How Medvolt's NCE module creates promising drugs.

Case Study

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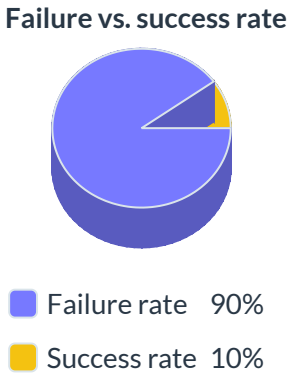
Creating a novel drug molecule with desired drug-like properties is a real challenge. It takes more than a decade to bring a successful drug to the market. Statistics show that nearly 90% of drugs fail in clinical trials. Eventually, the time and cost spent on these drugs go waste for the pharmaceutical companies. Most of these drugs fail because of their off-target effect, safety concern, and efficacy. Medvolt's NCE module overcomes the difficulties by using the inverse designing process wherein a new drug is designed with desired properties using AI and state-of-the-art insilico techniques. With the advancement in computational power and the introduction of AI, it is now possible to successfully employ inverse design in identifying a novel chemical entity (NCE).

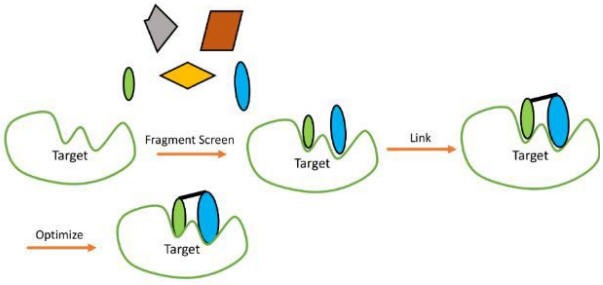


MEDVOLT'S STATE OF ART TECHNIQUES

Fragment-based de novo design

Medvolt has a dedicated fragment library which is highly diverse and is curated from literature using natural language processing (NLP). The use of the fragment as starting point to build drug molecules is highly advantageous to using large molecules as in the traditional approach. Some of the advantages include

- Fragments being small can explore the chemical space of the target and can identify new potential binding sites
- The fragments in addition to being small are comparatively less complex than large molecules, and can easily undergo multiple iterations to generate compounds with good efficiency, binding probability, and pharmacokinetic properties.
- Fragments can effectively be employed to develop drugs for undruggable targets.



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Inverse design using AI techniques

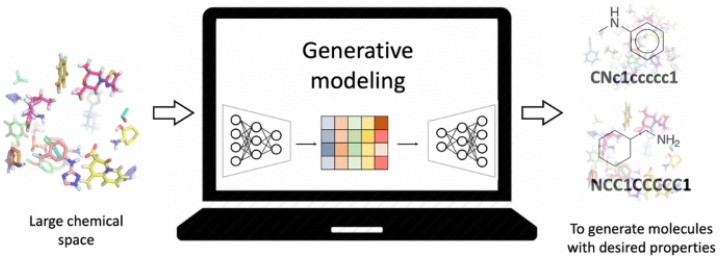
Inverse design generates compounds with predefined drug-like properties. The two neural networks viz., the generative model and reinforcement-based multiparameter optimization (RL-based MPO), work together to develop drugs with defined properties. The former generates the compound whereas the latter predicts and optimizes the properties of the compound.

Generative model

The generative model uses one of the neural networks viz., recurrent neural network (RNN), variational autoencoders (VAE), generative adversarial networks (GAN), and reinforcement-based models, to generate compounds. In the process of generation, the 3D structure of the compound is converted to either SMILES or graphic pattern and are fed to the neural networks. The neural network generates potent molecules represented as either SMILES or Graphic patterns. The 3D molecules are later developed from these representations. The generative models are considered promising for the computational creation of novel molecules due to their state-of-the-art results in the virtual synthesis of images, text, speech, and image captions.

RL-based MPO

The drug candidates usually fail in clinical trials owing to their poor pharmacological properties. Hence, it is a good practice to predict these properties very early at the generation stage to avoid failures in clinical trials. Our RL-based MPO neural networks predict the properties of the compounds generated by the generative model and also optimize the compounds to attain the desired values of properties.



Hit identification

Medvolt's NCE module has got molecular docking and ADMET property prediction tools to filter out and identify the hit compound.

Lead Optimization

The state of art molecular dynamics-Free energy perturbation (FEP) studies are used to optimize the lead compound.

Case Study

RESULT

Our AI-driven de novo designing platform accelerates the drug discovery process.

The use of a generative model coupled with RL-based MPO generates compounds with desired properties, thereby reducing the failures at a later stage of drug development.

Further with other state of art techniques our module develops a potential, synthesizable, safe, novel chemical entity for a particular therapeutic target.