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This book summarizes science and technology of a new generation of high-energy and insensitive explosives. The objective is to provide professionals with comprehensive information on the synthesis and the physicochemical and detonation properties of the explosives. Potential technologies applicable for treatment of contaminated wastestreams from manufacturing facilities and environmental matrices are also included. This book provides the reader an insight into the depth and breadth of theoretical and empirical models and experimental techniques currently being developed in the field of energetic materials. It presents the latest research by DoD engineers and scientists, and some of DoD's academic and industrial researcher partners. The topics explored and the simulations developed or modified for the purposes of energetics may find application in other closely related fields, such as the pharmaceutical industry. One of the key features of the book is the treatment of wastewaters generated during manufacturing of these energetic materials.

Poppy, the third volume in the series Medicinal and Aromatic Plants - Industrial Profiles presents up-to-date information on Poppy and related species. The introduction emphasizes the importance of Poppy, giving a historical evaluation. In the chapters describing the botany and taxonomy of the genus some novel aspects are discussed, e.g., special m

This book presents a range of current research topics in biological network modeling, as well as its application in studies on human hosts, pathogens, and diseases. Systems biology is a rapidly expanding field that involves the study of biological systems through the mathematical modeling and analysis of large volumes of biological data. Gathering contributions from renowned experts in the field, some of the topics discussed in depth here include networks in systems biology, the computational modeling of multidrug-resistant bacteria, and systems biology of cancer. Given its scope, the book is intended for researchers, advanced students, and practitioners of systems biology. The chapters are research-oriented, and present some of the latest findings on their respective topics.

Aqueous solubility is one of the major challenges in the early stages of drug discovery. One of the most common and effective methods for enhancing solubility is the addition of an organic solvent to the aqueous solution. Along with an introduction to cosolvency models, the Handbook of Solubility Data for Pharmaceuticals provides an extensive database of solubility for pharmaceuticals in mono solvents and binary solvents. Aqueous solubility data can be found in the Handbook of Aqueous Solubility Data by Samuel Yalkowsky and Yan He. Visit www.crcpress.com for more information. In addition to the experimental efforts to measure the solubility of drugs in mono and mixed solvents, this book discusses the advantages and limitations of a number of mathematical models used to predict the solubility in mono or mixed solvent systems. It covers the pharmaceutical cosolvents and other organic solvents that are used in syntheses,

separations, and other pharmaceutical processes. The solutes featured include the available data for official drugs, drug candidates, precursors of drugs, metabolites, and degradation products of pharmaceuticals. The author also presents the solubilities of amino acids since they play an important role in peptide drug properties. Collecting drug solubilities in various cosolvents, this time-saving handbook includes the mixtures and model constants needed to predict undetermined solubilities. It describes mathematical models that enable data to be derived and provides estimates on how drugs are likely to behave in a given cosolvent. A software program and associated user manual are available on the author's website.

This book is a printed edition of the Special Issue "Rietveld Refinement in the Characterization of Crystalline Materials" that was published in *Crystals*

Unity in Diversity and the Standardisation of Clinical Pharmacy Services represents the proceedings of the 17th Asian Conference on Clinical Pharmacy (ACCP 2017), held 28—30 July 2017 in Yogyakarta, Indonesia. The primary aim of ACCP 2017 was to bring together experts from all fields of clinical pharmacy to facilitate the discussion and exchange of research ideas and results. The conference provided a forum for the dissemination of knowledge and exchange of experiences. As such, it brought together clinical pharmacy scholars, pharmacy practitioners, policy makers and stakeholders from all areas of pharmacy society and all regions of the world to share their research, knowledge, experiences, concepts, examples of good practice, and critical analysis with their international peers. This year also marks the celebration of 20 years of ACCP. Central themes of the conference and contributed papers were Clinical Pharmacy, Social and Administrative Pharmacy, Pharmacy Education, Pharmacoeconomics, Pharmacoepidemiology, Complementary and Alternative Medicine (CAM) and a number of related topics in the field of Pharmacy.

The third edition of this popular work is revised to include the latest developments in this fast-changing field. Its interdisciplinary approach elegantly combines the chemistry and engineering to explore the fundamentals and optimization processes involved.

