ProFusion™ *… combine, collaborate, share*

Fully Automated Project Data Files

ProFusion facilitates collaborative structure based drug discovery research by delivering fully automated, expert project files to your scientists' desktops.

ProFusion session files provide a comprehensive overview of the structure based drug design research within a project, containing all key target data, all key ligand data and state-of-art protein-ligand interaction analysis. With this information in the one file, your project scientists have a better chance of discovering promising new compounds to synthesise.

Specifically, ProFusion combines a project's protein structure data (from crystallography and modeling) with results from robust computational methods, into a single, easy-to-use PyMol session file suitable for all users, both expert and non-expert. This means all chemists, crystallographers and modellers involved in a project can access up to date, fully functional and comprehensive project based session files at the click of a button.

What's really new about ProFusion is that you get fine-grained control over the display across multiple projects via fully automated processes … every project, every time.

Inclusions

ProFusion includes interactions and geometric water rank data generated by DesertSci's ViewContacts software and scoring results from our ground-breaking Scorpion software, based on networks and cooperativity in protein-ligand complexes.

ProFusion is fully integrated with DesertSci's Protein Structure Database and Visualisation System, Proasis3, providing you with a powerful and collaborative research tool.

ProFusion Features

- enables inhouse project data, off-target data, public domain data, modelling data and collaborators data to be easily combined
- wide range of alignment strategies available
- reference views for entire protein families can be defined
- includes ViewContacts interactions and Water Rank Scores
- includes Scorpion Scores to show binding hotspots in ligands
- allows grouping by Name, by ligand ID, by SMARTS, and by Project
- easy to inject customised pml
- easy to control the size of the viewed binding site region
- easy to control the alignment of specific monomers from multimeric protein structures
- saves aligned proteins for easy loading into dedicated modeling applications.
- saves aligned 3D ligands with correct Connection Tables, which can be organised into subdirectories according to scaffold
- colouring by relative B-factor histograms
- easy to manage command files
- automatic updating

ProFusion
SESSION FILES

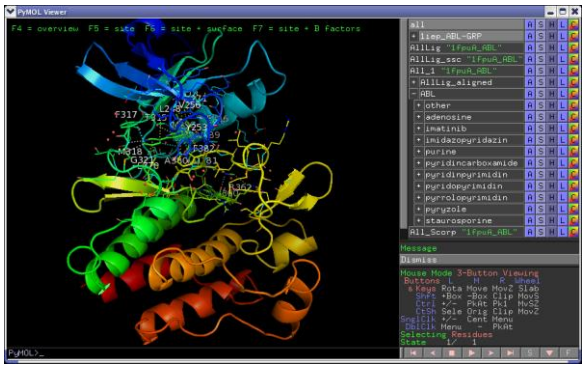
ProFusion … *In Action*

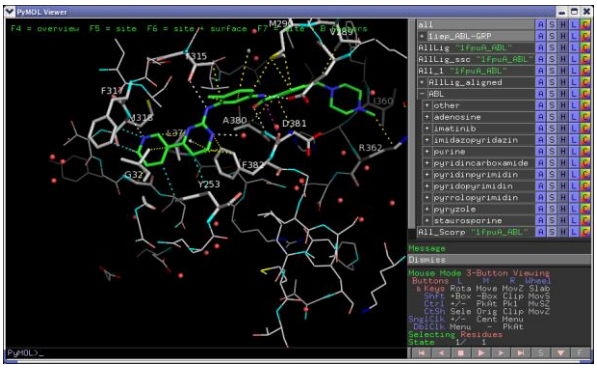
ProFusion collects all relevant protein structure data for a project and uses powerful alignment methods to overlay each onto a reference. Complexes can be organised according to structure name, ligand ID, SMARTS patterns, sub-project.

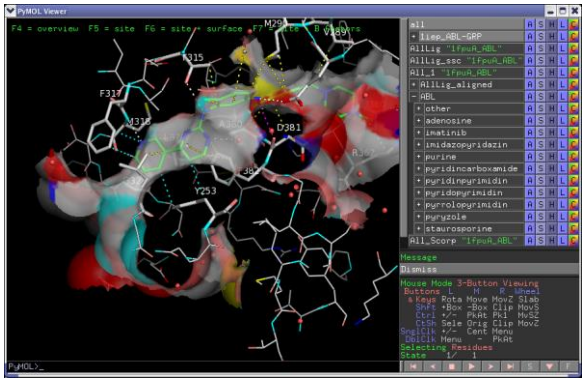
ProFusion session files have built-in scenes, views, objects, and groupings to facilitate easy navigation, particularly important when exploring many tens of structures.

