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Biomolecular Simulations in Structure-Based Drug Discovery-Francesco L. Gervasio 2019-04-29 A guide to

Biomolecular Simulations in Structure-Based Drug Discovery is an important resource that contains a review of the current generation of biomolecular simulation tools that have the potential to complement that used in multistage drug discovery projects. It also serves as a reference guide to the novel methods and strategies for the modeling of drug-target interactions within the framework of real-life drug design and development projects. The book also presents a review of the current state of the art in computational medicinal chemistry tools for real-life problems and presents solutions to commonly encountered problems. It shows how almost every step of the drug discovery pipeline can be optimized and accelerated by using biomolecular simulations – from the management of compound databases to targeted combinatorial synthesis, virtual screening and efficient hit-to-lead transition. An invaluable resource for drug developers and medicinal chemists, this book is also an essential guide for PhD students and academic researchers.

The Handbook of Medicinal Chemistry-Andrew Darlison 2015-07-07 Drug Discovery is a constantly developing and expanding field, and the reader has to keep up-to-date with the latest developments in order to be successful. This book contains a wide range of contributions that discuss specific aspects of the topic and provide up-to-date, comprehensive information. It is an essential resource for medicinal chemists, computational chemists and those in the pharmaceutical industry. The book covers the past, present and future of the entire drug development process. Highlighting the recent successes and future challenges that lie ahead, the book provides a comprehensive overview of current methods and applications of fragment-based drug discovery, as well as an outlook on where the field is headed.

Drug Metabolism Prediction-Johannes Kirchmar 2014-08-25 The first reference source on this highly interdisciplinary area of drug development, Drug Metabolism Prediction provides a comprehensive overview of computational tools and knowledge bases for drug metabolism research and their underlying principles. The aim is to convey their expert knowledge distilled from many years of experience in the field. The book is divided into four parts: the first part covers the fundamental principles and general concepts of drug metabolism, the second part presents the expert accounts of the latest experimental methodologies for investigating drug metabolism in four dedicated chapters, the third part devotes itself to the most important computational tools currently available and the fourth part presents a number of real world case studies. Co-vered in the book are the most important aspects of drug metabolism research and how to use the latest computational tools to real-life problems and presents solutions to commonly encountered problems. It shows how almost every step of the drug discovery pipeline can be optimized and accelerated by using biomolecular simulations – from the management of compound databases to targeted combinatorial synthesis, virtual screening and efficient hit-to-lead transition. An invaluable resource for drug developers and medicinal chemists, this book is also an essential guide for PhD students and academic researchers.

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Chemometrics in Drug Discovery-Sugo Kuhni 2006-03-06 Chemometrics brings together the most powerful concepts in modern chemistry and biology, linking combinatorial chemistry with potencies and protein structures. This introductory text to the subject focuses on the use of key statistical tools to improve the efficiency of drug discovery. Especially relevant in representing and analyzing high-dimensional data, chemometrics is an essential resource for designing, executing, and interpreting chemical experiments. The book includes several new and completely revised chapters on chemometrics.

Computational Tools for Chemical Biology-Sonsoles Martín-Santamaría 2017-11-01 The peroral application (swallowing) of a medicine for better drugs, elevated safety standards, and economic considerations have all led to a dramatic paradigm shift in drug administration. Topics include: drug design drug discovery natural products and supplements and medicinal chemistry of natural products. Drug discovery reviews the principles, advantages, and limitations involved with designing these compounds. The book describes the discovery and development of novel drugs, some of which will have a valuable addition to the pharmacological arsenal of pharmaceutical scientists and for industry professionals.

Prodrug Design: Perspectives, Approaches and Applications-Vivekkumar K Redasani 2015-07-07 Prodrug Design: Perspectives, Approaches and Applications-

3-D structure of biomolecules. These methods have been enhanced to improve the speed and quality of drug discovery. This book covers the history of the discovery and use of privileged scaffolds and addresses the various classes of these motifs, considering their role in the path of drug design. It presents contemporary research on molecular modeling techniques used in drug discovery and the drug development process. It considers key elements in the drug design cycle ranging from appropriateness of targets and disease models to the development of marketed compounds, the safety of promoieties, and a detailed classification of prodrugs organized by therapeutic profilm. It presents state-of-the-art summaries of platform technologies

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