This book provides up-to-date information on bioinformatics tools for the discovery and development of new drug molecules. It discusses a range of computational applications, including three-dimensional modeling of protein structures, protein-ligand docking, and molecular dynamics simulation of protein-ligand complexes for identifying desirable drug candidates. It also explores computational approaches for identifying potential drug targets and for pharmacophore modeling. Moreover, it presents structure- and ligand-based drug design tools to optimize known drugs and guide the design of new molecules. The book also describes methods for identifying small-molecule binding pockets in proteins, and summarizes the databases used to explore the essential properties of drugs, drug-like small molecules and their

targets. In addition, the book highlights various tools to predict the absorption, distribution, metabolism, excretion (ADME) and toxicity (T) of potential drug candidates. Lastly, it reviews in silico tools that can facilitate vaccine design and discusses their limitations.

Practical Aspects of Computational Chemistry II: An Overview of the Last Two Decades and Current Trends gathers the discussion of advances made within the last 20 years by well-known experts in the area of theoretical and computational chemistry and physics. The title reflects the celebration of the twentieth anniversary of the "Conference on Current Trends in Computational Chemistry (CCTCC)" to success of which all authors contributed. Starting with the recent development of modeling of solvation effect using the Polarizable Continuum Model (PCM) at the Coupled-Cluster level and the effects of extreme pressure on the molecular properties within the PCM framework, this volume focuses on the association/dissociation of ion pairs in binary solvent mixtures, application of graph theory to determine the all possible structures and temperature-dependent distribution of water cluster, generalized-ensemble algorithms for the complex molecular simulation, QM/MD based investigation of formation of different nanostructures under nonequilibrium conditions, quantum mechanical study of chemical reactivity of carbon nanotube, covalent functionalization of single walled-carbon nanotube, designing of functional materials, importance of long-range dispersion interaction to study nanomaterials, recent advances in QSPR/QSAR analysis of nitrocompounds, prediction of physico-chemical properties of energetic materials, electronic structure and properties of 3d transition metal dimers, the s-bond activation reactions by transition metal complexes, theoretical modeling of environmental mercury depletion reaction, organolithium chemistry and computational modeling of low-energy electron induced DNA damage. Practical Aspects of Computational Chemistry II: An Overview of the Last Two Decades and Current Trends is aimed at theoretical and computational chemists, physical chemists, materials scientists, and particularly those who are eager to apply computational chemistry methods to problems of chemical and physical importance. This book provides valuable information to undergraduate, graduate, and PhD students as well as to established researchers. Practical Aspects of Computational Chemistry II: An Overview of the Last Two Decades and Current Trends is aimed at theoretical and computational chemists, physical chemists, materials scientists, and particularly those who are eager to apply computational chemistry methods to problems of chemical and physical importance. This book provides valuable information to undergraduate, graduate, and PhD students as well as to established researchers.

Handbook of Neuroemergency Clinical Trials, Second Edition, focuses on the practice of clinical trials in acute neuroscience populations, or what have been called neuroemergencies. Neuroemergencies are complex, life-threatening diseases and disorders, often with devastating consequences, including death or disability. The overall costs are

staggering in terms of annual incidence and costs associated with treatment and survival, yet despite their significance as public health issues, there are few drugs and devices available for definitive treatment. The book focuses on novel therapies and the unique challenges their intended targets pose for the design and analysis of clinical trials. This volume provides neurologists, neuroscientists, and drug developers with a more complete understanding of the scientific and medical issues of relevance in designing and initiating clinical development plans for novel drugs intended for acute neuroscience populations. The editors provide the best understanding of the pitfalls associated with acute CNS drug development and the best information on how to approach and solve issues that have plagued drug development. Presents a comprehensive overview on clinical trials and drug development challenges in acute neuroscience populations Provides neurologists, neuroscientists and drug developers with a complete understanding of scientific and medical issues related to designing clinical trials Edited by leaders in the field who have designed and managed over 50 neuroemergency clinical trials

