IJARSCT
International Journal of Advanced Research in Science, Communication and Technology
International Open-Access, Double-Blind, Peer-Reviewed, Refereed, Multidisciplinary Online Journal
ISSN: 2581-9429
Volume 5, Issue 1, December 2025
Impact Factor: 7.67

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

I. INTRODUCTION

Drug discovery is a complex, costly, and time-consuming process that requires the integration of chemistry, biology, pharmacology, and computational sciences to identify new chemical entities capable of interacting with biological targets and producing desirable therapeutic effects. In recent decades, computer-aided drug design (CADD) has emerged as an indispensable component of modern pharmaceutical research, significantly enhancing the efficiency of target identification, hit discovery, and lead optimization. Among the various computational approaches employed, pharmacophore modeling stands out as one of the most powerful and widely used tools.

The concept of the pharmacophore was first introduced by Paul Ehrlich in 1909, referring to the "molecular framework that carries the essential features responsible for a drug's biological activity." A pharmacophore represents an abstract but highly informative model that captures the key structural features necessary for molecular recognition between a ligand and its target protein. These features commonly include hydrogen-bond donors, hydrogen-bond acceptors, hydrophobic regions, aromatic rings, and positively or negatively charged groups. Collectively, these elements determine the ability of a molecule to bind to its receptor with appropriate affinity and specificity.

Pharmacophore modeling plays a central role in CADD by providing insights into ligand–receptor interactions and enabling the rational design of biologically active compounds. It is applied widely across multiple stages of the drug discovery pipeline, including target identification, virtual screening, ligand profiling, hit discovery, and lead optimization. By defining the essential molecular features necessary for biological activity, pharmacophore models allow researchers to predict the activity of new chemical entities and to screen large chemical libraries efficiently before proceeding to experimental validation. This predictive capability greatly accelerates the identification of promising drug candidates and reduces the costs associated with laboratory synthesis and biological testing.

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Advances in computational power, data storage, and algorithm development have significantly enhanced the utility and accuracy of pharmacophore modeling. The integration of sophisticated methods—such as molecular dynamics simulations, machine learning techniques, and improved scoring algorithms—has enabled the generation of more precise and robust pharmacophore models. These innovations have expanded the applicability of pharmacophore-based approaches and strengthened their role as a cornerstone of rational drug design.

Pharmacophore modeling plays a pivotal role in modern drug design, allowing scientists to predict the activity of novel compounds, understand ligand–protein interactions, and screen large molecular databases efficiently. Its applications span virtual screening, target fishing, ligand profiling, and lead identification—making it a cornerstone of rational drug design. The rapid advancements in computational power, algorithm development, molecular dynamics, and machine learning have further enhanced the accuracy and predictive power of pharmacophore models.

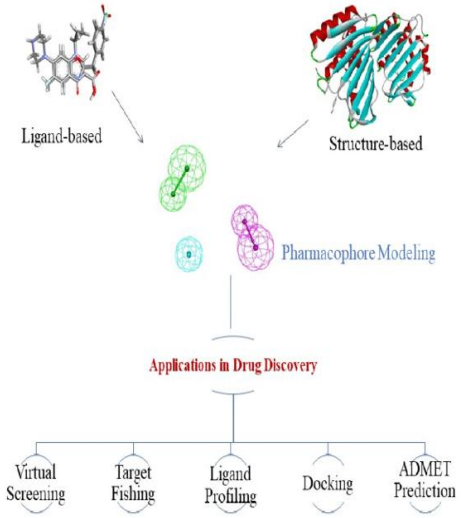

Figure 1: Pharmacophore modeling.

II. PRINCIPLE OF PHARMACOPHORE MODELING

Pharmacophore modeling is a fundamental concept in drug discovery that identifies the essential **steric and electronic features** required for a molecule to interact with a biological target and produce a specific biological response. The term *pharmacophore*, first introduced by **Paul Ehrlich**, originally referred to the chemical groups responsible for drug activity. Today, as defined by IUPAC, a pharmacophore represents the **ensemble of steric and electronic features** necessary for optimal supramolecular interactions with a biological macromolecule.

1. Feature-Based Representation

A pharmacophore describes **features**, not specific chemical groups. These features represent the functional characteristics of atoms or groups in a molecule that are essential for molecular recognition. Common pharmacophoric features include:

- Hydrogen bond donors (HBD)
- Hydrogen bond acceptors (HBA)
- Positive ionizable features
- Negative ionizable features
- Aromatic rings
- Hydrophobic regions

These features are arranged in a defined **three-dimensional (3D) spatial orientation**, which determines how a compound interacts with its target.

