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Editorial: Enhancing drug discovery through structure-based design and computational techniques

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Editorial on the Research Topic
Enhancing drug discovery through structure-based design and computational techniques

It is well-documented that discovering new drugs is a challenging and time-consuming process that requires substantial funding and well-equipped laboratory facilities for research and development (Pant et al., 2022; Pathak et al., 2020). Nowadays, computers play an essential role in research across various domains, including drug discovery. Computers and related algorithms and programs are widely used by scientists in both academia and industry to streamline and enhance the drug development process. As a result, several drugs developed with the help of computational tools have successfully reached the market and are continuously being used for the prevention and treatment of various diseases (Pathak et al., 2020).

As a hallmark of 21st-century science, bioinformatics, through computer-based investigations, has significantly revolutionized biological and pharmaceutical research. Recognizing its importance in drug discovery, numerous databases and tools have been developed, and many more are continuously being introduced to support the drug discovery process. Computational tools have made a significant contribution in resolving the drug target structure and drug-target interactions related issues very precisely. Additionally, existing resources are regularly updated to enhance their utility and facilitate ongoing drug discovery projects (Zhang et al., 2025). These computational tools enable the screening of large chemical libraries to identify potential lead compounds, thereby saving both time and resources. Among the core strategies in computer-aided drug discovery is structure-based design, which includes structural modeling, binding site prediction, molecular docking, virtual screening, ADMET prediction, molecular dynamics simulations, and binding energy calculations using the MM-PB/GBSA approach (Batool et al., 2019; Genheden and Ryde, 2015; Sadybekov and Katritch, 2023).

The current Research Topic "*Enhancing drug discovery through structure-based design and computational techniques*" received seven manuscripts. Four articles were accepted for publication in this special Research Topic.

The first article of this Research Topic, entitled "*Integrative Computational Approaches for Discovery and Evaluation of Lead Compounds for Drug Design*," explores how combining computational methods such as molecular docking, molecular dynamics simulations, and machine learning can enhance the identification and assessment of potential drug candidates. It emphasizes the importance of integrating these *in silico* techniques in streamlining drug discovery processes, improving prediction accuracy, and reducing the use of traditional experimental methods (Naithani and Guleria). The second article, entitled "*A Review on Dynamics of Permeability-Glycoprotein in Efflux of Chemotherapeutic Drugs*," highlights the role of P-glycoprotein (P-gp), a membrane-bound efflux transporter, emphasizing the Research Topic of multidrug resistance in cancer therapy. It discusses how P-gp actively transports a variety of chemotherapeutic agents out of cancer cells, thereby reducing drug efficacy. This review also explores strategies to inhibit P-gp function to enhance the effectiveness of chemotherapy (Rani et al.). The third article, entitled "*The Role of Physicochemical and Topological Parameters in Drug Design*," explores how molecular properties such as lipophilicity, molecular weight, and topological descriptors affect a compound's pharmacokinetics and pharmacodynamics. It emphasizes the importance of integrating these parameters in the early drug development to enhance efficacy and minimize toxicity (Darlami and Sharma). Concluding this Research Topic is the article entitled "*Identification of natural compounds as potential inhibitors of Interleukin-23: virtual screening, ADMET, drug-likeness, and dynamic simulation*." The article explores the use of virtual screening and molecular dynamics to identify natural lead compounds that could inhibit Interleukin-23, a target in inflammatory diseases. It highlights a computational strategy to streamline early-stage drug discovery (Gheidari et al.).

Given the current landscape and the growing demand for computational approaches in drug discovery, this series highlights the progress made in structure-based design and its value in identifying lead compounds for drug development. It offers a timely and key opportunity to explore how structure-based methods can contribute to societal welfare by reducing the need for animal testing, time, and experimental costs.

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Conflict of interest

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