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Sommario/riassunto

The book 'Computational Drug Discovery Methods and Applications' edited by Poongavanam and Vijayan Ramaswamy, provides a comprehensive overview of cutting-edge computational techniques in drug discovery. It covers a wide range of topics, including molecular dynamics, quantum mechanics, artificial intelligence, and more. The book is structured into thematic sections focusing on methods such as binding free energy calculations, solvation models, AI-based protein structure predictions, and virtual screening techniques. It aims to equip medicinal and computational chemists, as well as drug discovery professionals, with advanced knowledge and practical insights into the integration of computational tools in drug discovery processes. With contributions from experts in academia and industry, this volume serves as a valuable resource for understanding both theoretical and practical aspects of computational drug design.