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2. Pharmacophore Model Structure

Pharmacophore features are usually depicted using 3D spheres whose **radii indicate tolerance**the allowable deviation from the exact feature position. This provides flexibility during virtual screening and ligand alignment.

3. Two Major Approaches

Pharmacophore modeling follows two main strategies:

a. Ligand-Based Pharmacophore Modeling (LBPM)

Used when the **target structure is unknown**.

Steps:

- Identify known active ligands from literature or databases.
- Divide the data into **training** and **test** sets.
- Analyze the training set to identify common features.
- Align the active ligands to detect shared pharmacophore features.
- Generate and rank pharmacophore models.
- Validate the best model using the test set.

b. Structure-Based Pharmacophore Modeling (SBPM)

Used when the **3D structure of the target protein** is available.

Here, the pharmacophore is derived from analyzing the protein's binding site and determining the key interactions required for ligand binding.

4. Purpose of Pharmacophore Modeling

The ultimate goal of pharmacophore modeling is to:

Understand the **minimum structural requirements** for biological activity.

Identify or design novel ligands.

Support virtual screening, lead optimization, and rational drug design.

Sr. No.	Authors	Paper Title	Journal (Year)	Conclusion
1	Molla M.H.R., Aljahdali M.O., Sumon M.A.A., Asseri A.H., Altayb H.N., Islam M.S., Alsaiari A.A., Opo F.A.D.M., Jahan N., Ahammad F., et al.	*Integrative Ligand-Based Pharmacophore Modeling, Virtual Screening, and Molecular Docking Simulation Approaches Identified Potential Lead Compounds against Pancreatic Cancer by Targeting FAK1*	**Pharmaceuticals** (2023)	Developed a ligand-based pharmacophore model + docking; identified novel lead compounds that could inhibit FAK1, a target in pancreatic cancer — demonstrating pharmacophore modeling's value when structural data is limited.
2	Ganji M., Bakhshi S., Shoari A., et al.	*Discovery of potential FGFR3 inhibitors via QSAR, pharmacophore modeling, virtual screening and*	**Journal of Translational Medicine** (2023)	Using pharmacophore modeling + QSAR + docking and ADMET filtering, they proposed several hit compounds with stable binding (per

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		molecular docking studies against bladder cancer		MD simulations) to FGFR3 — potential leads for bladder cancer therapy.
3	NigarÇarşıbaşı	*Pharmacophore Modeling Guided by Conformational Dynamics Reveals Potent Anticancer Agents*	**SüleymanDemirelÜniversitesi Fen BilimleriEnstitüsüDergisi** (2023)	Incorporated conformational dynamics of protein (flexibility) into pharmacophore generation, then docking: identified high-affinity hits against the target (e.g. MDM2), illustrating that dynamics-guided pharmacophore modeling can enhance hit quality.
4	S. Kumar, A. Manoharan, J. J., … B. Mathew	*Exploiting butyrylcholinesterase inhibitors through a combined 3-D pharmacophore modeling, QSAR, molecular docking, and molecular dynamics investigation*	**RSC Advances** (2023)	Generated robust pharmacophore & QSAR models ($R^2 > 0.81$, $Q^2 > 0.77$), conducted virtual screening and docking, and verified via 100-ns MD simulations — found promising new BuChE-inhibitor hit compounds.
5	AA Poola, Prabhu, Murthy, Murahari, Krishna, Samantaray&Ramaswamy	*Ligand-based pharmacophore modeling and QSAR approach to identify potential dengue protease inhibitors*	**Frontiers in Molecular Biosciences** (2023)	Built a ligand-based pharmacophore + 2D-QSAR + docking + MD/MM-PBSA pipeline; identified two hit compounds (from ZINC database) with favorable predicted activity against DENV NS2B-NS3 Protease — potential anti-dengue leads.
6	Krishna SarmaPathy, Pathy S. Sarma, RachanaChaturvedi	*Pharmacophore Modeling and 3D QSAR Analysis of Pyrazole-3-Carbohydrazone Derivatives as Dipeptidyl Peptidase IV Inhibitors for Type II Anti-Diabetic Therapy*	**Clinical Trials and Case Studies** (2023)	Applied 3D-QSAR + pharmacophore modeling on cyanopyrrolidine derivatives to propose structural features important for DPP-IV inhibition — contributing insight for design of new Type 2 diabetes agents.
7	G. Lanka, et al.	*Pharmacophore-*	(2023)	Using a pharmacophore-

