DeepLigBuilder: An AI-Based Approach to *De Novo* Drug Design

Deep learning-based drug design approaches that can build molecular structures from scratch are gaining a lot of attention.

**Can a deep generative model for *de novo* molecular design generate 3D structures on target sites?**

**DeepLigBuilder**

**Combines:**

- Ligand Neural Network to generate valid 3D drug-like molecules
- Monte Carlo tree search to look for strong binding molecules

- Designs novel structures with high predicted binding affinity
- No additional atom placement or bond order inference needed
- Can accept user-defined seed structure

But most approaches find it difficult to generate 3D molecular structures.

DeepLigBuilder is a state-of-the-art tool for design and optimization of new drugs and functional organic molecules.

Structure-based de novo drug design using 3D deep generative models

Li, Pei and Lai (2021) | Chemical Science | DOI: 10.1039/d1sc04444c