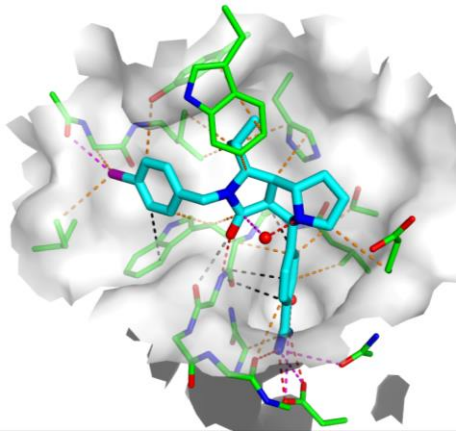
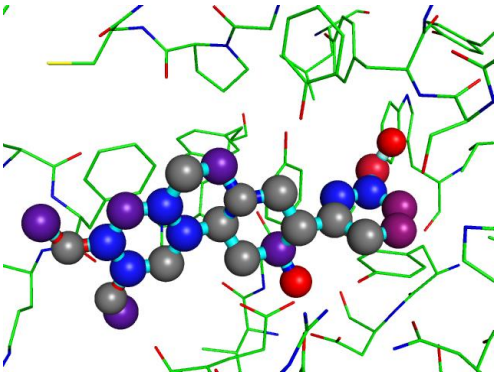
ViewContacts, Scorpion, Viper: 2020 Release Announcement

DesertSci's 2020 ViewContacts, Scorpion, Viper release includes wide ranging new extensions:

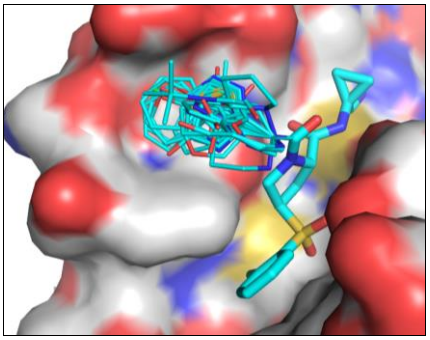
- new Viper interface for Proasis4
- new Viper fragment libraries
- new Viper SMIRKS scanning
- new automated Viper runs
- more API tools
- more control options
- more viewing options



ViewContacts *automatically classifies non-covalent interactions, finding commonly occurring and less-commonly occurring atom close-contacts. The system detects desolvation penalties and other sub-optimal close-contacts; and rank scores bound water molecules. A wide range of visualisation options are available*



Scorpion *is software for ligand affinity prediction based on ViewContacts interaction types, water rank scores, and novel network descriptors. It provides easy visualisation of ligand atoms, colour-coded according to predicted binding affinity*



Viper *is powerful ligand design software based on fast fragment scanning and fine-grained ranking of hits based on Scorpion Scores. The software suite includes: hotspot detection; atom scanning; SMIRKS scanning; and fragment scanning with a wide range of fragment libraries*

DesertScientific Software

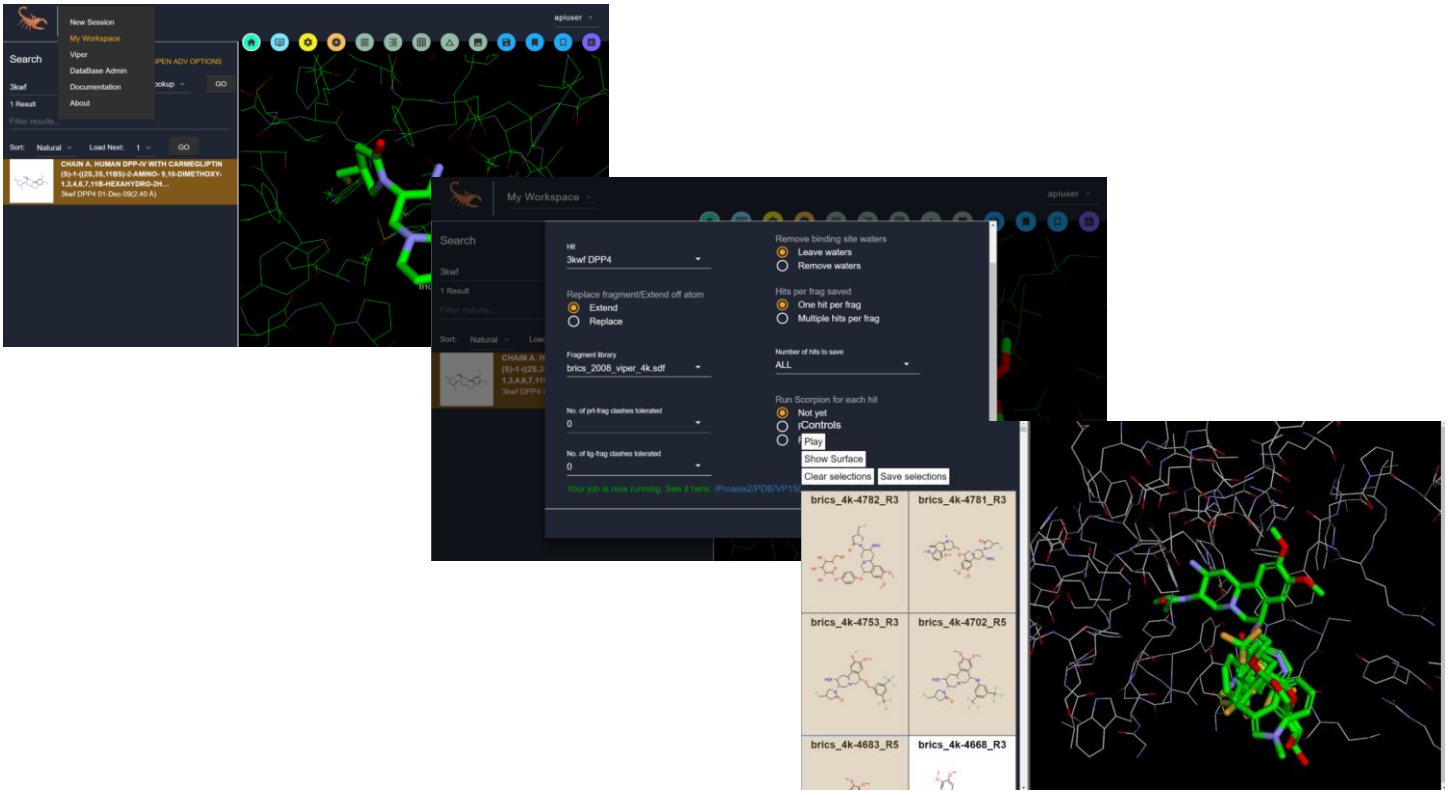
Extensions for ligand design: new Proasis4 GUI

