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The impact of Generative AI on the Efficiency and accuracy of drug discovery

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ABSTRACT

Drug discovery traditionally is a long and expensive process. It requires huge financial investment and can possibly take more than a decade to develop a single drug. In this paper, It has been explored how generative AI is changing this process. By using advanced models, generative AI can design new drug molecules, predict their properties, improve efficiency by reducing both time and cost required for research to get precise and accurate data. These models can generate drug candidates with better binding affinity and drug like properties, making the selection process more reliable. It is also being used across different stages of drug discovery, from identifying targets to monitoring drug safety. Although generative AI has great potential to transform drug discovery by making it faster, more efficient and accurate, there are still some challenges like the need for high quality data, lack of model transparency, regulatory concerns and more real world testing and comparison. These improvements are still needed for its full adoption.

Keywords: Generative AI, Drug Discovery, Molecular Design, Time Optimization, Cost Reduction, Predictive Modeling.

INTRODUCTION

Drug discovery is a complex and resource-intensive process that traditionally takes over a decade and can cost up to $1 billion for a single new drug. The process involves several stages, including target identification, hit discovery, lead optimization, and clinical development, each of which presents significant scientific and logistical challenges.

Traditionally, drug discovery has relied on methods such as high-throughput screening, iterative medicinal chemistry, and extensive experimental validation. While these approaches are effective, they are often time-consuming and limited in their ability to explore the vast chemical space or accurately predict complex biological interactions.

In recent years, generative AI has emerged as a transformative technology in this field. By leveraging advanced computational models, particularly deep learning and diffusion-based techniques, generative AI can design and optimize novel molecular structures more efficiently. It enables researchers to automate molecular generation, improve drug-like properties, and integrate diverse biological data for better decision-making. As a result, generative AI holds great potential to accelerate drug discovery, enhance candidate selection accuracy, and significantly reduce overall costs.

Key Findings

A. Efficiency: speed and cost reduction

Generative AI models have demonstrated impressive results in the speed and resource efficiency of drug discovery compared to traditional methods. For example, the IDOLpro generative chemistry AI platform was found to be over 100 times faster and less expensive than exhaustive virtual screening (Kadan et al., 2025). Similarly, the application of denoising diffusion probabilistic models (DDPMs) to molecular dynamics (MD)

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simulations reduced computational costs to one third of traditional umbrella sampling approaches, making high-throughput screening feasible for membrane partitioning studies (Obi et al., 2024).

B. Accuracy: Better Candidate Selection

Generative AI does not just save time, it also produces better candidates. IDOLpro generated ligands with binding affinities 10–20% higher than the next best method, and remarkably, it was the first approach to generate molecules that outperformed experimentally observed ligands in benchmark binding assays (Kadan et al., 2025). The DDPM models also showed strong accuracy, correctly predicting membrane interaction parameters and ligand orientations for a range of FDA approved drugs (Obi et al., 2024).

In a more disease-specific application, the CRISPR-TICA.ai pipeline combined functional genomics data with generative AI to prioritize drug candidates targeting key residues in acute myeloid leukaemia (AML). This kind of approach shows how generative AI can be tailored for specific biological contexts, potentially enabling more rational and targeted drug design (Vora et al., 2025).

It is worth noting, that different studies use different metrics to evaluate success binding affinity, quantitative estimate of drug likeness (QED), synthetic accessibility making it difficult to do detailed comparisons as the lack of universal validation standards remains a clear gap in the field.

C. Challenges and Limitations

Despite the promising results, there are real challenges that need to be addressed before generative AI can be fully trusted in drug discovery settings. Data quality is a big concern, if the training data is biased or incomplete, the models can produce misleading results (Abbas et al., 2024). Model interpretability is another issue: many generative AI models are essentially black boxes, which is a problem when regulators and clinicians need to understand why a particular candidate was selected (Abbas et al., 2024) (Bordukova et al., 2023).

Scalability and generalizability are also open questions. Most studies have demonstrated results for specific targets or disease areas, and it is not always clear how well these approaches would transfer to other contexts. The field also lacks the kind of systematic, benchmarking studies that would make it easier to compare different generative AI approaches against each other and against traditional methods (Zhang et al., 2024) (Lai et al., 2025).

Finally, there are regulatory and ethical considerations to keep in mind. As generative AI becomes more embedded in drug development, frameworks are needed to ensure that these tools are used safely with responsibility especially as they start influencing decisions that directly affect patient outcomes (Vanier et al., 2023).

