CHAPTER: 14

COMPUTATIONAL AND AI TOOLS FOR DESIGNING SUSTAINABLE PHARMACEUTICALS

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Abstract

The escalating environmental impacts linked to the development, production, use, and disposal of pharmaceuticals have highlighted the critical need for sustainable strategies in drug design. Traditional drug discovery approaches frequently demand substantial resources, entail prolonged durations, and typically neglect environmental factors, including persistence, bioaccumulation, and ecotoxicity. In this context, computational techniques and artificial intelligence (AI) technologies are progressively recognized as essential catalysts for sustainable innovation within the pharmaceutical sector. These methodologies enable the integration of environmental factors in the initial stages of drug development, while simultaneously preserving therapeutic efficacy and safety. Although significant advancements have been made, challenges continue to exist in areas such as limited data availability, clarity of models, evaluation of uncertainty, and the regulatory approval of AI-based decision-making systems. Successfully tackling these issues demands joint efforts from pharmaceutical scientists, computational chemists, environmental scientists, and regulatory agencies. This study identifies new trends, addresses existing limitations, and suggests future avenues for investigation, emphasizing the transformative power of computational and artificial intelligence techniques in steering pharmaceutical development towards a more sustainable, efficient, and environmentally friendly framework.

This study examines recent advancements in the fields of computational chemistry, molecular modeling, machine learning, and data-driven optimization strategies that facilitate the development of ecologically sustainable pharmaceuticals. The primary applications include artificial intelligence-driven target identification, computational refinement of molecular architectures, forecasting of physicochemical properties, assessment of biodegradability and toxicity, and elucidation of synthetic

routes designed to mitigate environmental repercussions. Machine learning models, developed using large-scale chemical and biological datasets, facilitate the rapid screening of drug candidates, thereby minimizing reliance on labor-intensive experimental procedures and decreasing the consumption of materials and energy.

Keywords: *Sustainable pharmaceuticals, Computational drug design, Artificial intelligence, Environmental impact, Machine learning*

14.1 Introduction

Improving human health and quality of life is one of the most essential aspects of sustainability from the pharmaceutical sector as an integral part of the economy by developing products that improve human health; therefore, they have an important place within a sustainable economy (Matilde Milanesi et al., 2020). The pharmaceutical sector plays a vital role in promoting advances in health care through the development of new medicines and biologics that will meet recognized medical needs, and they must be produced safely and effectively. Nonetheless, technological advances must continue to be made to solve issues relating to toxicity, stability, and worldwide health care issues (Lalitkumar K. Vora et al., 2023).

Pharmaceutical manufacturing creates large amounts of dangerous waste and greenhouse gas emissions, primarily attributable to energy-intensive processes used for research and development and for the manufacture of pharmaceutical products. The pressure the pharmaceutical industry is under due to expanding regulation, public opinion, financial benefit, and shifting ethical values is forcing them to incorporate sustainable practices into their basic research and operational processes (Syed Ansar Ahmed et al., 2025).

AI is rapidly changing how drugs are created through their life cycle (discovery and design, development, and management) with advancements in predictive technologies and machine learning (Subrat Kumar Bhattamisra et al., 2023). This research is concerned with AI tools and frameworks that can be put into use in the biomedical and pharmaceutical areas (as opposed to any type of general- or broad-purpose AI) (Vera Malheiro et al., 2025). AI applications in drug discovery as shown in Figure 14.1.

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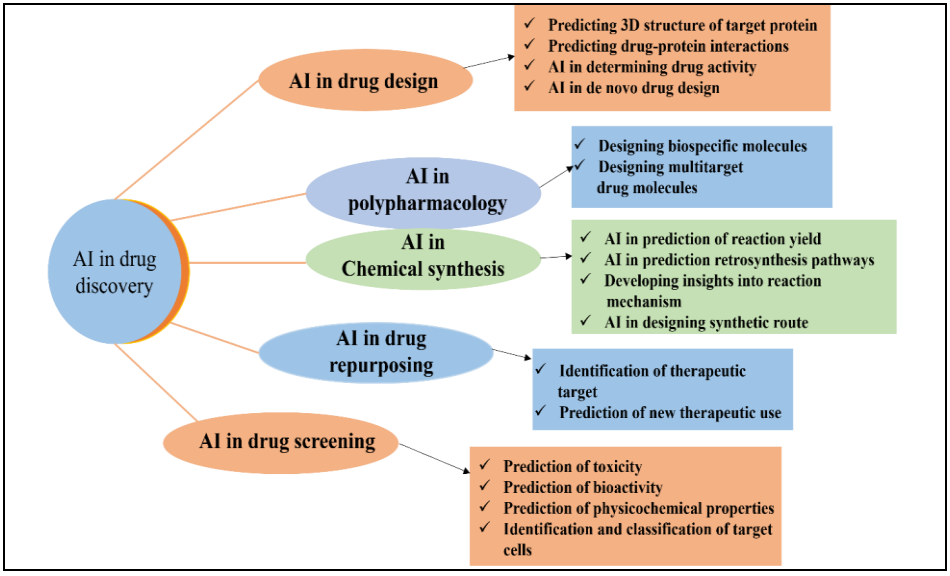