Of the thousands of novel compounds that a drug discovery project team invents and that bind to the therapeutic target, typically only a fraction of these have sufficient ADME/Tox properties to become a drug product. Understanding ADME/Tox is critical for all drug researchers, owing to its increasing importance in advancing high quality candidates to clinical studies and the processes of drug discovery. If the properties are weak, the candidate will have a high risk of failure or be less desirable as a drug product. This book is a tool and resource for scientists engaged in, or preparing for, the selection and optimization process. The authors describe how properties affect in vivo pharmacological activity and impact in vitro assays. Individual drug-like properties are discussed from a practical point of view, such as solubility, permeability and metabolic stability, with regard to fundamental understanding, applications of property data in drug discovery and examples of structural modifications that have achieved improved property performance. The authors also review various methods for the screening (high throughput), diagnosis (medium throughput) and in-depth (low throughput) analysis of drug properties. * Serves as an essential working handbook aimed at scientists and students in medicinal chemistry * Provides practical, step-by-step guidance on property fundamentals, effects, structure-property relationships, and structure modification strategies * Discusses improvements in pharmacokinetics from a practical chemist's standpoint

The oil palm is a remarkable crop, producing around 40% of the world's vegetable oil from around 6% of the land devoted to oil crops. Conventional breeding has clearly been the major focus of genetic improvement in this crop. A mix of improved agronomy and management, coupled with breeding selection have quadrupled the oil yield of the crop since breeding began in earnest in the 1920s. However, as for all perennial crops with long breeding cycles, oil palm faces

immense challenges in the coming years with increased pressure from population growth, climate change and the need to develop environmentally sustainable oil palm plantations. In *Oil Palm: Breeding, Genetics and Genomics*, world leading organizations and individuals who have been at the forefront of developments in this crop, provide their insights and experiences of oil palm research, while examining the different challenges that face the future of the oil palm. The editors have all been involved in research and breeding of oil palm for many years and use their knowledge of the crop and their disciplinary expertise to provide context and to introduce the different research topics covered.

Positron emission tomography (PET) is a very useful technique for medical diagnosis and drug development.

Radiopharmaceuticals are a key element in PET techniques and one of the pivotal factors influencing the applications of PET. The aim of this Special Issue of *Molecules* is to report on the recent research work on a number of aspects of PET radiopharmaceuticals and their preclinical and clinical use. More specifically, the content of this Special Issue includes but is not limited to radiolabeling design, radiosynthesis, synthesis techniques, quality control methodologies, GMP production methods, product formulation, in vitro and in vivo preclinical PET evaluations, clinical evaluations, dosimetry, stability study and metabolite analysis, and modeling.

A must-have resource to the booming field of sulfur-containing polymers *Sulfur-Containing Polymers* is a state-of-the-art text that offers a synthesis of the various sulfur-containing polymers from low-cost sulfur resources such as elemental sulfur, carbon disulfide (CS₂), carbonyl sulfide (COS) and mercaptan. With contributions from noted experts on the topic, the book presents an in-depth understanding of the mechanisms related to the synthesis of sulfur-containing polymers. The book also includes a review of the various types of sulfur-containing polymers, such as: poly(thioester)s, poly(thioether)s and poly(thiocarbonate)s and poly(thiourethane)s with linear or hyperbranched (dendrimer) architectures. The expert authors provide the fundamentals on the structure-property relationship and applications of sulfur-containing polymers. Designed to be beneficial for both research and application-oriented chemists and engineers, the book contains the most recent research and developments of sulfur-containing polymers. This important book: Offers the first comprehensive handbook on the topic Contains state-of-the-art research on synthesis of sulfur containing polymers from low-cost sulfur-containing compounds Examines the synthesis, mechanism, structure properties, and applications of various types of sulfur-containing polymers Includes contributions from well-known experts Written for polymer chemists, materials scientists, chemists in industry, biochemists, and chemical engineers, *Sulfur-Containing Polymers* offers a groundbreaking text to the field with information on the most recent research.

Offering comprehensive coverage of this hot topic, this two-volume handbook and ready reference treats a wide range of important aspects, from synthesis and catalytic properties of carbon materials to their applications as metal-free catalysts

in various important reactions and industrial processes. Following a look at recent advances in the development of carbon materials as carbon-based metal-free catalysts, subsequent sections deal with a mechanistic understanding for the molecular design of efficient carbon-based metal-free catalysts, with a special emphasis on heteroatom-doped carbon nanotubes, graphene, and graphite. Examples of important catalytic processes covered include clean energy conversion and storage, environmental protection, and synthetic chemistry. With contributions from world-leading scientists, this is an indispensable source of information for academic and industrial researchers in catalysis, green chemistry, electrochemistry, materials science, nanotechnology, energy technology, and chemical engineering, as well as graduates and scientists entering the field.

