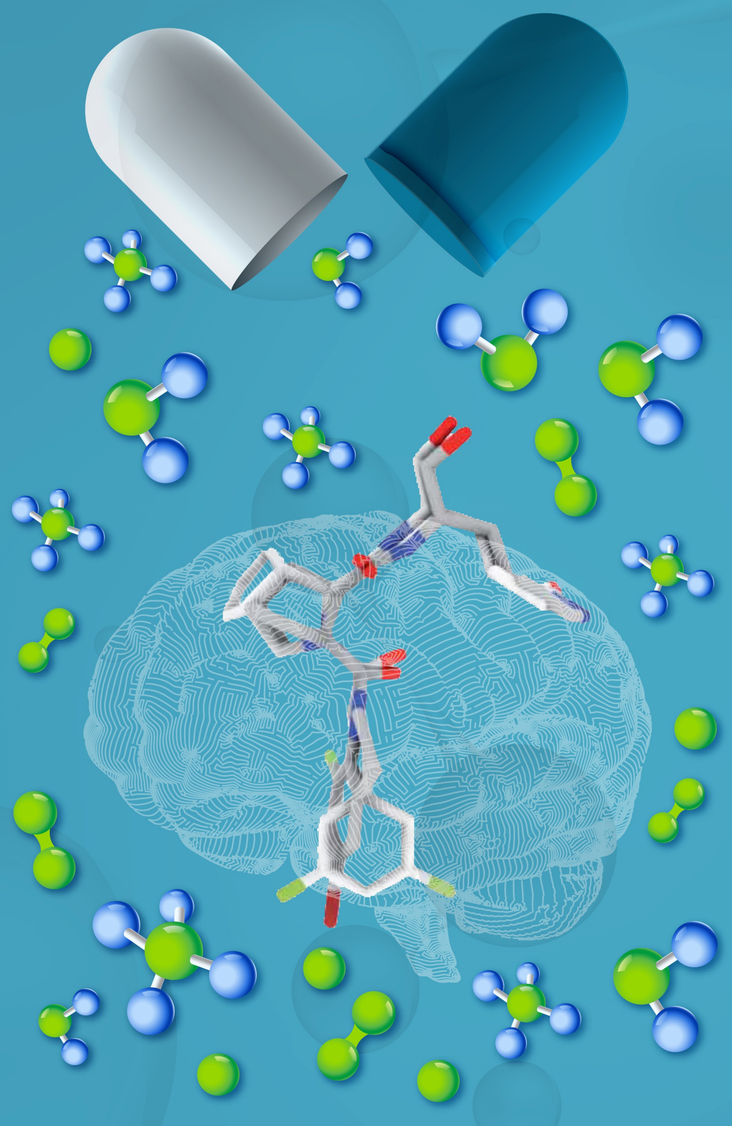
Electronic Supplementary Material (ESI) for Chemical Science.

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

Chemical Science

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



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

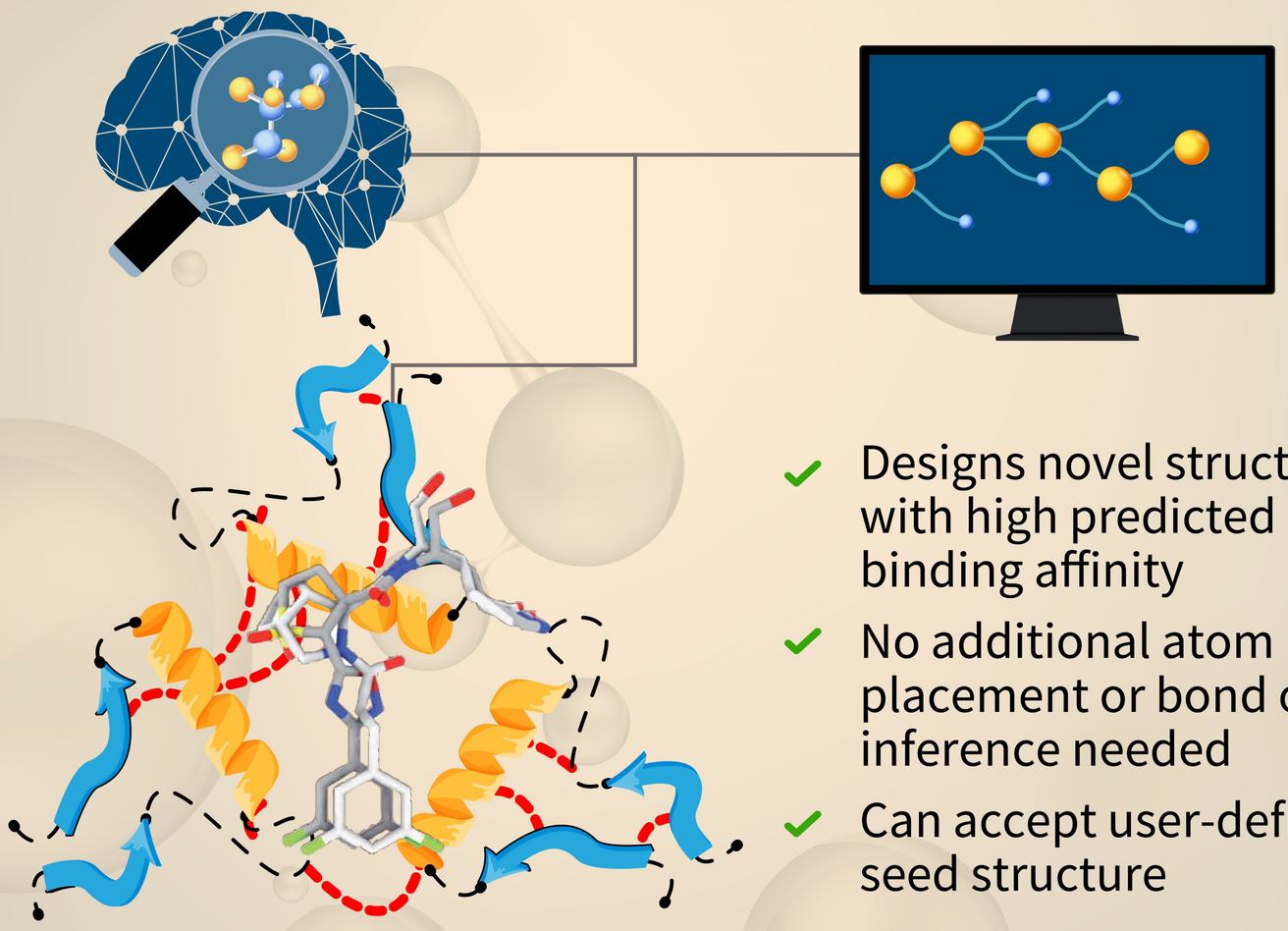
Can a deep generative model for *de novo* molecular design generate 3D structures on target sites?

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

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

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