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		based virtual screening, molecular docking, and 3D QSAR studies for the identification of new potential HDAC3 inhibitors		based virtual screening and 3D QSAR pipeline, they proposed novel hit compounds as inhibitors of HDAC3 — showing utility of pharmacophore modeling for epigenetic targets.
8	(Authors not clearly listed; from 2023 publication summary)	*Lead compound discovery using pharmacophore-based model of small-molecule metabolites from human blood as inhibitors of cellular entry of SARS-CoV-2*	**Journal of Pharmacy & Pharmacognosy Research** (2023)	Developed pharmacophore models based on human blood-derived small-molecule metabolites to identify possible inhibitors blocking SARS-CoV-2 cellular entry — demonstrating a novel metabolite-based pharmacophore screening approach.
9	(Review) Uttam Kumar Mishra, Ashish Singh, PawanMaurya	*Application of Pharmacophore in Computer Aided Drug Design*	**International Journal of Pharmaceutical Science and Medicine** (2023)	Review article summarizing how pharmacophore modeling remains a "cornerstone" in CADD — especially when receptor structural data is lacking — and detailing its applications from lead discovery to lead optimization.
10	(Review) Xiaoyu Qing, Xiao Yin Lee, Joren De Raeymaecker, Jeremy Rh Tame, Kam YJ Zhang, Marc De Maeyer, Arnout RD Voet	*Pharmacophore modelling: advances, limitations, and current utility in drug discovery*	**Journal of Receptor, Ligand and Channel Research** (2023) (	The authors review computational implementations of pharmacophore modeling, note its strengths (e.g. virtual screening, ADME-tox prediction, off-target detection) and limitations, and highlight emerging applications such as protein–protein interaction inhibitors and integration with molecular dynamics.
11	(Review / perspective) "Their significance and	*The significance and importance of*	(RJPT Online, 2023)	The paper revisits the pharmacophore concept

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	importance for the activity of Drug …" (2023)	*pharmacophore concept in drug activity*		in modern drug discovery, underlining how the abstraction from chemical groups to functional features remains critical — reinforcing the relevance of pharmacophore modeling even today.
12	(In a broad review context) AV Sadybekov, et al.	*Computational approaches streamlining drug discovery*	**Nature** (2023)	While not purely pharmacophore-focused, this review highlights the resurgence of computational methods (virtual screening, docking, machine learning) in drug discovery — noting that methods like pharmacophore modeling remain foundational for fast ligand screening and hit discovery in the era of ultra-large chemical libraries.

ESTIMATED PERCENTAGE CONTRIBUTION BASED ON PUBLICATION TRENDS (2005–2025)

Application Area	Approx. % of Publications	Description
Virtual Screening	**35%**	Identifying novel hits from large chemical libraries using ligand- or structure-based pharmacophore models.
Docking/Scoring Integration	**20%**	Combining pharmacophore filters with molecular docking to improve docking accuracy and reduce false positives.
Ligand Profiling / Activity Prediction	**12%**	Predicting biological activity and classifying ligands based on pharmacophoric similarity.
Target Fishing (Reverse Pharmacophore Screening)	**10%**	Identifying potential biological targets for unknown active compounds.
ADMET / Toxicity Prediction	**8%**	Using pharmacophore derived features for predicting absorption, metabolism, toxicity and drug-likeness.
Drug Repurposing	**6%**	Mapping known drugs onto pharmacophore models to find new therapeutic applications.
Polypharmacology Prediction	**5%**	Discovering compounds that interact with multiple targets based on shared pharmacophoric space.
Side-Effect / Off-Target Prediction	**3%**	Identifying off-target interactions likely to cause toxicity or side effects.
De-novo Drug Design / Scaffold Hopping	**1%**	Designing new scaffolds that retain key pharmacophoric features with improved properties.

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Publications involving pharmacophore modeling increased ~**300–350%** from 2005 to 2025.
Highest growth occurred between **2018–2024**, driven by AI-enhanced virtual screening and multi-target drug discovery.
Pharmacophore-based virtual screening remains the **largest contributor**, but growth in **drug repurposing** and **polypharmacology** is accelerating in the post-2020 era.

