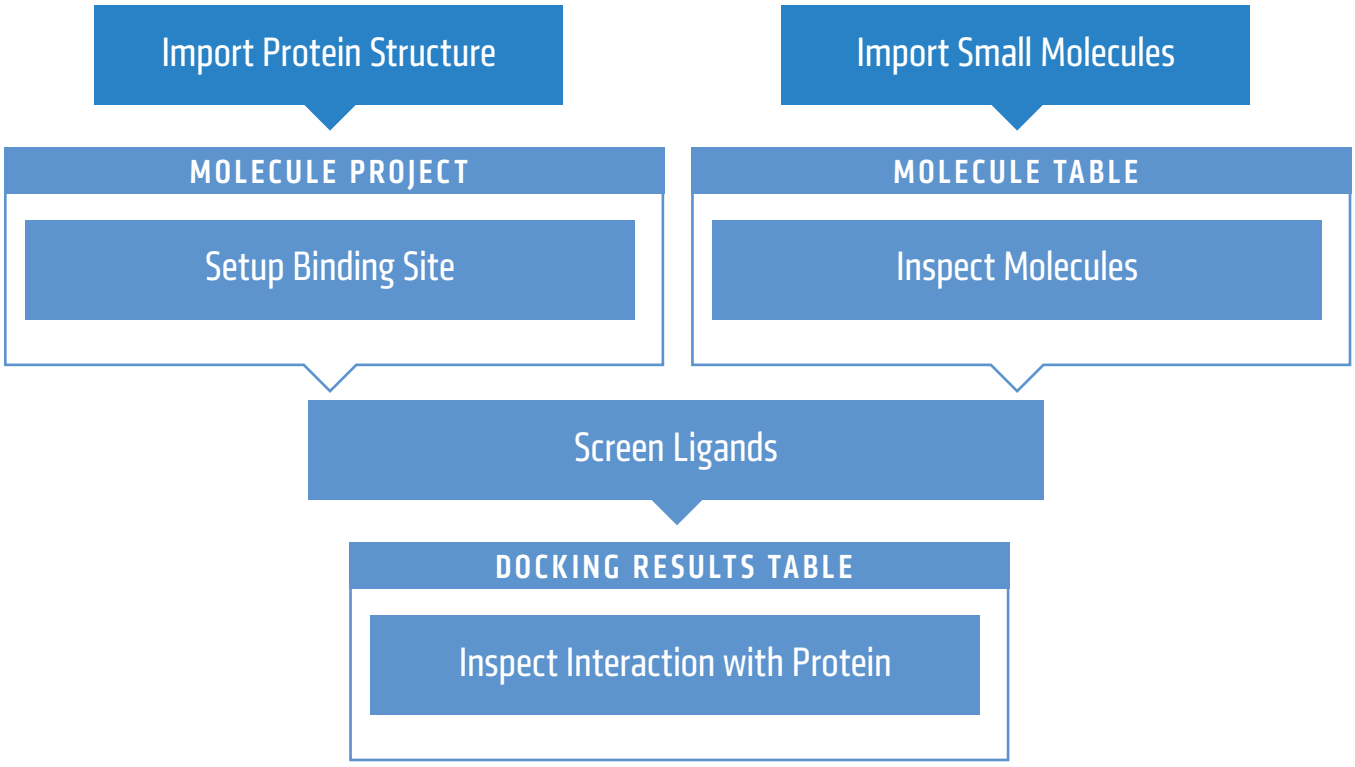
Quick Guide

CLC **Drug Discovery** Workbench

VIRTUAL SCREENING



A structure-based virtual screening is accomplished by docking all candidate ligands from a molecule library to a protein target binding site. Molecule libraries are stored in Molecule Tables for easy handling of large libraries. A scoring function is used to estimate which ligands bind to the protein with high affinity.

