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Artificial Intelligence for Drug Discovery-Resources, Application and Challenges

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Abstract: *Artificial intelligence (AI) has infused various sectors, including the drug discovery, where it has been utilized to efficiently identify new chemical moieties with desirable properties. Conventional wet laboratory testing, validations, and synthetic procedures are costly and time-consuming for drug discovery. The future in artificial intelligence (AI) techniques has revolutionized their applications to medicinal chemistry and drug discovery. Altogether with accessible data resources, AI techniques are changing the approach of drug discovery. In previous ten years, a series of AI-based models have been developed for various steps of drug discovery. Meanwhile, the algorithms used to modify AI-based models for drug discovery is argued. Subsequently, the applications of AI techniques in pharmaceutical analysis including predicting drug toxicity, drug bioactivity, and drug physicochemical property is discussed. Furthermore, AI-based models for de novo drug design, drug-target structure prediction, drug-target interaction, and binding affinity prediction is discussed. Moreover, it is also highlighted the modern applications of AI in drug activity prediction and nano-medicine design. Finally, the challenges and future perspectives on the applications of AI to drug discovery are discussed here*

Keywords: artificial intelligence; drug discovery; medicinal chemistry

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