Generative Artificial Intelligence in the context of drug discovery

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Since a few years, deep learning and generative artificial intelligence applied to medicinal chemistry has generated a strong interest. Although many promises have been made by this technology, there is yet to cross the gap from proof-of-concepts to real-life applications. Here, we compare two of the most studied generative models for chemistry in the literature, Variational-Auto Encoders and Recurrent Neural Networks, with regard to their performance in the setting of industrial drug discovery.

Bibliography:

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