

Generate new insights and score protein-ligand complexes on binding affinity

Rationalising molecular recognition and cooperativity through small-world network theory.



Beyond conventional scoring: The science of network cooperativity

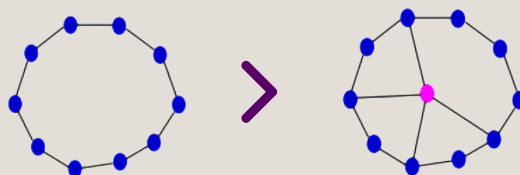
Cooperativity to provide a deeper, more predictive understanding of binding affinity. Traditional modelling approaches often treat interactions as isolated events. Scorpion breaks through this limitation by modelling the entire protein-ligand complex as an integrated small-world network.

Through the implementation of graph-theory properties, Scorpion offers completely new insights into important molecular recognition phenomena, allowing researchers to accurately rationalise tight binding and determine its long-term impact on drug discovery campaigns.



Theory and concepts in action

The core architecture of Scorpion is the integration of covalent and non-covalent interactions into a single, unified network of nodes and edges. **In this highly precise model, individual atoms (spanning amino acids, water molecules, and ligands) function as the network nodes.** All close contacts, including covalent bonds and favourable non-covalent interactions, form the connecting edges.

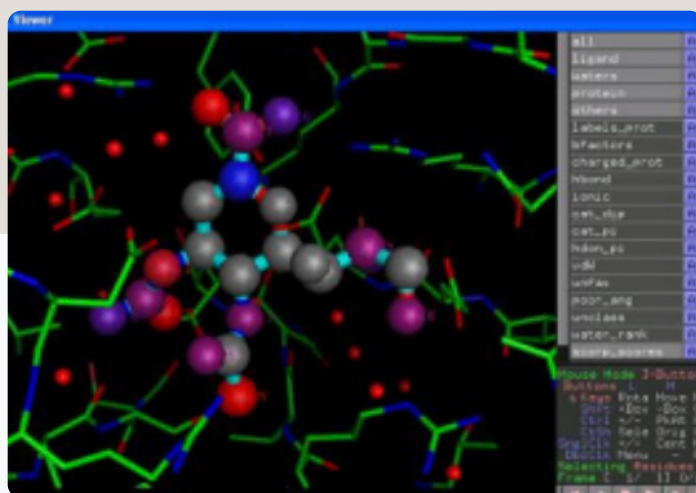
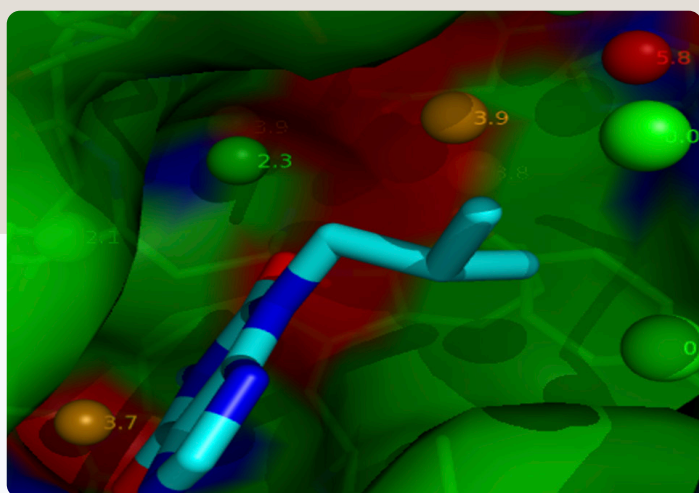


This small-world approach demonstrates how the addition of a ligand creates shorter path lengths between nodes across the binding site, mimicking the physical reality of how a molecule fits into a structural cavity to enhance overall network stability. By treating the complex as an interdependent interaction network, Scorpion encodes local cooperativity effects, considerably improving the quality of predicted binding affinities and identifying the exact parameters that drive local tight binding.



Visualising and scoring binding affinity

Scorpion provides powerful tools for understanding atomic contributions to binding through clear visual cues.



High-scoring atoms are colour-coded red within your visualisation environment, allowing researchers to pinpoint exactly where a ligand is most effectively engaged with the target.

The system operates via a derived scoring function that incorporates network terms alongside precise terms for favourable and unfavourable interactions.

This scoring function rewards strongly networked interactions in the final scores, providing new, unique, novel ligand design concepts for drug discovery.

The software also fully incorporates the Raptor toolset for finding and classifying non-covalent interactions alongside explicit geometric water rank scores.

Structural water molecules are classified based on their deviation from ideal tetrahedral coordination as observed in ice.

Using a clear green-to-red visual shorthand, Scorpion highlights water displacement potential:

Green

Denotes water molecules that are easy to replace.

Amber

Indicates locations where replacement is possible using suitable polar functionalities.

Red

Identifies deeply trapped, highly stable waters that are unlikely to be replaced.

Core technical features



HIGH-THROUGHPUT BATCH EVALUATION

Computes multi-mol SDF files, writing estimated binding affinities, individual interaction matrices, and network descriptors **cleanly into output files**.

COMPREHENSIVE TEXT QUERIES

Allows users to **search extensive text files of output** obtained from running Scorpion across massive in-house and public domain structures.

GRAPH-THEORETIC MOLECULAR DESCRIPTORS

Utilises a network description of molecular recognition based on **small-world network properties**.

ATOMIC CONTRIBUTION TRACKING

Provides distinct tools for **understanding individual atom and substituent contributions** to overall binding affinity.

SUB-NETWORK MOTIF DISCOVERY

Automatically finds binding site hotspots, mapping to specific, highly favourable ligand atoms that can **enhance ligand affinity**.

AUTOMATED SCRIPT GENERATION

Provides automated deployment scripts for rapid viewing and exploration in PyMOL and MOE.

ADVANCED AFFINITY SCORING

Incorporates **network stability** and **local cooperativity** directly into a derived scoring function.

ZERO PRE-PROCESSING PIPELINE

Supports the direct reading of raw PDB files with **no tedious pre-processing required**.

SPREADSHEET-COMPATIBLE DATA

Total scores and atomic contributions are saved natively in structured formats, allowing data to be **viewed in spreadsheets alongside clear chemical depictions**.

ECOSYSTEM INTEGRATION

Integrates fully with the Proasis database and enterprise visualisation system for **a completely streamlined research workflow**.

Collaborative innovation and industrial validation

Scorpion is not a theoretical exercise; it is the product of a joint collaboration between DesertSci and F. Hoffmann-La Roche, Basel, Switzerland.

This industry-led partnership ensured the software was fine-tuned against real-world research requirements, optimising the underlying SMARTS atom types and geometric parameters against strict quality control constraints.

The method and scoring metrics are fully documented and validated in peer-reviewed literature (Journal of Chemical Information and Modeling, 2011, 51(12), pp 3180–3198).

The software runs seamlessly on Linux servers and can be accessed via an intuitive web interface or integrated directly into automated data pipelines via command-line scripts and api resources, ensuring these ground-breaking insights can be shared effortlessly across your entire multi-disciplinary research team.



Stop relying on computational trial and error. To establish an evaluation licence or arrange a tailored technical walkthrough of the Scorpion scoring engine, contact our team.

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