

Applications of generative molecular AI in drug design

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Drug development is a traditionally long and very expensive task consisting of many steps including lead discovery and lead optimization. For this reason, a popular approach due to its cost-effectiveness currently is drug repurposing, in which one attempts to modify or even use an existing drug for new disease targets. Recent advancements in artificial intelligence (AI) have shown great potential in streamlining this process. Many applications of machine learning methodology in this approach necessitate an AI model capable of modifying the molecular structure of an initial drug according to relevant metrics to meet specific therapeutic requirements. In this study, we assess the performance of these AI models for molecular generation in drug design, focusing on their effectiveness in generating druglike and plausible molecules. We place particular emphasis on how the representation of molecules as input affects the training and outcomes of the models.

Keywords: generative AI, drug design, molecular representation