BioLuster Research Center Ltd

Medicinal Chemistry and Therapeutics

Editorial

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Artificial Intelligence in ADMET Prediction: Transforming Drug Safety and Pharmacokinetic Assessment

Artificial Intelligent for ADMET Prediction

Absorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET) properties are among the most critical determinants of whether a promising drug candidate ultimately reaches clinical use. It is estimated that a substantial proportion of drug candidates fail during preclinical and clinical development because of unfavorable pharmacokinetic behavior or unexpected toxicity, despite demonstrating excellent biological activity. Consequently, early evaluation of ADMET characteristics has become an essential component of modern medicinal chemistry. Artificial intelligence (AI) has significantly transformed this process by enabling rapid, accurate, and cost-effective prediction of ADMET properties before extensive experimental testing. By integrating machine learning (ML), deep learning (DL), and large-scale cheminformatics databases, AI supports the identification of compounds with favorable drug-like properties while reducing development costs and shortening discovery timelines (Vamathevan et al., 2019; Chen et al., 2018).

Early Toxicity Prediction

Drug-induced toxicity remains one of the primary causes of attrition during drug development and post-marketing withdrawal. Conventional toxicity evaluation relies heavily on in vitro assays and animal studies, which are expensive, time-consuming, and sometimes fail to accurately predict human responses. AI-driven predictive toxicology provides an efficient alternative by analyzing extensive toxicological datasets to identify structural features associated with adverse biological effects. Modern machine learning models can predict multiple toxicity endpoints, including hepatotoxicity, cardiotoxicity, nephrotoxicity, mutagenicity, carcinogenicity, hERG inhibition, and drug-induced liver injury (DILI). Deep learning algorithms further improve prediction accuracy by automatically extracting complex molecular features that influence toxicological outcomes. Early identification of potentially toxic compounds enables medicinal chemists to eliminate unsuitable candidates or modify their chemical structures before entering costly preclinical studies, thereby improving both safety and research efficiency (Chen et al., 2018; Bender & Cortés-Ciriano, 2021).

Pharmacokinetic Property Prediction

Beyond biological activity, successful drug candidates must possess favorable pharmacokinetic characteristics to achieve therapeutic efficacy. AI has become an indispensable tool for predicting critical ADME parameters, including intestinal absorption, blood-brain barrier permeability, plasma protein binding, cytochrome P450 metabolism, metabolic stability, clearance, and renal excretion.

Deep learning algorithms, graph neural networks, and quantitative structure–activity relationship (QSAR) models analyze molecular structures alongside experimental pharmacokinetic datasets to accurately estimate ADME behavior. These predictions enable medicinal chemists to prioritize compounds with optimal oral bioavailability, metabolic stability, and systemic exposure while minimizing undesirable pharmacokinetic properties. Early computational assessment reduces reliance on extensive laboratory experimentation and facilitates rational lead optimization (Mak & Pichika, 2019).

Reducing Late-Stage Drug Attrition

Late-stage clinical failure remains one of the most significant economic challenges in pharmaceutical development. Multi-parameter AI models simultaneously evaluate potency, selectivity, pharmacokinetics, toxicity, and synthetic accessibility, allowing researchers to prioritize compounds with the highest probability of clinical success. Continuous retraining using newly generated experimental and clinical datasets further improves predictive performance, enabling increasingly accurate identification of high-risk compounds during the earliest stages of drug discovery. Consequently, AI-assisted ADMET prediction contributes directly to lowering attrition rates, accelerating regulatory approval, and improving the overall productivity of pharmaceutical research (Paul et al., 2010; Vamathevan et al., 2019).

Widely Used AI-Based ADMET Prediction Platforms

Several computational platforms have become indispensable tools for predicting ADMET properties during modern drug discovery. These resources employ machine learning, deep learning, and cheminformatics algorithms to estimate pharmacokinetic and toxicity profiles before experimental validation. These platforms (**Table 1**) are widely used in both academia and the pharmaceutical industry to prioritize lead compounds, optimize pharmacokinetic profiles, and identify potential safety liabilities prior to experimental evaluation.

