Iwona Wawer,Bernd Diehl,2008-07-11 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 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

NMR Spectroscopy in Pharmaceutical Analysis Iwona Wawer,Bernd Diehl,2017-07-07 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 Pharmaceutical Analysis David C Lee,Michael L.

Webb,2009-02-12 The use of analytical sciences in the discovery development and manufacture of pharmaceuticals is wide ranging From the analysis of minute amounts of complex biological materials to the quality control of the final dosage form the use of analytical technology covers an immense range of techniques and disciplines This book concentrates on the analytical aspects of drug development and manufacture focusing on the analysis of the active ingredient or drug substance It provides those joining the industry or other areas of pharmaceutical research with a source of reference to a broad range of techniques and their applications allowing them to choose the most appropriate analytical technique for a particular purpose The volume is directed at analytical chemists industrial pharmacists organic chemists pharmaceutical chemists and biochemists NMR in Pharmaceutical Science Jeremy R. Everett,Robin K. Harris,John C. Lindon,Ian D. Wilson,2015-09-28 NMR in

Pharmaceutical Sciences is intended to be a comprehensive source of information for the many individuals that utilize NMR in studies of relevance to the pharmaceutical sector The book is intended to educate and inform those who develop and apply NMR 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 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

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Modern NMR Crystallography David L Bryce,2025-03-31 NMR crystallography has blossomed as a focussed field of research in recent years and is now acknowledged as such by the International Union of Crystallography The term NMR crystallography itself has proven to be inclusive of many NMR centric approaches which seek to solve or refine crystal structures Since the publication of a seminal book over ten years ago there have been numerous advances in experimental methodology in computational tools and in the fruitful combination of these to provide new insights into structure and dynamics in a range of solid materials This book presents insightful contributions describing these advances as well as a broad range of cutting edge applications to small molecules pharmaceuticals biomolecules energy materials and more It highlights the complementarity of NMR diffraction and computational approaches and presents several examples where complete structure solutions are only possible via this synergy Striking a balance between appealing to NMR experts and those outside the field it will appeal to practitioners of diffraction based crystallography and computational and theoretical chemists *NMR in Pharmaceutical Science* Jeremy R. Everett,Robin K. Harris,John C. Lindon,Ian D.

Wilson,2015-08-24 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

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Solid-State Properties of Pharmaceutical Materials Stephen R. Byrn,George Zografi,Xiaoming (Sean) Chen,2017-08-28 Presents a detailed discussion of important solid state properties methods and applications of solid state analysis Illustrates the various phases or forms that solids can assume and discusses various issues related to the relative stability of solid forms and tendencies to undergo transformation Covers key methods of solid state analysis including X ray powder diffraction thermal analysis microscopy spectroscopy and solid state NMR Reviews critical physical attributes of pharmaceutical materials mainly related to drug substances including particle size surface area hygroscopicity mechanical properties solubility and physical and chemical stability Showcases the application of solid state material science in rational selection of drug solid forms analysis of various solid forms within drug substance and the drug product and pharmaceutical product development Introduces appropriate manufacturing and control procedures using Quality by Design and other strategies that lead to safe and effective products with a minimum of resources and time **Essentials of Pharmaceutical Analysis** Muhammad Sajid Hamid Akash,Kanwal Rehman,2025-04-29 This 2nd edition of the comprehensive resource on

pharmaceutical analysis and analytical techniques builds upon the success of its first edition by incorporating updated methodologies expanded content and fresh insights into modern practices. Designed for students, researchers, and industry professionals alike, the book bridges theoretical principles with practical applications covering both classical methods and innovative approaches across spectrophotometry, chromatography, mass spectrometry, and thermal analysis. Detailed chapters elucidate method development, instrumentation, quality control, and regulatory compliance while enriched case studies and examples from environmental science, biomedical research, and materials science illustrate real world applications. New sections highlight the integration of miniaturized instruments, hyphenated techniques, and computational tools including machine learning and cloud based analytics. Enhanced diagrams, tables, and summaries further facilitate the understanding of complex analytical concepts. This edition not only reinforces essential foundational knowledge but also equips readers with advanced practical skills to meet evolving challenges in pharmaceutical research and quality assurance. Whether you are seeking a solid academic grounding or aiming to adopt cutting edge techniques, this book provides an indispensable guide to mastering contemporary pharmaceutical analysis and the future of analytical chemistry. With its rigorous and accessible approach, this book serves as an essential reference that inspires innovation in analytical sciences.

Applications of NMR Spectroscopy: Volume 9 M. Iqbal Choudhary, Atta-Ur-Rahman, 2021-12-29. 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 ^{1}H 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.

New Applications of NMR in Drug Discovery and Development Leoncio Garrido, Nicolau Beckmann, 2013-07-18. This book presents a review of recent developments in NMR applications in pharmaceutical research. Consideration is given to consolidated and emerging techniques and methods in NMR, many of which are not widely applied but are likely to provide new opportunities for drug design. The first part of the book is dedicated to the description of NMR as a tool for the analysis of chemicals and interaction with targets. Particular emphasis is put on applications with unexploited potential for drug discovery and development. The next seven chapters describe NMR approaches to investigate *in vivo* models of interest in drug discovery and development, with the attention focused on anatomy, function, metabolism, and molecular cellular aspects. Finally, consideration is given to the application of *in vivo* NMR to the identification and characterization of biomarkers with the aim of monitoring the outcome of therapeutic intervention in selected human diseases, including the study of drug

metabolism and toxicity Aimed at NMR spectroscopists and pharmaceutical scientists this title will be invaluable at putting NMR within context in its role in drug discovery and development This resource will be essential reading for those both new and already active in these areas *Modern Methods of Pharmaceutical Analysis* Roger E. Schirmer,1982

Pharmaceutical Excipients David E. Bugay,W. Paul Findlay,1999-02-23 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 *Applications of NMR Spectroscopy: Volume 9*

Atta-ur-Rahman,M. Iqbal Choudhary,2021-12-29 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 ^{1}H 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 *Analysis of Steroid Hormone Drugs*

S. Görög,György Szász,1978 *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

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