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Alan Hinchliffe

Molecular Modelling: Principles And Applications, 2/E Leach, 2009-09

An Introduction to Chemoinformatics Andrew R. Leach, V.J. Gillet, 2003-05-31 This book aims to provide an introduction to the major techniques of chemoinformatics. It is the first text written specifically for this field. The first part of the book deals with the representation of 2D and 3D molecular structures, the calculation of molecular descriptors and the construction of mathematical models. The second part describes other important topics including molecular similarity and diversity, the analysis of large data sets, virtual screening, and library design. Simple illustrative examples are used throughout to illustrate key concepts, supplemented with case studies from the literature.

Encountering Ability: On the Relational Nature of (Human) Performance Scott DeShong, 2016-07-18 In *Encountering Ability*, Scott DeShong considers how ability and its correlative, disability, come into existence. Besides being articulated as physical, social, aesthetic, political, and specifically human, ability signifies and is signified such that signification itself is always in question. Thus the language of ability and the ability of language constitute discourse that undermines foundations, including any foundation for discourse or ability. Drawing on Gilles Deleuze's theory of primary differentiation and Emmanuel Levinas's philosophy of ethical relationality, *Encountering Ability* finds implications of music, theology, and cursing in the signification of ability, and also examines various literary texts, including works by Amiri Baraka and Marguerite Duras.

Molecular Medical Microbiology Yi-Wei Tang, Musa Hindiyeh, Dongyou Liu, Andrew Sails, Paul Spearman, Jing-Ren Zhang, 2023-11-21 *Molecular Medical Microbiology*, Third Edition presents the latest release in what is considered to be the first book to synthesize new developments in both molecular and clinical research. The molecular age has brought about dramatic changes in medical microbiology, along with great leaps in our understanding of the mechanisms of infectious disease. This third edition is completely updated, reviewed and expanded, providing a timely and helpful update for microbiologists, students and clinicians in the era of increasing use of molecular techniques, changing epidemiology and prevalence, and increasing resistance of many pathogenic bacteria. Written by experts in the field, chapters include cutting-edge information and clinical overviews for each major bacterial group, along with the latest updates on vaccine development, molecular technology and diagnostic technology. - Completely updated and revised edition of this

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Molecular Modelling Andrew R. Leach,1996 This book provides a broad, practical introduction to the major techniques employed in molecular modelling and computational chemistry. It leads the reader through the relevant chemical and physical principles to an in-depth understanding of the methods.

Pharmacotherapeutics for Advanced Practice Virginia Poole Arcangelo,Andrew M. Peterson,2006 This advanced pharmacotherapeutics text for nurse practitioners and physician assistants offers guidelines on prescribing drugs for over 50 common diseases and disorders. The book is organized by disorder rather than drug class and includes algorithms and case studies that illustrate critical thinking aspects of prescribing, such as drug selection, lifespan considerations, therapeutic drug monitoring, adverse reactions, unexpected outcomes, and when to change therapy. This Second Edition has new chapters on oncologic disorders and complementary and alternative medicines. Improved case studies reflect more realistic practice issues in decision-making. Additional areas addressed include food-drug interactions, dietary considerations, and concerns regarding geriatric patients.

Mathematical Reviews ,2003

The Zoological Record ,2001

Chemical Applications of Molecular Modelling Jonathan M. Goodman,1998 This book explores the molecular modeling, enabling the nonspecialist to appreciate the power as well as the limitations of the computational tools available and giving a background to the methods used and how they were developed. It also provides examples of how molecular modeling has been used to address chemical questions commonly asked by the experimental chemist, and includes practical examples and case studies. 143 illus.

Molecular Modelling of Biological Activity James Andrew Lumley,2001

Molecular Modelling and Bonding E A Moore,2007-10-31 Why do molecules adopt particular shapes? What determines the physical and chemical properties of a material? Molecular Modelling and Bonding answers these questions by introducing the ideas behind molecular and quantum mechanics, using a largely non-mathematical approach. Atomic and molecular orbitals, computational chemistry and bonding in solids are also discussed. A Case Study, Molecular Modelling in Drug Design, explores ways in which computer modelling, in conjunction with experimental techniques, is used to design new drugs. The accompanying CD-ROM illustrates applications of molecular and quantum mechanics, and includes many of the structures and orbitals illustrated in the text. It provides the programs necessary to view orbitals and 3D structures. The

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A Molecular Modelling for Beginners Alan Hinchliffe, 2008

Modelling Molecular Structures Alan Hinchliffe, 2000-10-03 The application of mathematical models to molecules has now reached maturity. Scientists as diverse as astrophysicists, biologists, chemists, materials scientists and zoologists can reach for their PC, Mac or laptop to model molecular phenomena of unbelievable complexity. Following the highly successful first edition of *Modelling Molecular Structures*, this newly updated edition is your guide through the myriad of applications for molecular modelling. This easy-to-read, highly illustrated text covers all areas of molecular modelling, including molecular dynamics, quantum mechanics, and the Hartree-Fock self-consistent field model, providing background information and critically discussing the latest techniques in the field. Covering developments in the field since the first publication, this title also includes updated text and new material on: * Molecular Dynamics * Dealing with the Solvent This title is an indispensable introduction for all chemists, materials scientists, molecular biologists, and researchers working in, and interested in, the field of molecular modelling.

Molecular Modelling Sean C. Smith, Qiao Sun, Association of Molecular Modellers of Australia, 2010

Molecular Modelling: The Chemistry Of The 21st Century Marco Antonio Chaer Nascimento, 1994-03-28 This volume attempts to show molecular modeling as a new multidisciplinary area of research that transcends the boundaries traditionally separating biology, chemistry and physics. To this purpose, leading scientists present applications of molecular modeling to a variety of important problems such as: drug design, protein modeling, catalyst modeling, properties of glass, mechanical properties of materials and materials design. The emphasis here is on the atomistic approach.

Molecular Modelling in Real-time Anoop Singh Khurana, 1984

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