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A Review on Drug Design: Strategies, Advances, and Future Directions

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Abstract: *Drug design represents a cornerstone of modern pharmaceutical research, aiming to identify and optimize bioactive molecules that can modulate specific biological targets associated with disease. Over the past decades, drug discovery has transitioned from serendipitous findings and trial-and-error screening to rational, data-driven approaches guided by molecular biology, structural chemistry, and computational tools. This review provides an in-depth examination of traditional and contemporary drug design strategies, including structure-based drug design (SBDD), ligand-based drug design (LBDD), phenotypic screening, combinatorial chemistry, and novel modalities such as targeted covalent inhibitors, molecular glues, RNA therapeutics, and nanomedicine. The increasing role of artificial intelligence (AI) and machine learning (ML) in predictive modeling, virtual screening, and de novo molecular generation is discussed, alongside challenges in data quality, regulatory acceptance, and translational success. Finally, the paper outlines future perspectives, emphasizing the integration of multi-omics, explainable AI, and emerging chemical spaces to enhance the efficiency and success rate of drug discovery.*

Keywords: drug design, structure-based drug design, ligand-based drug design, molecular docking, artificial intelligence, molecular glues, combinatorial chemistry, nanomedicine

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