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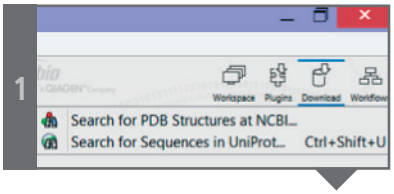
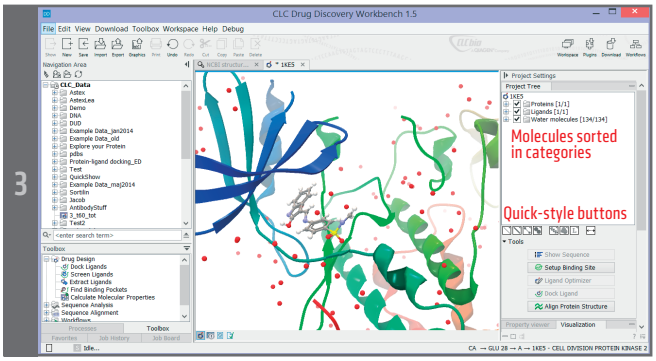
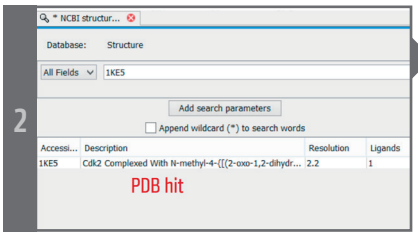
Import Protein Structure



Protein structures can be downloaded directly to the workbench from the Protein Data Bank.

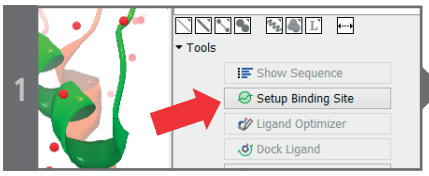


Specify keywords or a PDB ID in the search field, and a selection of hits appears below. Double-click a hit to open a Molecule Project with the content of the PDB file.

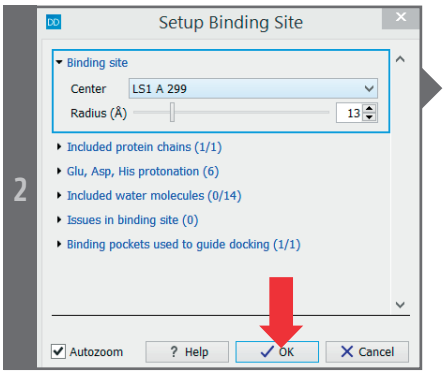


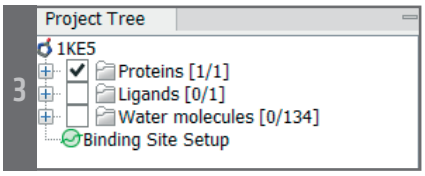
The molecules are automatically sorted in categories in the Project Tree. From the Project Tree, molecules can be hidden or displayed, and their visual representation can be customized via quick-style buttons.

Setup Binding Site

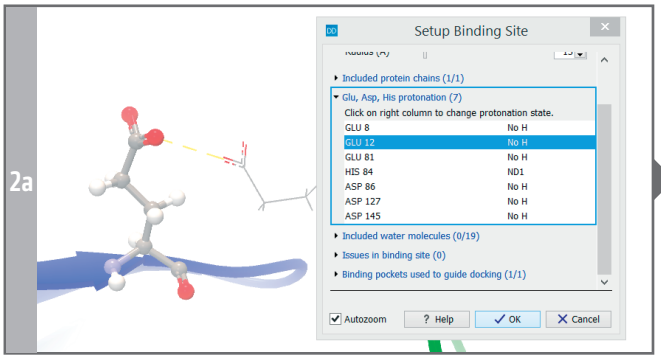


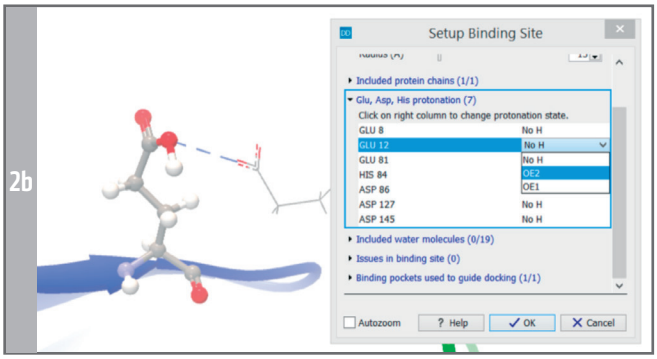
The imported protein structure can be set up for ligand binding studies in just two clicks.