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Table 1. Platform and their official websites for ADMET prediction

Platform	Primary Applications	Official Website
SwissADME	Drug-likeness, physicochemical properties, pharmacokinetics, medicinal chemistry filters	https://www.swissadme.ch
pkCSM	ADMET prediction using graph-based signatures	https://biosig.lab.uq.edu.au/pkcsm
ADMETlab 3.0	Comprehensive ADMET prediction, toxicity assessment, molecular optimization	https://admetlab3.scbdd.com
ProTox-3.0	Toxicity prediction, LD50 estimation, toxicity endpoints	https://tox.charite.de/protox3
DeepPK	AI-based pharmacokinetic parameter prediction	https://biosig.lab.uq.edu.au/deeppk
OCHEM	QSAR modeling, cheminformatics, ADMET prediction	https://ochem.eu
VEGA Hub	Toxicological prediction and QSAR models	https://www.vegahub.eu
FAF-Drugs4	ADMET filtering and drug-likeness assessment	https://fafdrugs4.rpbs.univ-paris-diderot.fr
StarDrop (Optibrium)	Commercial platform for ADMET optimization and multi-parameter drug design	https://www.optibrium.com/stardrop
Schrödinger QikProp	Commercial software for ADME property prediction	https://www.schrodinger.com/products/qikprop

Integrating such AI-enabled tools into medicinal chemistry workflows substantially reduces development time, minimizes experimental costs, and increases the probability of identifying clinically successful therapeutic candidates.

Relevance to the Scope of *Journal of Medicinal Chemistry and Therapeutics*

This editorial aligns well with the scope of the Journal of Medicinal Chemistry and Therapeutics by highlighting the growing role of artificial intelligence (AI) in ADMET prediction and its applications in modern drug discovery. It provides an overview of AI-driven approaches for toxicity and pharmacokinetic prediction, discusses widely used AI-based ADMET platforms, and demonstrates their significance in accelerating the discovery of safer and more effective therapeutics. By presenting current advances and practical computational tools, this editorial aims to stimulate researchers to explore and integrate AI-based ADMET prediction into medicinal chemistry and therapeutic research.

Editorial Note

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Conflict of Interest

The author declared that they have no conflict of interest.

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References

Bender, A., & Cortés-Ciriano, I. (2021). Artificial intelligence in drug discovery: what is realistic, what are illusions? Part 1: Ways to make an impact, and why we are not there yet. *Drug discovery today*, *26*(2), 511-524. https://doi.org/10.1016/j.drudis.2020.12.009

Chen, H., Engkvist, O., Wang, Y., Olivecrona, M., & Blaschke, T. (2018). The rise of deep learning in drug discovery. *Drug Discovery Today, 23*(6), 1241–1250. https://doi.org/10.1016/j.drudis.2018.01.039

Mak, K. K., & Pichika, M. R. (2019). Artificial intelligence in drug development: Present status and future prospects. *Drug Discovery Today, 24*(3), 773–780. https://doi.org/10.1016/j.drudis.2018.11.014

Paul, S. M., Mytelka, D. S., Dunwiddie, C. T., Persinger, C. C., Munos, B. H., Lindborg, S. R., & Schacht, A. L. (2010). How to improve R&D productivity: The pharmaceutical industry's grand challenge. *Nature Reviews Drug Discovery, 9*(3), 203–214. https://doi.org/10.1038/nrd3078

Vamathevan, J., Clark, D., Czodrowski, P., Dunham, I., Ferran, E., Lee, G., et al. (2019). Applications of machine learning in drug discovery and development. *Nature Reviews Drug Discovery, 18*(6), 463–477. https://doi.org/10.1038/s41573-019-0024-5

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