Applications of artificial intelligence in drug discovery and development

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The drug discovery process includes identification of drug targets, screening of hit compounds, the hit-to-lead phase, and lead optimization. These stages involve various scientific disciplines, including biology, chemistry, pharmacology, and computational science. The drug discovery process is slow, expensive, and complex and often relies on trial-and-error methods. Recently, artificial intelligence (AI) has been employed to effectively accelerate the drug discovery process. In this talk, I will present applications of AI for accelerating drug discovery and development, such as predictions of cardiotoxicity, metabolic stability, and identification of new drug target for drug repurposing. Further, I will discuss about the challenges faced with the use of AI in drug discovery and development.