The new Viper GUI in Proasis4 enables both expert and less-experienced modellers to run ligand design experiments directly from a desktop browser.

Ligand design based on fragment scanning, atom scanning, and SMIRKS scanning can be launched from the GUI, enabling ligand extensions and atom or substituent replacements.

Viper can be run from Proasis4 for complexes from the Proasis Database and also from pdb files uploaded from a local folder.

An extended set of scan options are available, such as allowing for the removal of binding site water molecules and using extended, customised fragment libraries.



The Viper GUI is designed to allow for fast, exploratory ligand design experiments to be run, followed up by more exhaustive scans with bigger libraries and comprehensive scoring of hits.

The system includes a new interface for exploring hits with a graphics application that runs within a browser. It provides links enabling hits to be exported into other molecular graphics applications, downloaded and saved, and then shared with colleagues.

DesertSci's Proasis system also allows for fully automated atom and fragment scanning, where a complete all-atom scanning is performed for all deposited inhouse protein-ligand complexes.

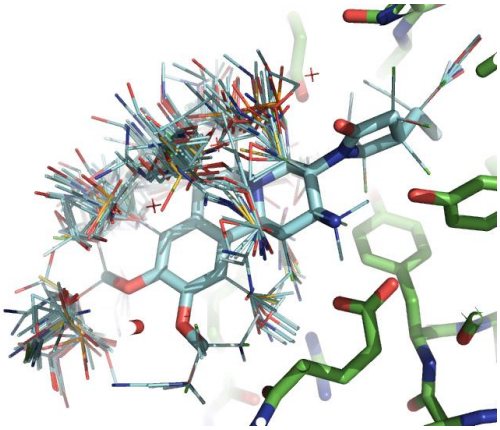
Extensions for ligand design: new SMIRKS scanning

Viper's new SMIRKS scanning greatly extends the power of DesertSci's fragment based ligand design toolset by enabling a wider range of chemical transformations and facilitating low-molecular weight fragment extensions. It allows for designers to encode their favourite set of fragments, such as those from matched molecular pair analyses.

SMIRKS scanning allows for a wide range of on-the-fly chemical transformations:

[#6:1][H:2]>>[#6:1][C:2]([F])([F])[F]	[#6:1][H:2]>>[#6:1][O:2][CH3]
[O:1][H:2]>>[#O:1]CC	[N:1][H:2]>>[N:1]CC
[c:1]1[a][a][a][a][a]1>>[n:1]1[a][a][a][a][a]1	[n:1]1[a][a][a][a][a]1>>[c:1]1[a][a][a][a][a]1

DesertSci provides a number of SMIRKS libraries of different sizes, obtained from a statistical analysis of all small substituents extracted from retro-synthetic analyses.



SMIRKS scanning *automatically scans every atom in a ligand, in the environment of the protein binding site, identifying the optimal low-molecular weight substitutions and chemical transformations that can lead to tighter ligand binding*

API Extensions

Many new features for the API-based command line tools have been created including:

- new resources for Viper fragment scanning, atom scanning, SMIRKS scanning
- new resources for reporting Viper results
- additional input and output options for ViewContacts and Scorpion resources
- extended test suites

The updated client tools, for Linux and WinPC, allow users to more easily run calculations from their workstations/desktops/laptops or when working remotely.

Extensions for viewing ViewContacts and Scorpion Results

The 2020 software release includes:

- extended pdb handling for the extraction of a single chain from a multimeric protein system
- identification and display of protein-ligand covalent bonds
- improved handling of pi-pi interactions for ligand-cofactor close-contacts in a binding site
- better handling of binding sites containing multiple, discrete small molecules
- created support for PyMol versions 2.X built with Python3
- updated and extended SMARTS atom types

Other 2020 improvements

The 2020 release includes:

- improved methods for fast scoring of Viper hits
- better handling of protons in Viper input files
- water molecules can be removed from the binding sites to enable more hits from Viper fragment scanning, atom scanning, SMIRKS scanning
- wider range of allowed chemical bonding for Viper fragment and SMIRKS scanning
- improved torsion checking for Viper secondary and tertiary amide bonding
- additional links with 3rd party modelling applications

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