Summary of Key Findings

- **Efficiency:** Generative AI models such as IDOLpro and DDPMs have demonstrated dramatic improvements in the speed and cost-effectiveness of early-stage drug discovery, with reported gains of up to 100-fold in speed and threefold reductions in computational cost compared to traditional methods (Kadan et al., 2025)(Obi et al., 2024).

- **Accuracy:** These models also enhance predictive accuracy, generating candidates with superior binding affinities and drug-like properties, and improving the reliability of membrane partitioning and safety assessments (Kadan et al., 2025)(Obi et al., 2024)(Mishra & Gupta, 2025).

- **Workflow Integration:** Generative AI is being integrated into multiple stages of the drug discovery pipeline, from hit identification and lead optimization to pharmacovigilance, supporting multi-objective optimization and data-driven decision-making (Kadan et al., 2025)(Vora et al., 2025)(Mishra & Gupta, 2025).

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- **Challenges:** Persistent challenges include data quality, model interpretability, regulatory compliance, and the need for more systematic benchmarking and real-world validation (Abbas et al., 2024)(Bordukova et al., 2023).

Gaps and Areas for Further Research

- **Quantitative Benchmarking:** More systematic, quantitative comparisons between generative AI and traditional approaches are needed across all stages of drug discovery.
- **Model Interpretability:** Improved transparency and explain ability are essential for regulatory acceptance and broader adoption.
- **Integration with Experimental Workflows:** Deeper integration and validation in real-world settings will be critical to demonstrate practical utility.

Ethical and Regulatory Frameworks: As generative AI becomes more pervasive, robust frameworks are needed to ensure safety, efficacy, and compliance

TABLE 1: generative AI impact across drug discovery stages

Stage	Efficiency Gains (AI vs. Traditional)	Accuracy Improvements	Integration Level	Notable Evidence Source(s)
Hit Identification	>100× faster, less expensive (Kadan et al., 2025)	Higher binding affinity (Kadan et al., 2025)	High	(Kadan et al., 2025)
Membrane Partitioning	3× reduction in computational cost (Obi et al., 2024)	Accurate PMF profiles (Obi et al., 2024)	Moderate	(Obi et al., 2024)
Lead Optimization	Not quantified (Zhang et al., 2024)	Not quantified	Moderate	(Zhang et al., 2024)
Clinical Trials/Digital Twins	Potential efficiency gains (Bordukova et al., 2023)	Not quantified	Low	(Bordukova et al., 2023)

Table 2: comparative performance metrics

Metric/Outcome	Generative AI (Best Reported)	Traditional Approach (Best Reported)	Relative Improvement	Source
Ligand Binding Affinity	>10–20% higher than SOTA	SOTA virtual screening	10–20% higher	(Kadan et al., 2025)
Computational Cost (Membrane Partitioning)	1/3 of umbrella sampling data needed	Full umbrella sampling	3× reduction	(Obi et al., 2024)

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Speed (Ligand Generation)	>100× faster	Exhaustive virtual screening	>100× faster	(Kadan et al., 2025)
Synthetic Accessibility	Generally better scores	Traditional methods	Improved	(Kadan et al., 2025)

DISCUSSION

Taken together, the evidence strongly suggests that generative AI is bringing meaningful changes to drug discovery, particularly in the early stages such as molecular design and candidate prioritization. Its ability to rapidly generate and evaluate novel compounds, while simultaneously optimizing multiple properties offers a clear advantage over traditional methods and opens up new possibilities for innovation.

Another important aspect is the versatility of generative AI. Beyond discovering new molecules, it is increasingly being used to model membrane interactions, predict adverse drug reactions, and simulate clinical trials. This wide range of applications indicates that generative AI has the potential to evolve into a core technology supporting the entire drug development pipeline, rather than remaining limited to specific tasks.

However, the field is still in its early stages. Many current studies are early implementations, and there is a strong need for validation in real world settings. The lack of standardized benchmarks also makes it difficult to accurately assess how well these models perform outside controlled environments. While these limitations do not undermine the promise of generative AI, they highlight the importance of cautious and realistic expectations.

Future Scope

Looking ahead, future research should focus on systematic comparisons between generative AI and traditional approaches across all stages of drug discovery. Improving model transparency will be essential for building trust among regulators and clinicians. Additionally, deeper integration with experimental workflows and the development of robust ethical and regulatory frameworks will be critical for long term success.

In conclusion, generative AI is not a complete replacement for existing methods, but it represents a powerful and transformative advancement in drug discovery. With continued improvement, validation, and responsible implementation, it has the potential to make drug development faster, more cost-effective, and more accurate ultimately benefiting patients worldwide.

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