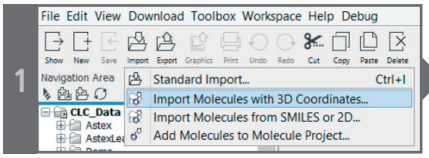
The Molecule Project now contains a Binding Site Setup.



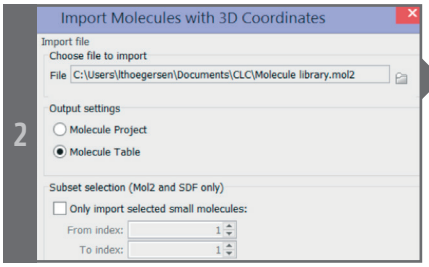


The Setup Binding Site dialog box is interactive, and the relevant molecules, residues, and interactions will automatically be displayed in the 3D view for easy inspection. The view is continuously updated when changes are made.

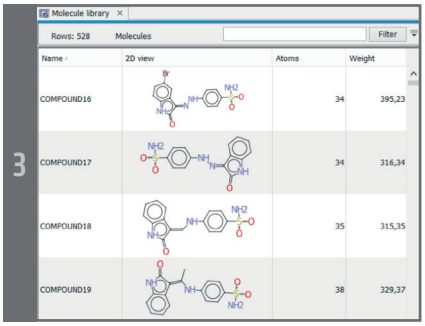
Import Small Molecules



Molecule libraries in SDF, Mol2, and SMILES formats can be imported. For SMILES and molecules with only 2D information, 3D structures are generated on import.

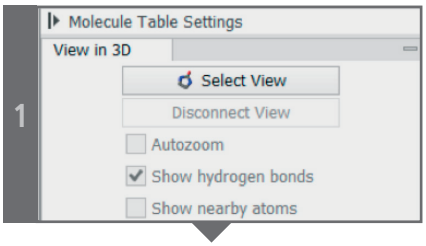


Molecules are imported to a Molecule Table.

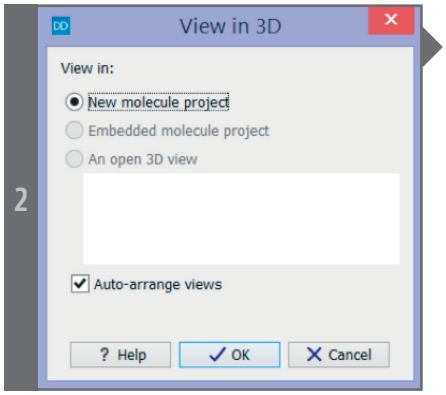


Molecule Table showing 2D molecule depictions.

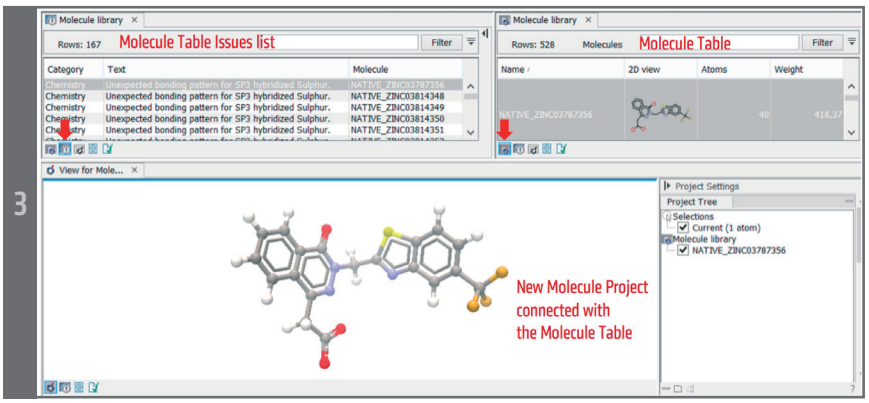
Inspect Molecules



Molecules in tables can also be viewed in 3D...

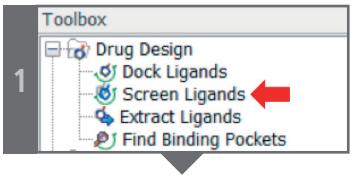


...either in a new, empty Molecule Project view or in an already opened Molecule Project.