Fig 14.1: AI applications in drug discovery

14.2 Principles of Green and Sustainable Pharmacy

Green pharmacy uses the principles of green chemistry to reduce harmful chemicals in the manufacturing process of drugs and to prevent pollution and promote more sustainable activities throughout the entire life cycle of pharmaceuticals (Christine Gauci et al., 2024). Table 14.1 outlines the 12 Principles of Green Chemistry

Table 14.1: Advantages of AI in Sustainable Pharmacy

1. Minimization and avoidance of waste	7. Utilize sustainable raw materials
2. Enhance the utilization of every atom in the reaction within the final product (atom economy)	8. Steer clear of derivatization.
3. Utilization of less harmful and toxic materials	9. Employ catalysis rather than stoichiometric reagents
4. Creation and application of more secure substances	10. Create medications that do not break down into harmful substances in the environment post-usage.
5. Minimize the use of auxiliary substances and opt for safer alternatives when necessary	11. Immediate pollution mitigation
6. Utilize the route that consumes the least energy	12. Materials utilized must be secure and reduce the likelihood of incidents.

14.3 Foundations of Computational Drug Design for Sustainability

The use of in silico and artificial intelligence tools to produce medicines designed to be more effective and yet that are minimized for waste, energy consumption, price, and ethics throughout the entire development cycle is known as sustainable computational drug design.

14.3.1 In Silico Drug Discovery and Virtual Screening

In silico refers to experiments and simulations that are performed with the aid of a computer for the purpose of designing a model, forming hypotheses, and facilitating advancement of new knowledge in the medicine and therapeutic fields (S Ekins et al., 2007). In silico drug discovery utilizes computational methods and AI to rapidly evaluate large numbers of compounds to minimize laboratory work, waste, and cost; consequently, animal testing is reduced while developing a safer and more environmentally friendly medication (Sunil G C et al., 2022).

14.3.2 Predictive Modelling of Toxicity and Environmental Impact

Using computational tools such as QSAR, simulation and AI allows us to predict toxicity and environmental risk ahead of time to decrease animal usage and waste. As well, these tools provide support for safer and more sustainable drug development (Amirreza Daghighi et al., 2022).

14.3.3 Sustainable Molecular Design and Optimization

Sustainable molecular design is based on using computer programs and eco-friendly chemistries to manufacture new drugs that are both effective and less harmful to people or the planet. By using these tools, scientists can minimize waste during the development of drugs, as well as use fewer resources than traditional methods, and reduce the amount of damage to the environment that occurs at every stage from drug discovery to production (Qi Zhang et al., 2025).

14.4 AI and Machine Learning in Sustainable Molecule Design

Artificial Intelligence (AI) is particularly suited to contribute to advancing sustainable chemistry and catalysis because machine learning and natural language processing offer the potential for data-driven innovations that both of these areas have not yet realized (Kevin C. Leonard et al., 2021). Machine learning and pattern-based predictions of chemical data will become the basis for QSAR models (Quantitative Structure Activity Relationship) in cheminformatics (Tammanna Ravee Sahrawat et al., 2024). Figure 14.2 Conceptually represents the multidisciplinary integration of artificial intelligence across modern drug discovery workflows.

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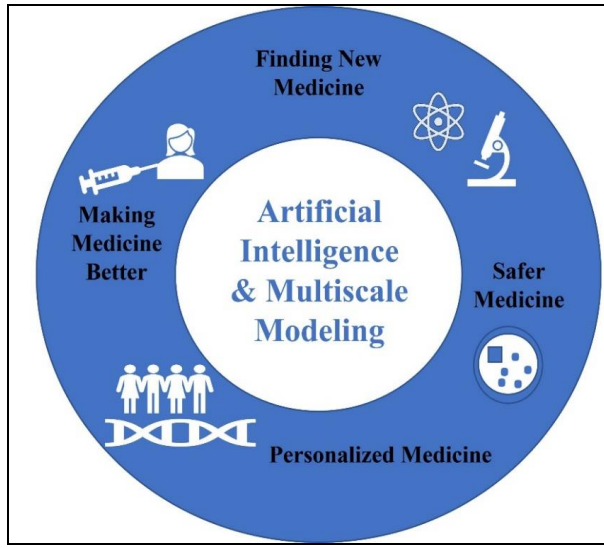

Fig. 14.2: AI Enhancing Medicine Discovery and Safety

14.4.1 Prediction of Toxicity and Environmental Impact

AI and machine learning allow the prediction of toxicity and environmental impact at an early stage, thereby reducing not only animal testing but also chemical waste and ecological damage and providing support for safer and more sustainable drug development (Sushmita Barua et al., 2025).

