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Case Report

Case Report book review: Computer-aided drug development

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The book "Computer-Aided Drug Development" offers a comprehensive exploration of the integration of computer applications in pharmaceutical research and development. With a detailed syllabus covering various aspects of computer applications in drug development, the book provides a structured and insightful approach to understanding the complexities and advancements in this interdisciplinary domain.

The first section of the book provides a historical overview of computers in pharmaceutical research and development, tracing the evolution of computational techniques and their impact on the industry. It also delves into statistical modeling, distinguishing between descriptive and mechanistic modeling, and covering essential statistical parameters, estimation methods, confidence regions, sensitivity analysis, optimal design, and population modeling. This foundational knowledge sets the stage for readers to grasp the subsequent advanced topics.

The book also delves into Quality-by-Design (QbD) principles in pharmaceutical development, introducing the ICH Q8 guideline and discussing regulatory perspectives alongside industry views on QbD. Through scientifically based QbD examples, readers gain insights into how these principles are applied in real-world scenarios, enhancing their understanding of quality-driven approaches in drug development.

Another significant section explores computational modeling of drug disposition, focusing on modeling techniques related to drug absorption, solubility, permeation, distribution, excretion, and active transport mechanisms. The inclusion of specific transporters such as P-gp, BCRP, nucleoside transporters, and others adds depth to the discussion, highlighting the intricate processes involved in drug dynamics within biological systems.

The book's coverage extends to computer-aided formulation development, emphasizing the concept of optimization, factorial design, and screening design in pharmaceutical formulations. It also addresses legal and ethical considerations regarding innovative uses of computers in R&D, shedding light on intellectual property rights and ethical practices in pharmaceutical research.

Furthermore, the book delves into computer-aided biopharmaceutical characterization, including gastrointestinal absorption simulation, in vitro dissolution, in vitro-in vivo correlation, and biowaiver considerations. It also explores computer simulations in pharmacokinetics and pharmacodynamics, providing a holistic view of computer applications at various levels, from whole organisms to proteins and genes.

The final section of the book discusses emerging technologies such as artificial intelligence (AI), robotics, and computational fluid dynamics (CFD) in the pharmaceutical industry. It covers pharmaceutical automation, applications of AI and robotics, and outlines the advantages, disadvantages, current challenges, and

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future directions in leveraging these technologies for drug development.

Overall, "Computer-Aided Drug Development" is a comprehensive and insightful resource that bridges theoretical concepts with practical applications in pharmaceutical research and development. The expertise of the authors, coupled with a structured syllabus and in-depth coverage of key topics, makes this book an essential read for students, researchers, and professionals in the pharmaceutical and computational sciences domains.

The authors of this book, namely Dr. Amit Nerkar, Dr. Narendra Mulchand Gowekar, Dr. Gita Chaurasia, and Dr. Bhushan D. Varpe, are highly regarded experts in their respective fields. Dr. Nerkar, possessing a Ph.D. from SVKM's NMIMS University, has extensive experience in pharmacy and medicinal chemistry, having served as a Senior Research Fellow for the Indian Council of Medical Research. Currently holding the position of Professor and Research Head at CAYMET's Siddhant College of Pharmacy, he specializes in clinical pharmacology, medicinal chemistry, and computer-aided drug design. Dr. Gowekar, with more than two decades of teaching experience in pharmacy and a Ph.D. from SRTM University, is a distinguished academic focusing on analytical method development, impurity profile study, and validation of analytical methods. Dr. Chaurasia, an Assistant Professor with 18 years of academic experience and a Ph.D. in Pharmaceutics, contributes expertise in pharmaceutical sciences, including patents and research publications. Dr. Varpe, an Indian Patent Agent and holds Ph.D. degree in pharmaceutical chemistry from the University of Pune, brings expertise in medicinal chemistry, patents, and bioanalytical research to the table. Together, these esteemed authors significantly enhance the book with their wealth of knowledge, making it an indispensable resource for professionals and students in the pharmaceutical and computational sciences domains. The Book is published by A.F.S.E.R International Publishers, publishers in all types of books.

Conflict of Interest

None.

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