

Bring together people, data, and ideas to collaborate on discoveries

Fully automated project data files
delivering unified 3D structure
intelligence directly to your desktop.



Coalescent

Consolidating data for collaborative breakthrough.

Coalescent facilitates collaborative, structure-based drug discovery by delivering fully automated, expert level project files directly to your team's desktops.

These unified session files provide a comprehensive overview of a project's research, containing all key target and ligand data alongside state-of-the-art protein-ligand interaction analysis. By consolidating this critical information into a single functional file, Coalescent empowers project scientists to move past fragmented workflows to efficiently discover and synthesise promising new compounds.

Specifically, the software combines a project's protein structure data derived from crystallography and modeling with results from robust computational methods, **rendering them into a single, easy-to-use PyMOL session file suitable for both expert modellers and non-expert chemists.**

Seamless integration and automated insights.

The true power of Coalescent lies in its ability to provide fine - grained control over the display across multiple projects via fully automated processes. Every chemist, crystallographer, and modeller involved in a project can access fully functional, up-to-date session files at the click of a button.

These files are automatically enriched with critical scientific data, including interactions and geometric water rank data from Raptor, alongside advanced scoring results from our ground-breaking Scorpion software.

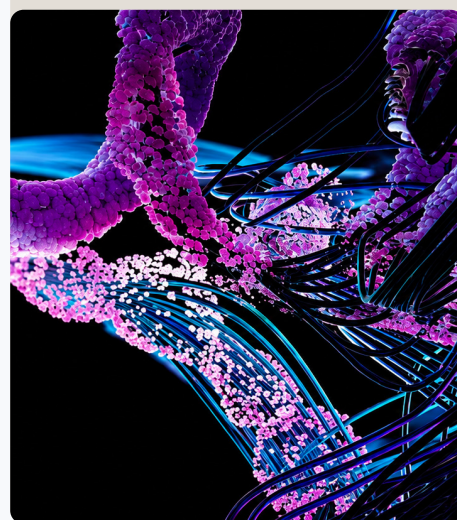
Treating the system as the central operational hub, **Coalescent rationalises tight binding by highlighting interaction networks and hotspots within protein-ligand complexes.**

Fully integrated with our Proasis database:

Coalescent acts as a powerful collaborative tool that bridges the gap between raw experimental data and actionable research.



Proasis



Coalescent in action

Coalescent automatically collects relevant protein structure data and utilises powerful alignment strategies to overlay each structure onto a reference format.