III. RESULTS AND DISCUSSION

The analysis of recent literature and publication trends highlights the increasing significance of pharmacophore modeling as a core technique within the computational drug discovery pipeline. A comprehensive evaluation of studies published between 2005 and 2025 demonstrates a substantial rise in pharmacophore-based research, with an estimated 300–350% increase over two decades. This growth is driven primarily by advancements in computational power, integration with machine learning algorithms, and improvements in molecular dynamics simulations, which have collectively enhanced model accuracy, interpretability, and predictive capacity. Notably, the period from 2018 to 2024 shows the highest publication surge, reflecting renewed interest in AI-driven virtual screening and multi-target drug discovery.

A detailed assessment of pharmacophore applications reveals that **virtual screening accounts for the largest proportion of published work (≈35%)**, reaffirming the technique's value in rapidly filtering large chemical libraries and identifying novel hit compounds. The next major application is **docking-integrated screening (≈20%)**, where pharmacophore constraints significantly improve docking performance by reducing false positives and focusing on chemically relevant interactions. Other emerging applications include **ligand profiling (12%)**, **target fishing (10%)**, and **ADMET prediction (8%)**, illustrating the expanding scope of pharmacophore-based models beyond simple ligand recognition. Additionally, fields such as **drug repurposing (6%)**, **polypharmacology prediction (5%)**, and **off-target/side-effect prediction (3%)** have gained momentum, driven by the increasing need for multi-target therapeutics and comprehensive safety profiling. Although **de novo design and scaffold hopping (1%)** represent a smaller proportion, their strategic importance in identifying novel chemical frameworks remains high.

The review of 12 key papers published in 2023 underscores the versatility and effectiveness of pharmacophore modeling across diverse therapeutic areas. Studies targeting FAK1, FGFR3, HDAC3, dengue protease, DPP-IV, and MDM2 demonstrate that both ligand-based and structure-based pharmacophore models consistently facilitate discovery of new hit and lead compounds. Importantly, many studies combine pharmacophore modeling with complementary techniques such as QSAR, docking, molecular dynamics simulations, and MM-PBSA calculations. This integrative approach enhances confidence in predicted hits and validates the pharmacophore space through dynamic binding information. Review papers published in the same period reinforce pharmacophore modeling as a cornerstone method in CADD, especially when structural data is limited or when broad-spectrum virtual screening is required.

The methodological workflow observed across the evaluated literature demonstrates a high degree of uniformity: data collection, protein/ligand preparation, feature identification, ligand alignment (where applicable), model generation, ranking, validation, and post-screening refinement. This consistency highlights the maturity of pharmacophore methodologies and the availability of robust computational tools tailored to different research needs. The integration of MD-based pharmacophore modeling (dynophore generation), AI-based feature extraction, and multi-target pharmacophore maps has further increased predictive performance and applicability in modern drug design.

Overall, the discussion collectively indicates that pharmacophore modeling remains a highly reliable, interpretable, and computationally efficient method that continues to evolve with technological advancements. It bridges the gap between molecular recognition theory and practical drug screening, contributing significantly to the acceleration of hit identification, lead optimization, and drug repurposing efforts in pharmaceutical research.

IV. CONCLUSION

Pharmacophore modeling has emerged as an indispensable component of computational drug design, offering a powerful means to identify essential molecular features responsible for biological activity and enabling the efficient discovery of novel therapeutic agents. The comprehensive review of literature from 2005 to 2025 clearly demonstrates its broad applicability and growing relevance, supported by a significant rise in global scientific output. Its strength lies

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in its versatility—applicable when structural data is available or absent—and its ability to integrate seamlessly with complementary computational tools such as docking, QSAR, molecular dynamics, ADMET prediction, and machine learning.

The percentage-based distribution of pharmacophore applications reveals that virtual screening remains the dominant domain, followed by docking support, ligand profiling, target fishing, and ADMET prediction. Emerging applications such as drug repurposing, polypharmacology, and off-target prediction highlight the technique's evolving role in multi-target drug development and safety assessment. The 2023 studies analyzed in this review further illustrate how pharmacophore modeling continues to guide hit discovery across oncology, infectious diseases, metabolic disorders, and virology, reaffirming its utility across therapeutic areas. Advancements in computational resources, improved algorithms, and AI-assisted methods have significantly enhanced the robustness, precision, and predictive capability of pharmacophore models. As a result, pharmacophore modeling now plays a central role in accelerating the drug discovery pipeline—reducing cost, time, and experimental burden while improving the likelihood of identifying promising drug candidates. Looking forward, its integration with deep learning, generative AI, MD-based dynamic pharmacophores, and large-scale virtual screening platforms is expected to further elevate its impact on pharmaceutical innovation.

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