

Discover viable and effective prospects more quickly with AI-powered ligand design

Automated fragment-based lead optimisation utilising predictive small-world network hotspots.



Automated ligand design for high-affinity network cooperativity.

Viper AI is a high-performance ligand design software suite that enables researchers to identify new ligand substituents that substantially improve binding affinities without the need to add large, complex chemical groups. By utilising a completely new approach to designing tight-binding ligands, the software identifies specific chemical transformations for improving protein–ligand interaction networks and local cooperativity. This advanced system allows structural biologists and medicinal chemists to discover more viable prospects more quickly through precise, data-driven insights into molecular recognition.

Innovation through Scorpion technology.

Viper AI is built natively upon DesertSci's proprietary Scorpion technology, which provides a sophisticated computational description of molecular recognition and hotspots. This foundation treats the entire protein–ligand complex as a small-world network to rationalise binding physics, offering entirely new insights into complex molecular recognition phenomena. By incorporating these network topology concepts, Viper AI provides research teams with a unique toolkit for exploring binding metrics and designing novel molecules with enhanced network stability.

Viper AI in action: the three-stage computational pipeline

A typical fragment design workflow within Viper AI is executed seamlessly across three automated stages:

PHARMACOPHORE SEARCH:

Maps the geometry and chemical features of the target pocket.

FRAGMENT SCAN:

Queries chemical libraries to link substituents to the core template.

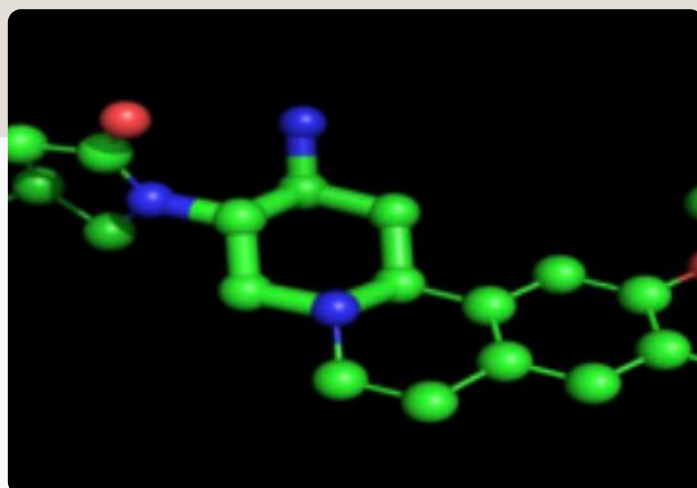
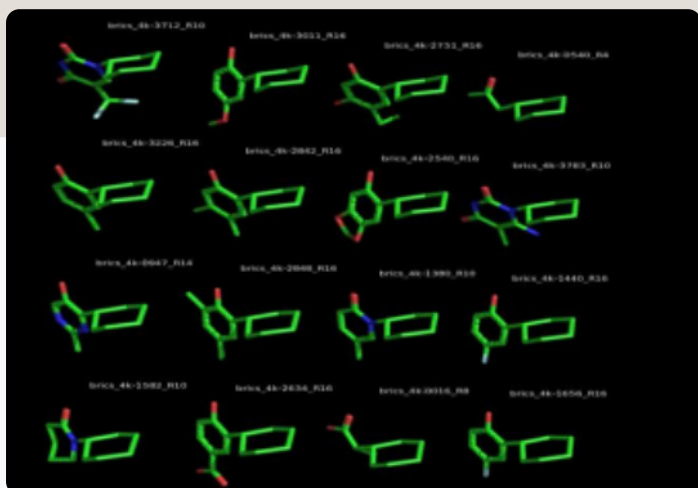
FULL SCORPION SCORING:

Evaluates the resulting design combinations against strict network stability algorithms.

Multiple fragment scan computations can be performed rapidly using the results derived from a single, initial pharmacophore search. The search for explicit ligand substituents can be directed to maximise total calculated binding affinity or fine-tuned in a wide variety of ways, enabling optimisation of pharmacological profiles.

