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Titolo Artificial Intelligence and Machine Learning in Drug Design and

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Sommario/riassunto The book is a comprehensive guide that explores the use of artificial

intelligence and machine learning in drug discovery and development covering a range of topics, including the use of molecular modeling, docking, identifying targets, selecting compounds, and optimizing drugs. The intersection of Artificial Intelligence (AI) and Machine Learning (ML) within the field of drug design and development represents a pivotal moment in the history of healthcare and pharmaceuticals. The remarkable synergy between cutting-edge technology and the life sciences has ushered in a new era of possibilities, offering unprecedented opportunities, formidable challenges, and a tantalizing glimpse into the future of medicine. Al can be applied to all the key areas of the pharmaceutical industry, such as drug discovery and development, drug repurposing, and improving productivity within a short period. Contemporary methods have shown

promising results in facilitating the discovery of drugs to target different diseases. Moreover, AI helps in predicting the efficacy and safety of molecules and gives researchers a much broader chemical pallet for the selection of the best molecules for drug testing and delivery. In this context, drug repurposing is another important topic where AI can have a substantial impact. With the vast amount of clinical and pharmaceutical data available to date, Al algorithms find suitable drugs that can be repurposed for alternative use in medicine. This book is a comprehensive exploration of this dynamic and rapidly evolving field. In an era where precision and efficiency are paramount in drug discovery, AI and ML have emerged as transformative tools, reshaping the way we identify, design, and develop pharmaceuticals. This book is a testament to the profound impact these technologies have had and will continue to have on the pharmaceutical industry, healthcare, and ultimately, patient well-being. The editors of this volume have assembled a distinguished group of experts, researchers, and thought leaders from both the AI, ML, and pharmaceutical domains. Their collective knowledge and insights illuminate the multifaceted landscape of AI and ML in drug design and development, offering a roadmap for navigating its complexities and harnessing its potential. In each section, readers will find a rich tapestry of knowledge, case studies, and expert opinions, providing a 360-degree view of AI and ML's role in drug design and development. Whether you are a researcher, scientist, industry professional, policymaker, or simply curious about the future of medicine, this book offers 19 state-of-the-art chapters providing valuable insights and a compass to navigate the exciting journey ahead. Audience The book is a valuable resource for a wide range of professionals in the pharmaceutical and allied industries including researchers, scientists, engineers, and laboratory workers in the field of drug discovery and development, who want to learn about the latest techniques in machine learning and AI, as well as information technology professionals who are interested in the application of machine learning and artificial intelligence in drug development.