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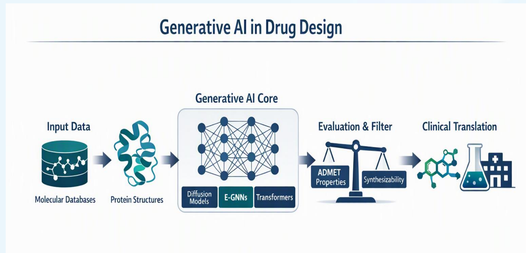


Generative AI for Multi-Objective ADMET Optimization in De Novo Drug Design: A Systematic Review of Molecular Generation Strategies and Evaluation Metrics

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Backgrounds

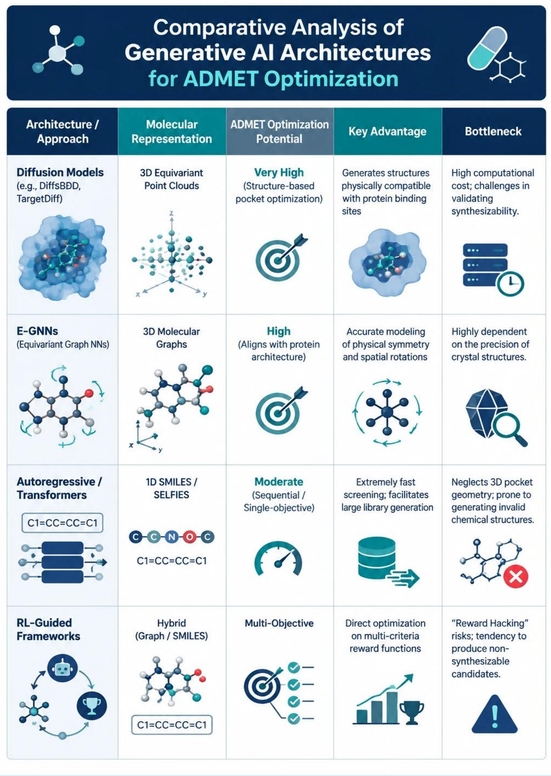
- **The Core Bottleneck:** While generative AI models effectively explore hyper-dimensional chemical spaces (~10^{60} potential compounds), late-stage clinical attrition remains alarmingly high due to unfavorable Pharmacokinetics and Toxicity (ADMET).
- **The Multi-Objective Dilemma:** Designing ligands solely for maximum target binding affinity frequently yields unstable, insoluble, or toxic molecules. Co-optimizing affinity alongside ADMET properties creates conflicting mathematical objectives.
- **Translational Imperative:** Shifting from serendipitous screening to physics-informed, target-aware computational "co-pilots" that bridge the gap between *in silico* generation and *in vitro* wet-lab synthesizability.

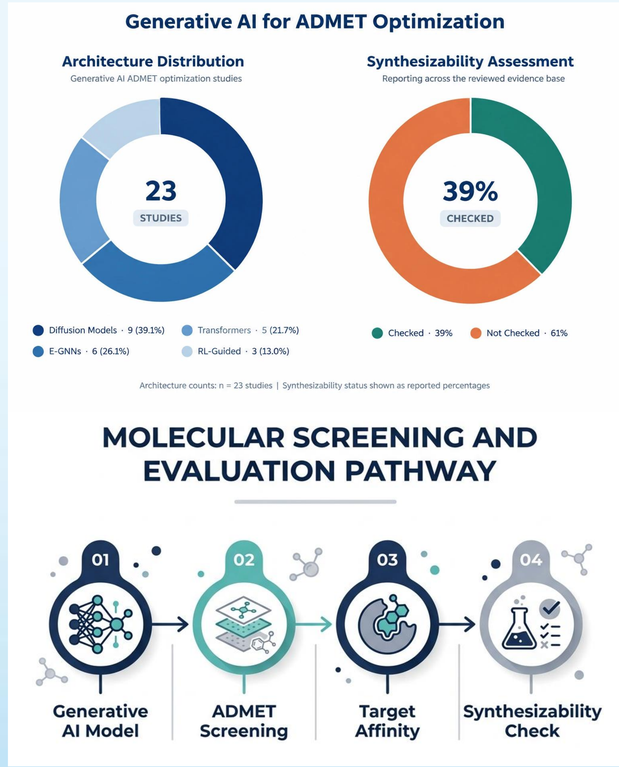
Methods

1. **Study Design:** Conducted in strict adherence to the **PRISMA 2020** guidelines.
2. **Search Strategy:** Comprehensive search performed across PubMed, Scopus, IEEE Xplore, and Web of Science for literature published between 2025 and 2026.
3. **Data Selection:** An initial pool of 600 records was systematically filtered. After duplicate removal, title/abstract screening, and full-text eligibility assessment, 23 foundational studies were included for narrative synthesis.
4. **Quality Assessment:** Methodological rigor evaluated using MINORS criteria.

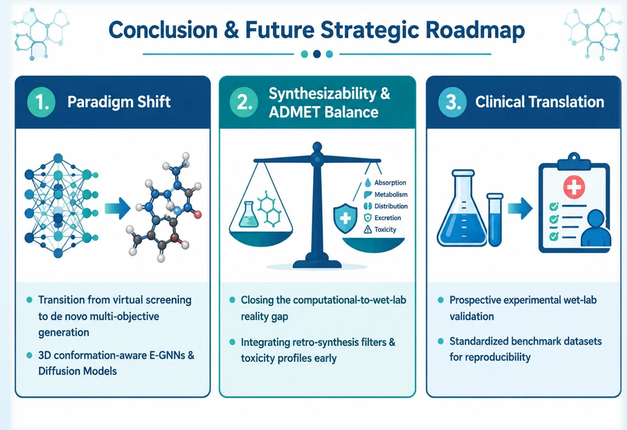


Findings





Conclusion



References

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3. Zarei A, Javidnezhad E, Meysami MS. Deep Markov Neural Clustering: An Optimized Framework for Accurate Detection of Hepatitis B. In: 2026 International Biennial Conference on Advances in Artificial Intelligence and Data Science (IBAAIDS); 2026. p. 1-7.