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Pharmacophore Modeling in Computational Drug Design: A Critical Review

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Abstract: *Pharmacophore modeling defines the essential molecular features required for the biological activity of a compound and serves as a valuable tool in modern drug discovery. By utilizing structural information from active ligands or biological targets, Pharmacophore models enable the identification of novel compounds that exhibit desired biological properties. This technique plays a crucial role across multiple stages of the drug discovery pipeline, including virtual screening, molecular docking, target fishing, ligand profiling, and ADMET prediction. The effectiveness of pharmacophore modeling depends on selecting appropriate computational tools, as several software programs are available for different research needs. Recent advancements—such as integration with molecular dynamics simulations, machine learning approaches, and improved computational resources—have significantly enhanced model accuracy and performance. These developments have accelerated drug discovery, reducing cost and time while increasing efficiency. Overall, the evolution of pharmacophore modeling continues to improve the reliability and quality of generated models, further strengthening its impact on pharmaceutical research*

Keywords*:* Molecular docking, Drug discovery, ADMET Prediction, Ligand-based design

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