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Computational Methods in Drug Development

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Advances in computational techniques have profoundly transformed the drug development process, providing innovative solutions to accelerate the discovery and enhancement of therapeutic agents. These techniques encompass a range of technologies, from molecular modeling to artificial intelligence, and are involved at various stages of development. Recently, their use has grown in areas such as predicting the structures of proteins, RNA, drug molecules, and their complexes, discovering new drug targets, and optimizing drug–receptor interactions. Since experimental methods for determining molecular structures can be costly and time-consuming, computational approaches serve as effective alternatives, helping to elucidate complex biological systems, screen large chemical libraries, and reduce the time and expense of traditional methods. This Reprint compiles recent research and reviews on computational strategies in drug development, including molecular mechanisms, discovery techniques, disease-specific therapeutics, and future research directions. Highlighting these advancements underscores the transformative role of computational methods in creating new, effective therapeutics.

