

Uncover hidden connections in drug discovery with fast, vector-based searching

Drug repurposing and lead hopping based on interaction searches.

Chameleon uses fast vector-based searching to identify unexpected similarities between unrelated drug discovery projects.

It surfaces connections across therapeutic areas that would otherwise go unnoticed, and helps teams identify positive changes to make in a project by drawing on what has already worked elsewhere. Rather than comparing molecules by shape alone, Chameleon searches on the non-covalent interactions a ligand actually makes with its protein. Select the contacts that matter, and Chameleon finds the other binding sites in the Proasis database that make the same ones, whatever the protein family.



Chameleon

Key capabilities:

- Fingerprint searching of non-covalent interactions, typically returning results in seconds.
- Searches experimental protein-ligand structure data held in the Proasis database.
- Sorts hits by binding affinities.
- Searches by interaction type, with or without residue-residue distance constraints.
- Kinase-specific queries against the ATP binding site.
- Similarity searching across whole binding sites or defined sub-pockets.
- Runs in the browser as part of Proasis4, with hits overlaid in 3D.

Built for:

- Drug repurposing.
- Scaffold and lead hopping.
- Cross-project and cross-therapeutic-area discovery.



Chameleon in practice: One query, twenty-six hits

A Chameleon search begins with a structure. Take the sugar ligand bound to xylose isomerase (PDB 5xim), select a few of the contacts it makes with the protein, and run the search.

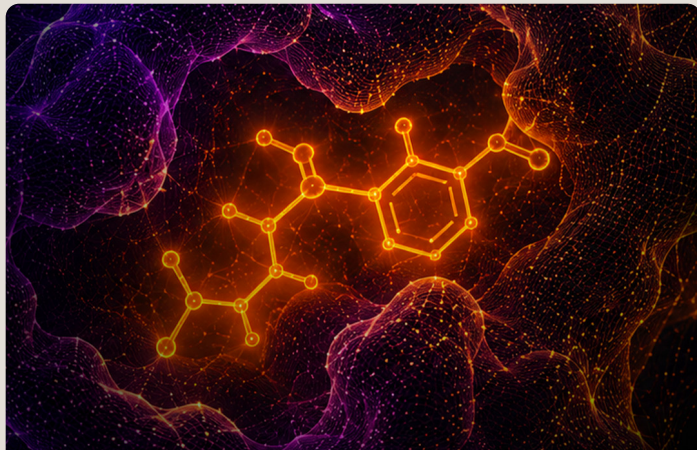
Chameleon returns 26 hits. Alongside the expected isomerases sit beta-galactosidase structures from *E. coli*, an enzyme from an entirely different family, reproducing the same set of interactions.

That is the kind of connection Chameleon exists to find.



Chameleon

What sits behind it



GROUNDING IN EXPERIMENTAL STRUCTURE DATA

Chameleon matches query fingerprints against data derived from protein-ligand crystal structures stored in the Proasis database. Searches typically take less than a few seconds.



INTERACTIONS, FOUND AND CLASSIFIED

DesertSci's ViewContacts software finds and classifies all close contacts between ligands and proteins. These are stored as vectors, which enables very fast searches and immediate results.



RANKED BY BINDING AFFINITY

A unique feature of Chameleon is the ability to sort hits binding affinities, using affinity results stored from DesertSci's Scorpion software. Results come back not just matched, but ranked.



BUILT FOR KINASE WORK

Chameleon also stores information about the kinase ATP binding site in its vectors, enabling kinase-specific queries. All pairwise distances between residues around a ligand are also computed and stored, so residue-residue distance constraints can be built into queries.

Other things you can ask Chameleon

- Find all sites with grouped interaction types, such as all favourable polar contacts to any sidechain.
- Find all sites and sort the hits by Scorpion score.
- Search all kinases for interactions involving specific residues in the ATP site.
- Similarity search on the residues around a ligand, on interaction and residue types, or on a defined sub-pocket.
- Generate a histogram of binned distances for a given interaction type.



Chameleon
by DesertSci

Contact us to arrange an obligation-free Chameleon demonstration, by video conference or site visit.

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