Repair and regeneration of musculoskeletal tissues is generating substantial interest within the biomedical community. Consequently, these are the most researched tissues from the regeneration point of view. *Regenerative Engineering of Musculoskeletal Tissues and Interfaces* presents information on the fundamentals, progress and recent developments related to the repair and regeneration of musculoskeletal tissues and interfaces. This comprehensive review looks at individual tissues as well as tissue interfaces. Early chapters cover various fundamentals of biomaterials and scaffolds, types of cells, growth factors, and mechanical forces, moving on to discuss tissue-engineering strategies for bone, tendon, ligament, cartilage, meniscus, and muscle, as well as progress and advances in tissue vascularization and nerve innervation of the individual tissues. Final chapters present information on musculoskeletal tissue interfaces.

Comprehensive review of the repair and regeneration of musculoskeletal individual tissues and tissue interfaces Presents recent developments, fundamentals and progress in the field of engineering tissues Reviews progress and advances in tissue vascularization and innervation

Natural Polymers, Biopolymers, Biomaterials, and Their Composites, Blends, and IPNs focuses on the recent advances in natural polymers, biopolymers, biomaterials, and their composites, blends, and IPNs. Biobased polymer blends and composites occupy a unique position in the dynamic world of new biomaterials. The growing need for lubricious coatings and surfaces in medical devices—an outcome of the move from invasive to noninvasive medicines/procedures—is playing a major role in the advancement of biomaterials technology. Natural polymers have attained their cutting-edge technology through various platforms, yet there is a lot of novel information about them that is discussed in the book. This important work covers topics such as chitosan composites for biomedical applications and wastewater treatment, coal biotechnology, biomedical and related applications of second generation polyamidoamines, silk fibers, PEG hydrogels, bamboo fiber reinforced PE composites, jute/polyester composites, magnetic biofoams, and many other interesting aspects of importance to polymer research today.

Plants have served mankind as an important source of foods and medicines. While we all consume plants and their products for nutritional support, a majority of the world population also rely on botanical remedies to meet their health needs, either as their own “traditional medicine” or as “complementary and alternative medicine”. From a pharmaceutical point of view, many compounds obtained from plant sources have long been known to possess bio/pharmacological activities, and historically, plants have yielded many important drugs for human use, from morphine discovered in the early nineteenth century to the more recent paclitaxel and artemisinin. Today, we are witnessing a global resurgence in interest and use of plant-based therapies and botanical products, and natural products remain an important and viable source of lead compounds in many drug discovery programs. This Special Issue on “Plant Natural Products for Human Health” compiles a series of scientific reports to demonstrate the medicinal potentials of plant natural products. It covers a range of disease targets, such as diabetes, inflammation, cancer, neurological disease, cardiovascular disease, liver damage, bacterial, and fungus infection and malarial. These papers provide important insights into the current state of research on drug discovery and new techniques. It is hoped that this Special Issue will serve as a timely reference for researchers and scholars who are interested in the discovery of potentially useful molecules from plant sources for health-related applications.

Understand and assess the design, delivery, and efficacy of orally administered drugs A practical guide to understanding oral bioavailability, one of the major hurdles in drug development and delivery, Oral Bioavailability: Basic Principles, Advanced Concepts, and Applications is designed to help chemists, biologists, life science researchers, pharmaceutical scientists, pharmacologists, clinicians, and graduate and students become familiar with the fundamentals and practices of the science of oral bioavailability. The difference in rate and extent between a drug taken orally and the actual amount of a drug reaching the circulatory system, oral bioavailability is an essential parameter for determining the efficacy and adverse effects of new and developing medications, as well as finding an optimal dosing regimen. This book provides a much-needed one-stop resource to help readers better understand and appreciate the many facets and complex problems of oral bioavailability, including the basic barriers to oral bioavailability, the methods used to determine relevant parameters, and the challenges of drug delivery. In addition, this comprehensive book discusses biological and physicochemical methods for improving bioavailability, integrates physicochemistry with physiology and molecular biology, and includes several state-of-the-art technologies and approaches—Caco-2 cell culture model, MDCK, and other related cell culture models—which are used to study the science of oral bioavailability.

