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Short Communication

Artificial Intelligence-Driven Drug Discovery: Reimagining the Journey from Molecule to Medicine

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DESCRIPTION

Artificial intelligence is transforming drug discovery by introducing computational methods capable of processing enormous collections of biological, chemical and clinical information. Traditional drug development can require extensive time and substantial financial resources because identifying a promising therapeutic molecule involves many stages, from selecting a biological target to evaluating molecular activity, safety and pharmacological properties. Artificial intelligence can accelerate several of these stages by recognizing patterns within complex datasets, predicting molecular characteristics and helping prioritize the most promising candidates. The process often begins with identifying a biological target associated with a disease mechanism. Genomic information, protein profiles, molecular networks and clinical observations can provide clues about proteins or pathways that may influence disease progression. Artificial intelligence models can integrate these different information sources and identify relationships that may be difficult to recognize through conventional computational approaches. Target prioritization can consequently become more systematic, particularly when thousands of possible molecular candidates are available [1,2].

Once a target has been selected, computational systems can help identify molecules capable of interacting with it. Machine learning models can analyze chemical structures and learn relationships between molecular features and biological activity. Deep learning methods can represent molecules using graphs, sequences or numerical descriptions and estimate how structural changes may influence their properties. These predictions can reduce the number of compounds requiring extensive laboratory evaluation and help chemists focus on candidates with more favourable characteristics. Virtual screening is another area strongly influenced by artificial intelligence. Large chemical libraries may contain millions of compounds, making direct evaluation impractical. Computational models can rank these molecules according to predicted binding potential, activity, selectivity or other properties. Molecular docking can provide structural information about possible interactions between a compound and a protein, while machine learning can help refine rankings by considering multiple molecular characteristics simultaneously [3,4].

Generative artificial intelligence introduces a different approach by creating new molecular structures rather than simply evaluating existing compounds. Generative models can propose molecules with desired characteristics, such as particular binding properties, molecular sizes or chemical features. The generated structures can then be assessed using additional computational filters. This approach creates opportunities for designing compounds that may not be present in existing chemical libraries. Drug safety is another important area where artificial intelligence can contribute. Predictive models can estimate potential toxicity, metabolic behavior, solubility and interactions with biological systems before a candidate advances to later stages. Early identification of undesirable properties can reduce wasted resources and help prioritize molecules with more favourable profiles. However, computational predictions cannot completely replace biological evaluation because complex physiological responses may not be fully represented by available datasets [5,6].

It can also support drug repurposing, in which existing medicines are considered for additional therapeutic applications. Computational models can connect drugs with genes, proteins, pathways, diseases and clinical information to identify unexpected relationships. A medicine developed for one condition may influence a molecular pathway relevant to another condition, creating an opportunity to explore an alternative application without starting the entire development process from the beginning. A model trained on limited or unbalanced data may produce unreliable predictions when applied to unfamiliar molecules or biological populations. Careful data curation,

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validation and independent evaluation are therefore essential for developing dependable computational systems [7,8].

Interpretability is equally important. Some advanced artificial intelligence models can generate highly accurate predictions while providing limited explanations for their decisions. In pharmaceutical applications, understanding why a molecule is predicted to interact with a target or display a particular property can guide chemical optimization and increase confidence in computational results. Explainable artificial intelligence can help identify molecular features that contribute to predictions and make computational outputs easier for specialists to assess. Integration with multi-omics technologies is expected to broaden the capabilities of artificial intelligence in pharmaceutical development [9,10].

CONCLUSION

Genomic, transcriptomic, proteomic, metabolomic and clinical information can be combined to create detailed representations of disease biology. Such integration may support more precise target selection, patient stratification and treatment design. Personalized drug development could increasingly consider molecular differences among individuals when predicting therapeutic responses. By shortening computational cycles and revealing previously overlooked molecular possibilities, artificial intelligence has the potential to make drug discovery more efficient, targeted and adaptable to the complex biology of human disease.

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