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AI-based Smart Molecular Design

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The ultimate goal of chemistry is to make new molecules with desired properties. It is challenging because chemical space is very large and discrete with a wide variety of molecules. For example, there are only 108 molecules synthesized as potential drug candidates, but 1060 molecules are estimated to be existing. High-throughput virtual screening approach has attracted great attention but still requires large costs and time. In this talk, we propose to use a molecular generative model based on deep learning algorithm as an alternative. It is specialized in controlling multiple molecular properties simultaneously, embedding them in namely the latent space. As a proof of concept, we will show that it can be used to generate a number of molecules as drugs with specific properties. We also apply it to design of new molecules with promising binding energy for a specific target protein and use them as potential drug candidates that are not in the database.

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