Multi-volume major reference work bringing together histories of companies that are a leading influence in a particular industry or geographic location. For students, job candidates, business executives, historians and investors.

Guidelines from ACS to help authors and editors in preparing scientific texts.

In the time since the second edition of The ACS Style Guide was published, the rapid growth of electronic communication has dramatically changed the scientific, technical, and medical (STM) publication world. This dynamic mode of dissemination is enabling scientists, engineers, and medical practitioners all over the world to obtain and transmit information quickly and easily. An essential constant in this changing environment is the requirement that information remain accurate, clear, unambiguous, and ethically sound. This extensive revision of The ACS Style Guide thoroughly examines electronic tools now available to assist STM writers in preparing manuscripts and communicating with publishers. Valuable updates include discussions of markup languages, citation of electronic sources, online submission of manuscripts, and preparation of figures, tables, and structures. In keeping current with the changing environment, this edition also contains references to many resources on the internet. With this wealth of new information, The ACS Style Guide's Third Edition continues its long tradition of providing invaluable insight on ethics in scientific communication, the editorial process, copyright, conventions in chemistry, grammar, punctuation, spelling, and writing style for any STM author, reviewer, or editor. The Third Edition is the definitive source for all information needed to write, review, submit, and edit scholarly and scientific manuscripts.

Chemoinformatics is equipped to impact our life in a big way mainly in the fields of chemical, medical and material sciences. This book is a product of several years of experience and passion for the subject written in a simple lucid style to attract the interest of the student community who wish to master chemoinformatics as a career. The topics chosen cover the entire spectrum of chemoinformatics activities (methods, data and tools). The algorithms, open source databases, tutorials supporting theory using standard datasets, guidelines, questions and do it yourself exercises will make it valuable to the academic research community. At the same time every chapter devotes a section on development of new software tools relevant for the growing pharmaceutical, fine chemicals and life sciences industry. The book is intended to assist beginners to hone their skills and also constitute an interesting reading for the experts. This is the first complete book of polymer terminology ever published. It contains more than 7,500 polymeric material terms. Supplementary electronic material brings important relationships to life, and audio supplements include pronunciation of each term.

An authoritative, systematic, and comprehensive description of current CMP technology Chemical Mechanical Planarization (CMP) provides the greatest degree of planarization of any known technique. The current standard for integrated circuit (IC) planarization, CMP is playing an increasingly important role in other related applications such as microelectromechanical systems (MEMS) and computer hard drive manufacturing. This reference focuses on the chemical aspects of the technology and includes contributions from the foremost experts on

specific applications. After a detailed overview of the fundamentals and basic science of CMP, *Microelectronic Applications of Chemical Mechanical Planarization*: Provides in-depth coverage of a wide range of state-of-the-art technologies and applications Presents information on new designs, capabilities, and emerging technologies, including topics like CMP with nanomaterials and 3D chips Discusses different types of CMP tools, pads for IC CMP, modeling, and the applicability of tribometry to various aspects of CMP Covers nanotopography, CMP performance and defect profiles, CMP waste treatment, and the chemistry and colloidal properties of the slurries used in CMP Provides a perspective on the opportunities and challenges of the next fifteen years Complete with case studies, this is a valuable, hands-on resource for professionals, including process engineers, equipment engineers, formulation chemists, IC manufacturers, and others. With systematic organization and questions at the end of each chapter to facilitate learning, it is an ideal introduction to CMP and an excellent text for students in advanced graduate courses that cover CMP or related semiconductor manufacturing processes.

The book covers theoretical background and methodology as well as all current applications of Quantitative Structure-Activity Relationships (QSAR). Written by an international group of recognized researchers, this edited volume discusses applications of QSAR in multiple disciplines such as chemistry, pharmacy, environmental and agricultural sciences addressing data gaps and modern regulatory requirements. Additionally, the applications of QSAR in food science and nanoscience have been included – two areas which have only recently been able to exploit this versatile tool. This timely addition to the series is aimed at graduate students, academics and industrial scientists interested in the latest advances and applications of QSAR.