Hotspot searching and automated grid sampling

To suggest optimal pharmacophores for strong protein–ligand network interactions, Viper AI performs grid-like sampling of multiple atom types across a target binding site. It determines precise network interaction scores at each distinct site point based on the underlying Scorpion scoring function, achieving excellent alignment between theoretical predictions and experimental crystal structures. The interactions radiating from each computed pharmacophore site to neighbouring protein atoms can be easily exported and explored natively within your visualisation environment.



Advanced scanning capabilities

To refine lead development with absolute scientific rigor, the software suite incorporates three specialised screening engines:

FRAGMENT SCANNING:

Guided directly by network hotspots, this process optimises ligand binding affinity by linking explicit substituents from libraries, such as the BRICS fragment library, to the template structure. The engine automatically accounts for allowed chemical reaction rules and internal ligand strain, highlighting candidates that deliver enhanced network stability.

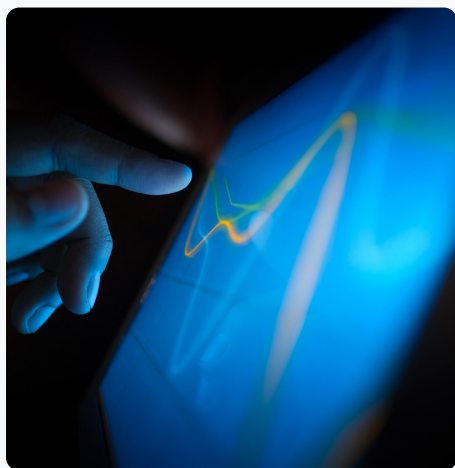
ATOM SCANNING:

This process identifies explicit single-atom substitution patterns that yield high network scores in binding sites, computing all ligand variations and ordering results systematically from lowest to highest affinity.

SMIRKS SCANNING:

Specifically engineered for fine-tuning molecules based on libraries of small chemical fragments for lead optimisation.

Core technical features



AI-POWERED LIGAND GENERATION

Highlights pharmacophores that **maximise local interaction networks** and structural cooperativity.

HOTSPOT-GUIDED LIBRARY SCREENING

Scans **extensive fragment libraries** at any **user-defined ligand position** and ranks results cleanly via Scorpion scoring.

MULTIVALENT GRID SAMPLING

Evaluates target pockets using combinations of Raptor **non-covalent interaction rules**.

SOLVATION INTELLIGENCE

Automatically identifies **highly favourable water binding sites** to guide water-displacement strategies.

BUILT-IN CHEMISTRY KNOWLEDGE

Applies **rigorous synthetic chemistry** constraints and rules during all fragment-linking simulations.

BUNDLED SOFTWARE CORE

Includes **full operational licences** for the Scorpion binding affinity prediction engine and the Raptor interaction visualisation tool.

ENTERPRISE ECOSYSTEM INTEGRATION

Integrates seamlessly with the central Proasis protein structure database for an **automated, high-throughput research workflow**.

Professional integration and platform requirements

Viper AI was developed through an intensive, joint industry collaboration between DesertSci and F. Hoffmann-La Roche, Basel, Switzerland. This partnership ensured the software natively meets the strict data curation and predictive accuracy requirements of industrial drug discovery pipelines. **Accelerate your design-make-test cycles with validated machine learning.**

Client access:

End users can access the system via command-line scripts, api resources, or through the intuitive Proasis web interface.

Server infrastructure:

Viper AI server software runs under Linux environments and requires RHEL 8 or 9 or equivalent.

Visualisation interoperability:

Complex interaction networks, network hotspots, and fragment-linking arrays are exported via automated scripts for direct viewing in industry-standard tools like Proasis, PyMOL and MOE.



Viper AI
by DesertSci

To establish an evaluation licence or arrange a tailored technical demonstration of the Viper AI suite, contact our expert team.

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