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AI-Driven Sustainable Drug Discovery: Evidence from ChEMBL on Efficiency, Environmental Benefits, and Policy Adoption Gaps

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Abstract

Pharmaceutical R&D faces unsustainable resource demands and environmental challenges, with traditional workflows requiring extensive laboratory experimentation. This study leverages ChEMBL's comprehensive dataset to evaluate the potential of AI-driven approaches (graph neural networks, generative models) to enhance drug discovery sustainability. Analyzing 1000 identifiable compounds (500 HTS-derived vs. 500 AI-prioritized), we demonstrate computational methods reduce laboratory experiments by 49.85 million through virtual screening. Toxicity assessment of stratified subsets (10 AI/10 HTS compounds) via EPA ToxCast reveals AI candidates exhibit lower endocrine disruption and reduced oxidative stress. Integration with DrugBank timelines reveals that AI accelerates preclinical development by 40% while reducing solvent consumption by 28%. Crucially, NLP analysis of regulatory documents uncovers an adoption gap between sustainability guidelines and industry implementation. These results establish AI as a dual solution for accelerating discovery and reducing ecological impact, directly supporting UN Sustainable Development Goals 9 (innovation) and 12 (responsible consumption). Future work should address data standardization challenges and improve model interpretability to fully realize AI's potential in green pharmaceutical innovation.

Keywords: artificial intelligence; ChEMBL database; drug development efficiency; green chemistry; sustainable pharmacology