2018 Version Release Announcement:
ViewContacts, Scorpion, Viper

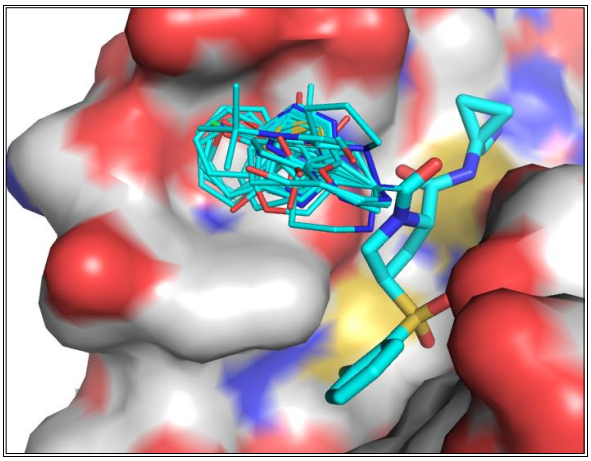
The 2018 release versions of ViewContacts, Scorpion and Viper incorporate a wide range of new extensions including:

- new constraints options
- new molecular recognition motifs
- api extensions
- additional report options
- an array of miscellaneous improvements

Background:

- Viper software detects hotspots as well as providing atom and fragment scanning
- Scorpion software predicts ligand binding affinity
- ViewContacts classifies and visualises protein-ligand interactions.
- WaterRank analyses bound water molecules in protein binding sites.

***Viper** is powerful ligand design software based on fast fragment scanning and fine-grained ranking of hits*



Extensions for ligand design: new constraints options

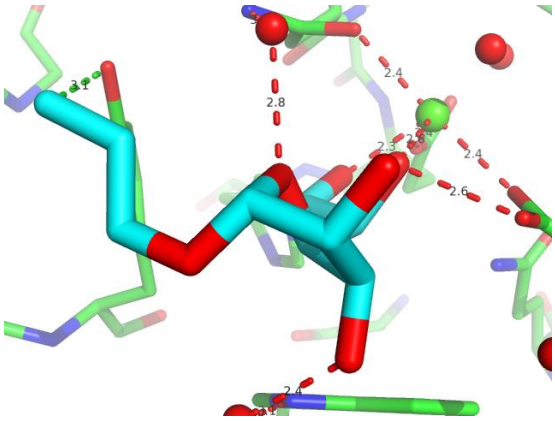
New functionality is available allowing ViewContacts calculations to be easily done with:

1. relaxed constraints - that is, with less stringent cutoff parameters, and
2. tighter constraints - with more stringent cutoff parameters.

With relaxed constraints you see more contacts, including more distal binding site atoms that you are close to hitting with your ligand designs. With tight constraints you see fewer contacts, that is, only those that are close to optimal in their distances and angles.

Example results shown for the binding of Galactofuranose to Intelectin-1 (pdb ID: 4wmy)

Fig A. *ViewContacts results for 4wmy with regular parameters, showing both H-bonding and H-bonding into pi interactions*



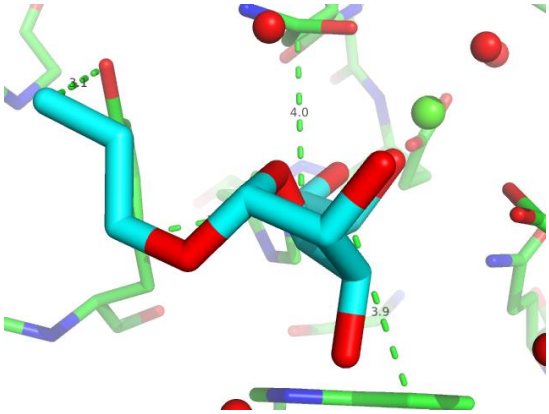
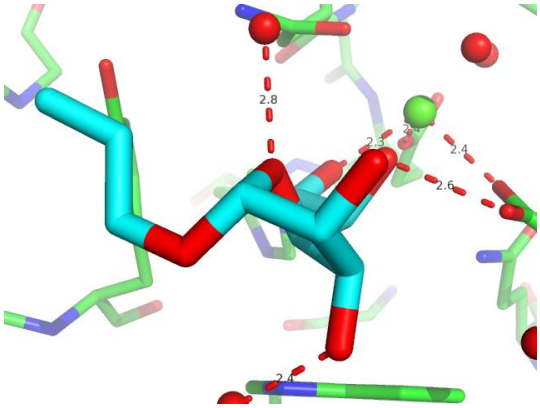


Fig B. *ViewContacts results for 4wmy with relaxed constraints, showing additional H-bonding into pi interactions. The contact to the TRP is particularly interesting*

Fig C. *ViewContacts results for 4wmy with tight constraints, showing fewer H-bonding and H-bonding into pi interactions*



A new command line option is provided allowing for fine-tuning the relaxation of the maximum distance cutoff for all close-contact interactions.

The additional constraint options provide powerful new tools for chemists and modellers analysing ligand designs docked into binding sites, and for crystallographers when analysing lower resolution structures.

Extensions for ligand design: new interaction motifs

The detailed analysis of close contacts in signaling proteins, particularly involving carbohydrate binding, has led to the identification of new molecular recognition motifs.

New favourable interactions are now identified for a range of newly defined carbon atom types that are in close proximity to pi systems. An example is shown in Fig. B above.

The new interaction motifs provide additional improvements in the recognition of surrounding interactions, and improvements in the analysis of interaction networks. Scorpion results are correspondingly more insightful.

The new interaction motifs provide many new opportunities for drug design.

Extensions for structure analysis and viewing: API extensions

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

- short-cuts for ligand identification
- json output can include more detailed, fine-tuned interactions
- additional output options

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

Extensions for reporting

The 2018 software release includes:

- additional data export options, such as new json objects for different grouping schemes for different interaction types
- tab separation for table output
- new reporting of close-contacts that are just beyond the cutoff distance constraints, allowing for easier recognition of sub-optimal molecular recognition
- for Table output, enabled -n options to come into effect

Ease of use: connectivity to third party applications

The 2018 release includes:

- updated and more efficient connectivity to third party modelling applications
- additional option for ViewContacts for creating output files containing fine-grained interaction details for reading into third party modelling applications
- additional option allowing for original atoms names to be used in output files

Miscellaneous improvements

The 2018 release includes:

- Viper fragment searching now saving hits with unique names when saving multiple hits for each fragment
- ViewContacts analysis of all protein-protein interactions between all pairs of chains in any multi-domain pdb file is now routine
- ViewContacts analysis of all non-covalent interactions within any protein structure, whether a complex or not
- Improved methods for the automatic assignment of correct ligand atom bond orders
- ViewContacts and Scorpion documentation extended to better clarify different results that can be obtained using different input options
- ViewContacts and Scorpion documentation extended to better explain close contacts that are neither favourable nor unfavourable

Evaluation Licenses Available

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