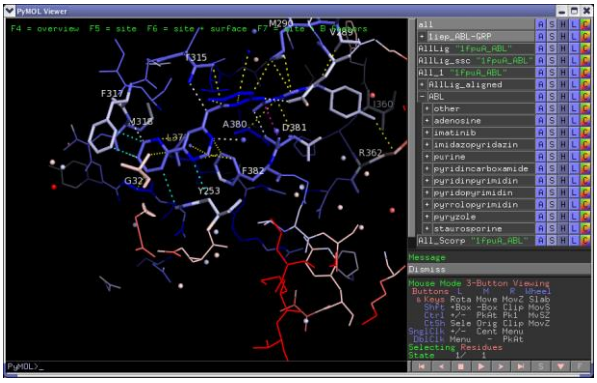
ProFusion session files provide all key target data and all key ligand data from a project. With the information in the one file, your project scientists have at their fingertips the relevant information needed to find promising new compounds to synthesise. For instance, the files enable the viewing of all overlayed ligands, showing the full extent of how a binding site has been scooped, and indicating pockets not yet explored. With all complexes aligned, any pair of structures can be immediately compared and contrasted, ***enabling design concepts in one chemical series to be easily analysed in other series***. Furthermore, the files provide key data for better understanding protein-ligand interactions, ligand binding and water binding, computed using DesertSci's ViewContacts and Scorpion software.

The images below show the four stored scenes for session files in an Abl Kinase project. The menu on the right illustrates how complexes can be separated according to ligand substructures, in this case, the hinge binding group.









DesertSci

ProFusion is loaded with data from Proasis3, which is always up-to-date with inhouse and public protein structure data. ProFusion can be integrated with Proasis3 so that the deposition of a new structure into the Proasis3 database triggers the creation of a new session file for the structure's project. Protein structure complexes not in Proasis3, for example, those generated by modellers, can be simply stored on the file system and then loaded into a session file using the powerful xml input syntax provided.

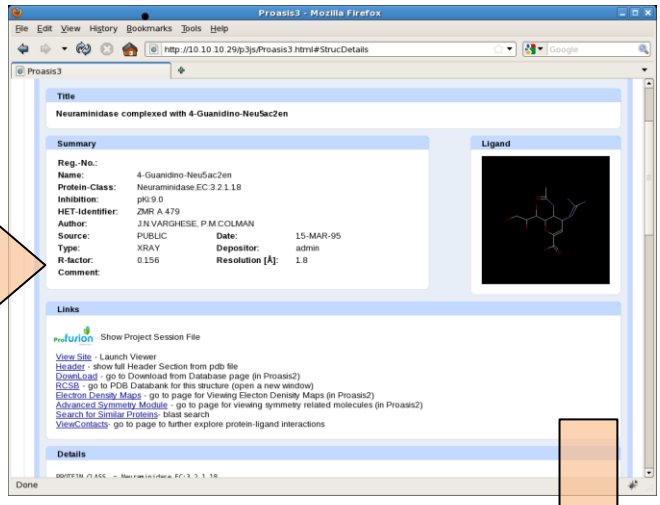
Access

Scientists simply click on a link in Proasis3 to view a project session file associated with a particular project.

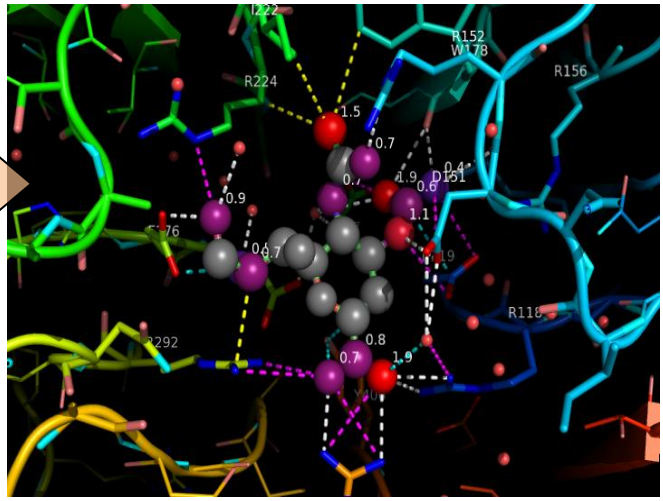
ProFusion software also ***creates directories loaded with aligned pdb files***, enabling other modeling pacjkages, such as MOE and BW3DE, to be used.

With such a vast resource of structural data and computed properties, ProFusion session files provide modellers and other drug design experts the opportunity to load their own predicted results, and to compare and contrast against all previous experimental results. Thus, ProFusion session files offer a new and efficient process for evaluating not only their design ideas, but also the results from new computational methods.

ProFusion Link in Proasis3



Session File viewed in PyMol



Automated Updating

A common task for many modellers working in industry is maintaining project files for all project members. This usually includes adding new structures from inhouse crystallography, adding new structures from the RCSB, and loading results from computational chemistry tools when new versions of software become available. These tasks take significant time. ProFusion completely alleviates this burden. The automated building of project session files gives modellers more time to focus their expertise on the discovery of new drug candidates.

Acknowledgements

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- from Python community - Python
- from the late Warren DeLano and Schrodinger - PyMol
- from OpenBabel community - openbabel

Desert Scientific Software gratefully acknowledges all of the authors and contributors to the above mentioned packages. All intellectual property rights associated with these packages remain at all times with the respective intellectual property right holders. All copyright notices associated with these packages must remain at all times with the packages.

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