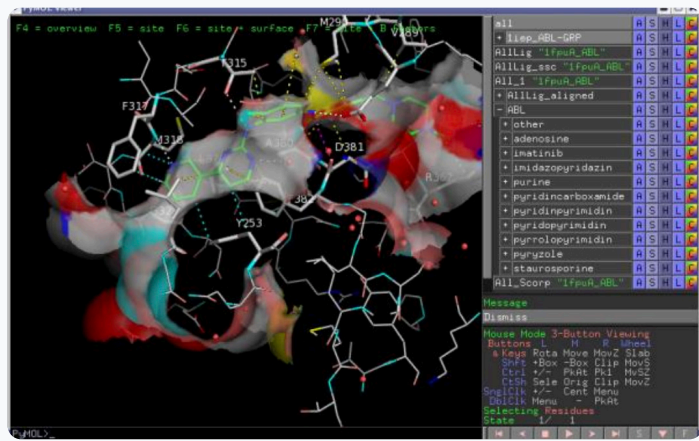
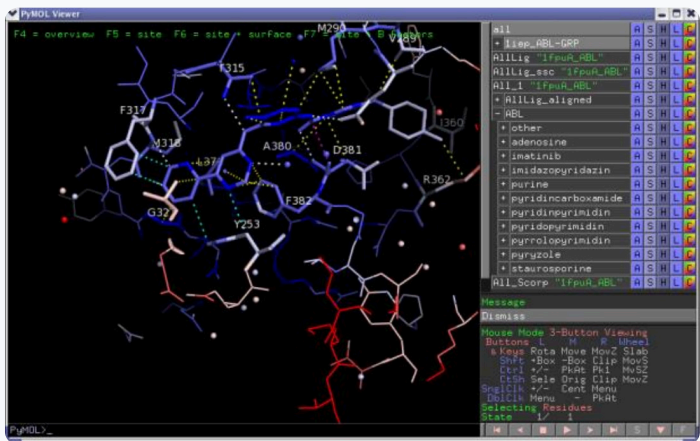
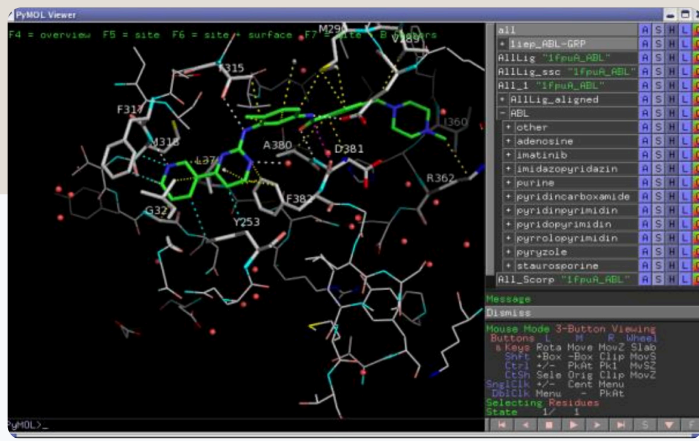
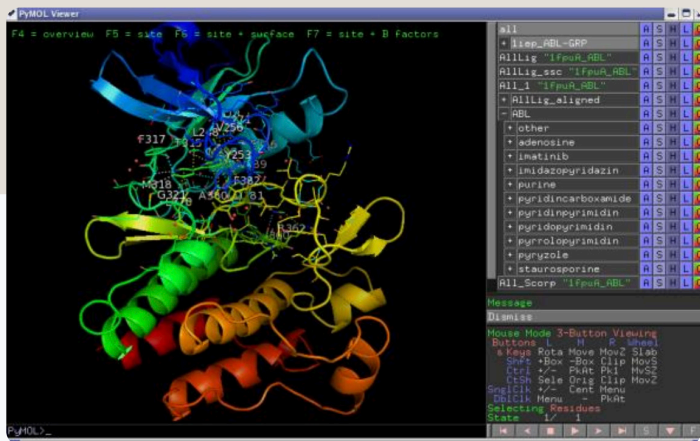
This allows for the immediate comparison and contrast between any pair of structures, enabling design concepts in one chemical series to be easily analysed across entirely separate series. The software features built-in scenes, views, and objects that make navigating tens of complex structures highly intuitive.

By providing a clear visual map of how a binding site has been scoped, **Coalescent highlights unexplored pockets, giving scientists a distinct tactical advantage when developing ligand designs.**

Beyond internal visualisation, the software automatically creates directories of aligned PDB files compatible with other industry-standard modeling packages such as MOE and Benchware 3D (BW3DE).

This functionality provides an efficient process for evaluating new design ideas against a vast resource of previous experimental results.

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.



Core technical capabilities



MULTI-SOURCE DATA AMALGAMATION

Combines in-house project data, off-target data, public domain records, and collaborator datasets into a single searchable environment.



ADVANCED ALIGNMENT ENGINES

Provides a wide range of alignment strategies and reference views across entire protein families.



INTEGRATED INTELLIGENCE

Built-in Raptor interaction tracking, Water Rank Scores, and Scorpion network stability results.



FLEXIBLE STRUCTURAL SORTING

Organises complexes cleanly by name, ligand ID, SMARTS patterns, or specific sub-projects.



FINE-GRAINED DISPLAY CONTROLS

Offers precise control over the size of the viewed binding site region and the alignment of specific monomers from multimeric protein structures.



CUSTOMISABLE SCRIPT INJECTION

Supports the seamless injection of customised command files and PML scripts for advanced computational users.



SCAFFOLD DIRECTORY ORGANISATION

Saves aligned proteins and 3D ligands with correct connection tables, neatly organised into subdirectories according to scaffold lines alongside relative b-factor histograms.



EXTERNAL COORDINATE LOADING

Permits structure complexes not yet deposited in Proasis (such as those generated by external modellers) to be loaded directly via a robust XML input syntax.



TRIGGERED AUTOMATED UPDATING

Features automatic background processes that re-calculate and update session files the moment a new structure is deposited into the Proasis database.

Alleviating the computational burden

In many industrial settings, expert molecular modellers spend significant time manually maintaining project files, adding new structures from in-house crystallography, or re-loading results when software versions change.

Coalescent completely alleviates this administrative burden through automated updating. When a new structure is deposited into the Proasis enterprise system, **Coalescent automatically triggers the creation of an updated project session file.**

This automation ensures the entire project team is permanently working with the latest intelligence, removing version drift and allowing your modellers to shift their focus back toward the discovery of clinical drug candidates.



Coalescent
by DesertSci

Redefine your research collaboration.
For more information or to request
a technical walkthrough, please
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