Profusion
Session File Software

Profusion: Fully Automated Project Data Files

FEATURES

- Allows in-house project data, off-target data, public domain data, modeling data and collaborators data to be easily combined
- Wide range of alignment strategies available
- Reference views for entire protein families can be defined
- Includes proprietary ViewContacts interactions and geometric water rank data
- Includes Scorpion Scores to show binding hotspots in ligands
- Allows grouping by Name, ligand ID, SMARTS and by Project
- Easy to inject customized pml
- Easy to control the size of viewed binding site region
- Easy to control the alignment of specific monomers from multimeric protein structures
- Saves aligned proteins for easy loading into dedicated modelling applications
- Saves aligned 3D ligands with Connection Tables which can then be organized into subdirectories according to scaffold
- Colouring by relative B-factor histograms
- Easy to manage command files
- Automatic updating

Profusion: providng a fully automated, overview of all key project data, ligand data and state of the art protein-ligand interaction data in one comprehensive file…NOT just a spreadsheet

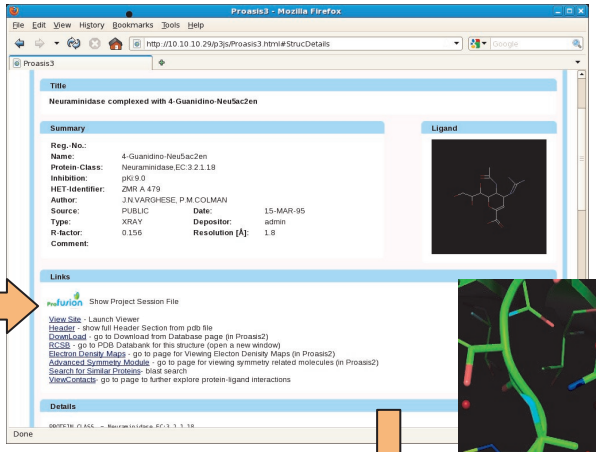
Every Project, Every Time

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

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

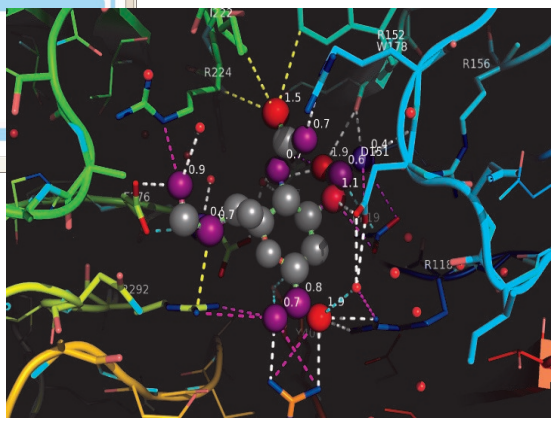
Scientists simply click on a link in Proasis3 to view a project session file associated with a particular project or, for non-proasis users, the session files can be built with minimal effort via with a command line tool provided by DesertSci.

ProFusion link in Proasis3



ProFusion allows researchers to load their own predicted results and compare and contrast against all previous experimental results

Session File viewed in graphics package



ProFusion offers a new and efficient process for evaluating scientists' design ideas and the results from new computational methods

For more information on any of our products or services please visit us on the Web at: www.desertsci.com

DesertScientific Software
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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 in-house 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.

ACKNOWLEDGMENTS

Desert Scientific Software gratefully acknowledges the contributions of scientists from Genentech, CA, USA, particularly Huifen Chen and Jeff Blaney.

The development and execution of ProFusion makes use of these packages:

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

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.

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.

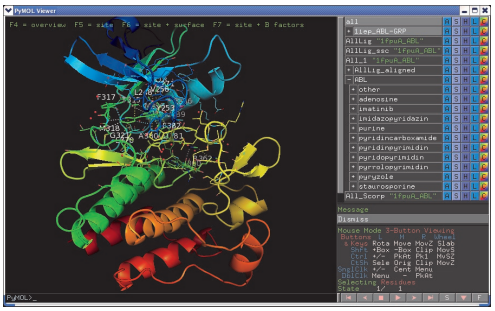
⇒ ProFusion session files have built-in scenes, views, objects, and groupings to facilitate easy navigation, particularly important when exploring many tens of structures.

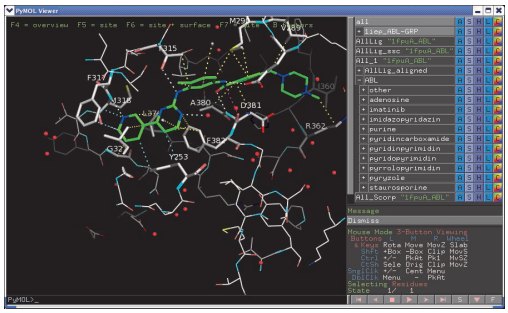
With the information in the one file, project scientists have all the relevant information needed to find promising new compounds to synthesise.

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.

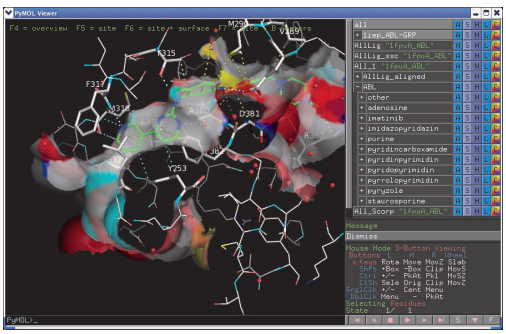
With all complexes aligned, any pair of structures can be immediately compared and contrasted, ***enabling design concepts in one chemical series to be easily analysed in other series***.

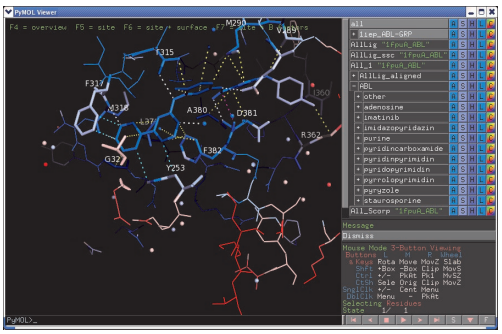
ProFusion is loaded with data from Proasis3, which is always up-to-date with in-house and public protein structure data. ProFusion can be integrated with Proasis3 so that the deposition of a new structure into the Proasis3 database triggers the creation of a new session file for the structure's project. 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.





These images 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.





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