Deep drug design: Advancing from hits to leads

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Molecular design is an iterative, constructive process grounded in pattern recognition. Generative AI empowers automated molecular design, replicating and often surpassing chemists' capacity to connect molecular structure, synthetic routes, and molecular properties. These systems consider domain-specific data during the molecule construction process. A key benefit of generative AI in drug design is its potential to develop data-driven, implicit models that effectively navigate the complexities of chemical search. Deep networks and hybrid ensembles enhance both the prediction of pharmacological properties and the planning of chemical syntheses. We will present a selection of AI methods applicable to de novo drug design, with a focus on approaches that have demonstrated effectiveness and reliability in hit and lead structure generation. Prospective case studies will be examined, emphasizing the use of graph neural networks for both molecular design and reaction prediction, as well as the application of active learning for molecule optimization.