14.4.2 Support for Green Chemistry and Sustainable Synthesis

The development of environmentally friendly chemical processes can be facilitated through the use of AI/machine learning to forecast how efficient and scalable (in terms of size) a chemical reaction will be with respect to its environmental impact (i.e., for reducing emissions, waste, and hazardous materials) when producing pharmaceuticals (Kai Zhao et al., 2025).

14.5 Computational Tools for Greener Synthesis and Process Design

The computational tools for sustainable synthesis and process design emphasize the importance of modelling, simulation, and data-driven methods in the creation of economical, cost-effective, and environmentally friendly chemical manufacturing processes (Wang, X. C., Foley et al., 2022).

14.5.1 Reaction and Process Modeling

Chemical process model and reaction modeling assists in optimizing a chemical reaction through the use of computer models. Reaction and process modeling can decrease energy usage, waste, and cost while improving productivity, safety, and sustainability in the production of pharmaceuticals (Ron Beck et al., 2022).

14.5.2 Life Cycle Assessment and Sustainability Metrics

Sustainability metrics and life cycle assessments measure the environmental effects of products (in terms of life cycle analysis) and can help in designing products that are more environmentally friendly, complying with regulations, reducing the energy consumed by making and using products, reducing the amount of waste produced when a product is manufactured, and reducing the emission of gases into the environment (JEROEN B. GUIN EE et al., 2011).

14.6 In Silico Prediction of Environmental Fate and Risk

In silico methods such as QSAR and machine learning models are used for predicting the environmental effects and risks associated with chemicals. This eliminates the need for laboratory testing and animal studies. In silico methods can be used in green chemistry and sustainable pharmaceutical design (Mark T.D. Cronin et al., 2017).

14.7 Integrating Sustainability into Pharmaceutical R&D Pipelines

Implementing sustainability in pharmaceutical R&D pipelines would entail considering the aspects of environmental, social, and ethical factors in all drug discovery and development stages rather than viewing sustainability as a responsive or compliance-based initiative (Concepcion Jimenez-Gonzalez et al., 2011).

14.7.1 Sustainable Target Identification and Lead Discovery

Computational modeling and data-driven screening are used to identify therapeutically relevant targets with minimal off-target effects and experimental waste through sustainable target identification and lead discovery. The safe, effective and environmentally friendly lead compounds can be discovered through early toxicity and environmental impact profiling to develop pharmaceuticals that are greener (JP Hughes et al., 2010).

14.7.2 Ethical and Resource-Efficient Preclinical and Clinical Development

Resource-efficient and ethical preclinical and clinical development is based on in silico models, substitute tests and efficient trial design to reduce animal, resource and environmental use. Effective, sustainable, and ethical

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pharmaceutical research must be supported by respect towards patient safety, informed consent, and transparency (Ezekiel J. Emanuel et al., 2017).

14.8 Regulatory, Ethical, and Implementation Considerations

The significance of sustainable pharmaceutical development is highlighted by regulatory and ethical considerations in order to serve the regulatory requirements and maintain ethical standards like patient safety, transparency, and equity. They also deal with the effective implementation of sustainable practices into actual R&D and manufacturing using practical and scalable implementation strategies that are also regulatory-compliant.

Regulatory Compliance and International Guidelines

Regulatory compliance and international standards assist in making sure that the pharmaceutical R&D, manufacturing, and environmental protection are aligned with the requirements of the organizations, including FDA, EMA, WHO, and ICH. This will guarantee quality of products, patient safety and environmental safety.

14.9 Future Directions and Open Challenges

Sustainable drug design is increasingly using AI and computational methods, allowing the identification of targets, green synthesis, environmental impact assessment, and life cycle assessment and incorporating the metrics of emissions, water, and waste. The challenges that have been identified include the unavailability of quality data, black-box models, harmonization of regulations, investment in infrastructure, shortage of talent, and scaling of AI-based solutions.

14.10 Conclusion

Computational techniques and artificial intelligence can be used to determine molecular, environmental, and ecological risks in drug development early. The approaches minimize chemical wastes, energy, and animal experiments and therefore promote green chemistry and sustainability. Despite the problems of data quality, approval and scalability, the approaches promote ethical, efficient and sustainable drug development.