Regenerative Engineering of Musculoskeletal Tissues and Interfaces Woodhead Publishing

At last, here is a baseline book for anyone who is confused by cryptic computer programs, algorithms and formulae, but wants to learn about applied bioinformatics. Now, anyone who can operate a PC, standard software and the internet can also learn to understand the biological basis of bioinformatics, of the existence as well as the source and availability of bioinformatics software, and how to apply these tools and interpret results with confidence. This process is aided by chapters that introduce important aspects of bioinformatics, detailed bioinformatics exercises (including solutions), and to cap it all, a glossary of definitions and terminology relating to bioinformatics.

Zeolite synthesis is an active field of research. As long as this continues, new phases will be discovered and new techniques for preparing existing phases will appear. This edition of *Verified Synthesis of Zeolitic Materials* contains all the recipes from the first edition plus 24 new recipes. Five new introductory articles have been included plus those from the first edition, some of which have been substantially revised. The XRD patterns have been recorded using different instrument settings from those in the first edition and are intended to conform to typical X-ray diffraction practice. In most cases, only the XRD pattern for the product as synthesised is printed here. The exceptions are those phases which show marked changes in the XRD pattern upon calcination.

Soil is an irreplaceable resource that sustains life on the planet, challenged by food and energy demands of an increasing population. Therefore, soil contamination constitutes a critical issue to be addressed if we are to secure the life quality of present and future generations. Integrated efforts from researchers and policy makers are required to develop sound risk assessment procedures, remediation strategies and sustainable soil management policies. *Environmental Risk Assessment of Soil Contamination* provides a wide depiction of current research in soil contamination and risk assessment, encompassing reviews and case studies on soil pollution by heavy metals and organic pollutants. The book introduces several innovative approaches for soil remediation and risk assessment, including advances in phytoremediation and implementation of metabolomics in soil sciences.

The search for extremophiles conjures the image of daring adventurers exploring dramatic geologic or climatologic phenomena. Berkeley Pit Lake, however, is not buried deep in the ocean, cradled in a volcanic caldera, or marooned at the southern tip of Antarctica. Instead, it is nestled in a mineral-rich formation in the Rocky Mountains in Butte, Montana. The Berkeley Pit evolved from an open-pit copper mine to an acid mine waste lake in less than 20 years. Today, Berkeley Pit Lake is part of the largest Superfund site in the USA. The Environmental Protection Agency and Montana residents view the Berkeley Pit as an ecological time bomb, but it is something more—an evolving and dynamic ecosystem, a classic by-product of the industrial age. Although conditions within the Pit Lake system are toxic for “normal” aquatic biota, these same conditions provide an ideal environment for extremophiles. Since 1995, we have isolated over 60 fungi and bacteria from the waters and basal sediments of the Pit Lake. Specific signal transduction enzyme inhibition assays were used to guide the isolation of bioactive secondary metabolites from broth cultures of selected microbes. Compounds that were isolated based on their ability to inhibit matrix metalloproteinase-3 have demonstrated selective activity against specific cancer cell lines in the National Cancer Institute's human cancer cell line screen. Caspase-1 inhibitors have shown selective cytotoxicity toward leukemia cell lines and have demonstrated the ability to mitigate the production of proinflammatory cytokines in induced inflammasome assays. This review describes the compounds isolated from this hostile environment and compares them to secondary metabolites isolated from other acid mine waste lakes.

This book is comprised of reviews on the chemotherapy of mycobacterial infections, as well as descriptions of established methods and new techniques for drug susceptibility testing. Some of the fascinating topics examined include the activity of conventional and experimental antimicrobial agents, the rationale of drug combinations in chemotherapy, pharmacokinetics, and the problems of drug susceptibility of mycobacteria analyzed using standards established in other fields of clinical microbiology. Any physician or researcher involved with the therapy of tuberculosis, leprosy, *M. avium* in AIDS patients and other mycobacterial infections, and drug susceptibility testing will discover a wealth of information in this comprehensive volume.