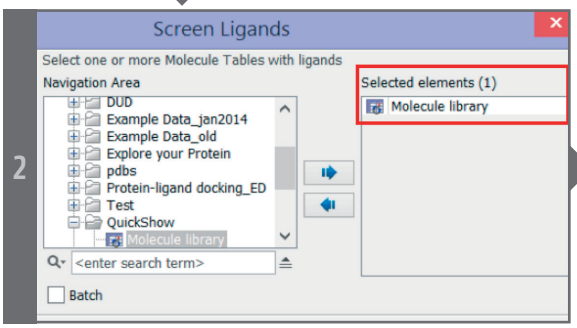


Molecules selected in the Molecule Table are visualized in the connected Molecule Project view. Issues related to the molecule representation are raised on import, and updated when changes are made to molecules. Selecting an issue from the Issues list will select the implicated molecule in the Molecule Table, and show the molecule in the 3D view, with the relevant atoms selected.

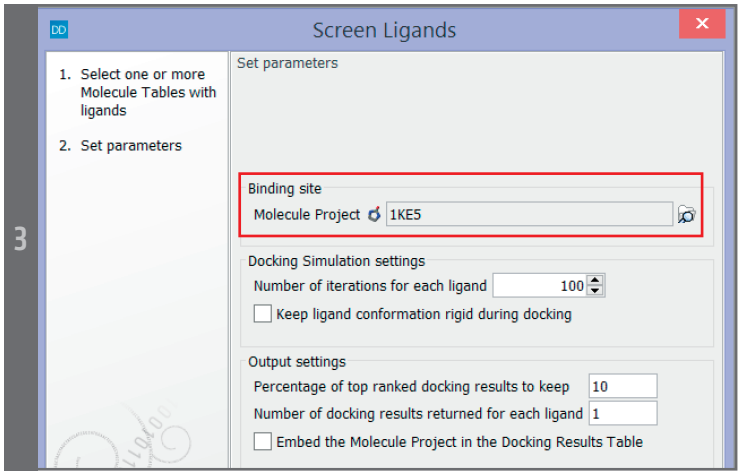
Screen Ligands



Invoke the Screen Ligands tool from the Toolbox.

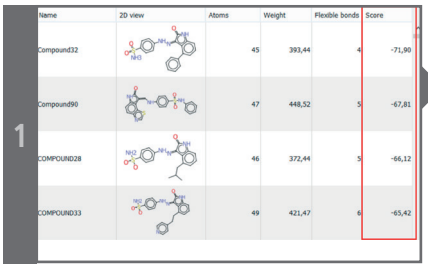


Select the Molecule Tables containing the ligands to screen.

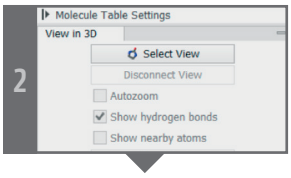


Specify which Molecule Project holds the Binding Site Setup. The screening will start, and the progress can be followed using the Processes tab in the Toolbox.

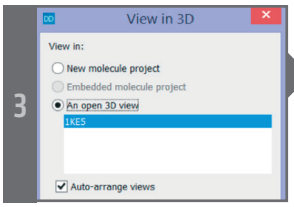
Inspect Interaction with Protein



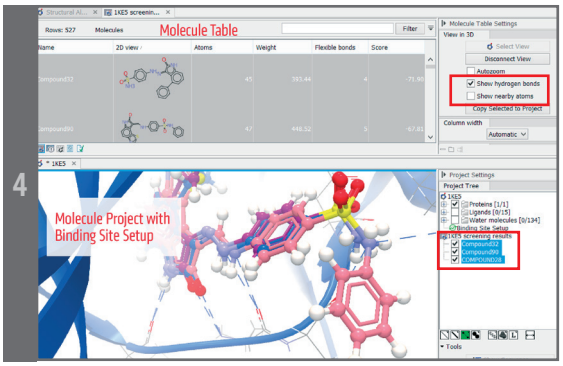
The screening outputs a Molecule Table with a column listing the score for each screened ligand.



The ligand binding modes can also be viewed in 3D...



...by choosing to see the screening results in the Molecule Project containing the Binding Site Setup.



Molecules selected in the table appear in the Molecule Project. Visualize the binding modes of the top scoring results to find common functional groups and structural elements.

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