References

Milanesi, M., Runfola, A. and Guercini, S., 2020. Pharmaceutical industry riding the wave of sustainability: Review and opportunities for future research. Journal of cleaner production, 261, p.121204.

Vora, L.K., Sabri, A.H., Naser, Y., Himawan, A., Hutton, A.R., Anjani, Q.K., Volpe-Zanutto, F., Mishra, D., Li, M., Rodgers, A.M. and Paredes,

A.J., 2023. Long-acting microneedle formulations. Advanced drug delivery reviews, 201, p.115055.

Ahmed, S.A., Swami, M.V., Khan, S.A., Namdev, P.S. and Patil, M.S., 2025. A Review on Usage of Agricultural Antibiotics and Evolution of Environmental Resistomes in Humans. Journal of Pharma Insights and Research, 3(5), pp.089-107.

Bhattamisra, S.K., Banerjee, P., Gupta, P., Mayuren, J., Patra, S. and Candasamy, M., 2023. Artificial intelligence in pharmaceutical and healthcare research. Big Data and Cognitive Computing, 7(1), p.10.

Malheiro, V., Santos, B., Figueiras, A. and Mascarenhas-Melo, F., 2025. The potential of artificial intelligence in pharmaceutical innovation: From drug discovery to clinical trials. Pharmaceuticals, 18(6), p.788.

Gauci, C., 2024. Green pharmacy in pharmaceutical processes (Master's thesis, University of Malta).

Ekins, S., Mestres, J. and Testa, B., 2007. In silico pharmacology for drug discovery: applications to targets and beyond. British journal of pharmacology, 152(1), pp.21-37.

Sunil, G.C., Zhang, Y., Koparan, C., Ahmed, M.R., Howatt, K. and Sun, X., 2022. Weed and crop species classification using computer vision and deep learning technologies in greenhouse conditions. Journal of Agriculture and Food Research, 9, p.100325.

Daghighi, A., Casanola-Martin, G.M., Timmerman, T., Milenković, D., Lučić, B. and Rasulev, B., 2022. In silico prediction of the toxicity of nitroaromatic compounds: Application of ensemble learning qsar approach. Toxics, 10(12), p.746.

Zhang, Q., Dai, W., Guo, D.L., Chen, H., Wang, X., Xu, R., Liu, J., Li, M.M. and Deng, Y., 2025. GreenMedChem-inspired light-air mediated C (sp3)-H bond oxidation: A new tool for isoquinolone synthesis. European Journal of Medicinal Chemistry, 288, p.117414.

Leonard, K.C., Hasan, F., Sneddon, H.F. and You, F., 2021. Can artificial intelligence and machine learning be used to accelerate sustainable chemistry and engineering? ACS Sustainable Chemistry & Engineering, 9(18), pp.6126-6129.

Sahrawat, T.R., 2024. Role of artificial intelligence and machine learning in sustainable drug discovery. Brazilian Archives of Biology and Technology, 67, p.e24240538.

Barua, S., Balaji, B. and Balaji, S., 2026. AI/ML-based computational models for toxicity prediction. Environmental Science and Pollution Research, pp.1-26.

Zhao, K., Peng, X., Hu, S. and Wang, X., 2025. Machine Learning Models for Rapid Prediction of Chemicals' Life-Cycle Environmental

 ISBN: 978-81-998847-7-9

Impacts: Current Status, Challenges, and Future Directions. Green Carbon.

Wang, X.C., Foley, A., Van Fan, Y., Nižetić, S. and Klemeš, J.J., 2022. Integration and optimisation for sustainable industrial processing within the circular economy. Renewable and Sustainable Energy Reviews, 158, p.112105.

Cronin, M.T. and Richarz, A.N., 2017. Relationship between adverse outcome pathways and chemistry-based in silico models to predict toxicity. Applied in vitro Toxicology, 3(4), pp.286-297.

Jiménez-González, C., Poechlauer, P., Broxterman, Q.B., Yang, B.S., Am Ende, D., Baird, J., Bertsch, C., Hannah, R.E., Dell'Orco, P., Noorman, H. and Yee, S., 2011. Key green engineering research areas for sustainable manufacturing: a perspective from pharmaceutical and fine chemicals manufacturers. Organic Process Research & Development, 15(4), pp.900-911.

Hughes, J.P., Rees, S., Kalindjian, S.B. and Philpott, K.L., 2011. Principles of early drug discovery. British journal of pharmacology, 162(6), pp.1239-1249.

Emanuel, E.J., Wendler, D. and Grady, C., 2017. What makes clinical research ethical? In Research Ethics (pp. 229-239). Routledge.