Quantitative Structure-Activity Relationships (QSARs) are increasingly used to predict the harmful effects of chemicals to humans and the environment. The increased use of these methods in a variety of areas (academic, industrial, regulatory) results from a realization that very little toxicological or fate data is available on the vast amount of chemicals to which humans and the environment are exposed. Predicting Chemical Toxicity and Fate provides a comprehensive explanation of the state-of-the-art methods that are available to predict the effects of chemicals on humans and the environment. It describes the use of predictive methods to estimate the physiochemical properties, biological activities, and fate of chemicals. The methods described may be used to predict the properties of drugs before their development, and to predict the environmental effects of chemicals. These methods also reduce the cost of product development and the need for animal testing. This book fills an obvious need by providing a comprehensive explanation of these prediction methods. It is a practical book that illustrates the use of these techniques in real life scenarios. This book will demystify QSARs for those students unsure of them, and professionals in environmental toxicology and chemistry will find this a useful reference in their everyday working lives.

This volume focuses on computational modeling of the ecotoxicity of chemicals and presents applications of quantitative structure–activity relationship models (QSARs) in the predictive toxicology field in a regulatory context. The extensive book covers a variety of protocols for descriptor computation, data curation, feature selection, learning algorithms, validation of models, applicability domain assessment, confidence estimation for predictions, and much more, as well as case studies and literature reviews on a number of hot topics. Written for the Methods in Pharmacology and Toxicology series, chapters include the kind of practical advice that is essential for researchers

everywhere. Authoritative and comprehensive, Ecotoxicological QSARs is an ideal source to update readers in the field with current practices and introduce to them new developments and should therefore be very useful for researchers in academia, industries, and regulatory bodies. This book presents the unique mechanical, electrical, and optical properties of nanomaterials, which play an important role in the recent advances of energy-related applications. Different nanomaterials have been employed in energy saving, generation, harvest, conversion, storage, and transport processes very effectively and efficiently. Recent progress in the preparation, characterization and usage of 1D, 2D nanomaterials and hybrid architectures for energy-related applications and relevant technologies and devices, such as solar cells, thermoelectronics, piezoelectronics, solar water splitting, hydrogen production/storage, fuel cells, batteries, and supercapacitors is covered. Moreover, the book also highlights novel approaches in nanomaterials design and synthesis and evaluating materials sustainability issues. Contributions from active and leading experts regarding important aspects like the synthesis, assembly, and properties of nanomaterials for energy-related applications are compiled into a reference book. As evident from the diverse topics, the book will be very valuable to researchers working in the intersection of physics, chemistry, biology, materials science and engineering. It may set the standard and stimulates future developments in this rapidly emerging fertile frontier of nanomaterials for energy.

Gradient elution demystified Of the various ways in which chromatography is applied today, few have been as misunderstood as the technique of gradient elution, which presents many challenges compared to isocratic separation. When properly explained, however, gradient elution can be less difficult to understand and much easier to use than often assumed. Written by two well-known authorities in liquid chromatography, High-Performance Gradient Elution: The Practical Application of the Linear-Solvent-Strength Model takes the mystery out of the practice of gradient elution and helps remove barriers to the practical application of this important separation technique. The book presents a systematic approach to the current understanding of gradient elution, describing theory, methodology, and applications across many of the fields that use liquid chromatography as a primary analytical tool. This up-to-date, practical, and comprehensive treatment of gradient elution: * Provides specific, step-by-step recommendations for developing a gradient separation for any sample * Describes the best approach for troubleshooting problems with gradient methods * Guides the reader on the equipment used for gradient elution * Lists which conditions should be varied first during method development, and explains how to interpret scouting gradients * Explains how to avoid problems in transferring gradient methods With a focus on the use of linear solvent strength (LSS) theory for predicting gradient LC behavior and separations by reversed-phase HPLC, High-Performance Gradient Elution gives every chromatographer access to this useful tool. Covers the area of lipidomics from fundamentals and theory to applications Presents a balanced discussion of the fundamentals, theory, experimental methods and applications of lipidomics Covers different characterizations of lipids including Glycerophospholipids; Sphingolipids; Glycerolipids and Glycolipids; and Fatty Acids and Modified Fatty Acids Includes a section on quantification of Lipids in Lipidomics such as sample preparation; factors affecting accurate quantification; and data processing and interpretation Details applications of Lipidomics Tools including for Health and Disease; Plant Lipidomics; and Lipidomics on Cellular Membranes

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