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A generative AI method for do novo design of ligands with drug-like properties (SAGE)

Stanford researchers have developed SAGE, an AI-powered drug discovery platform that designs novel drug molecules directly within a target protein's binding pocket in 3D space, accelerating the identification of promising drug candidates.

Breakthroughs in structural biology have provided unprecedented insights into biomolecular functions and drug targets. However, translating this knowledge into effective drugs remains slow and inefficient due to outdated and limited discovery tools.
To overcome these challenges, SAGE leverages advanced generative AI and physics-based scoring to design high-quality drug-like molecules with optimized binding, stability, and synthesizability. By building potential drugs directly inside a target protein's binding pocket, SAGE systematically balances key factors such as molecular interactions, ease of synthesis, and overall drug-likeness, streamlining the drug discovery process.

Stage of Development:
Research – in vitro. Next steps involve benchmarking studies, and potentially further methodological improvements.

Applications

- Enabling efficient drug design
- Lead optimization for novel therapeutics

Advantages

- Faster and cheaper than virtual screening
- More desirable properties than those designed by existing methods
- Can be used to design multiple chemical classes of compounds

Innovators

- Alex Powers
- Ron Dror

Licensing Contact

Imelda Oropeza

Senior Licensing Manager, Physcial Sciences

Email