

CLC **Drug Discovery** Workbench

EXPLORING PROTEIN-LIGAND BINDING

Using fast track docking

Import Protein Structure

MOLECULE PROJECT

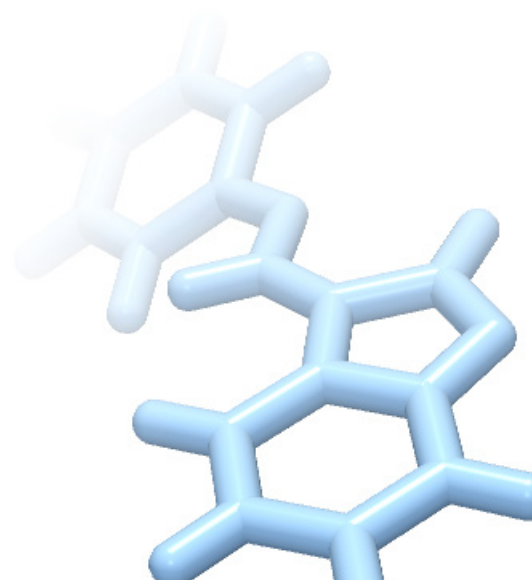
Setup Docking Target

Copy-Paste Molecules from 2D Sketcher

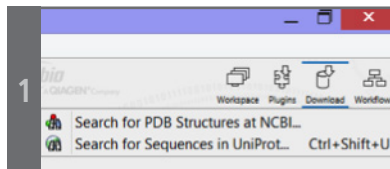
One-click Docking

Inspect Interaction with Protein

Protein-ligand binding is explored using molecular docking, to fit the ligand in a binding pocket on the target protein. The ligands are stored in a Molecule Project together with the protein structure, for fast track docking in a 3D view.

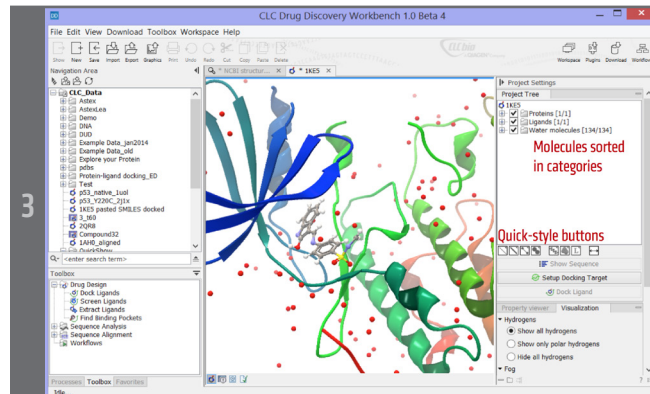
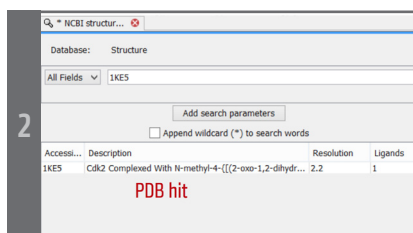


Import Protein Structure



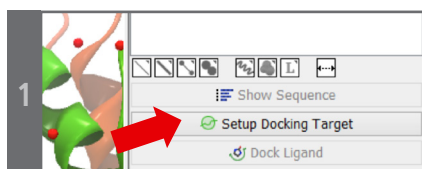
Protein structures can be downloaded directly from the Protein Data Bank through the built-in Search for PDB Structures at NCBI option.

Specify keywords or a PDB ID in the search field, and a selection of hits appears below. Double-click a hit to open a 3D view of the molecule structures.

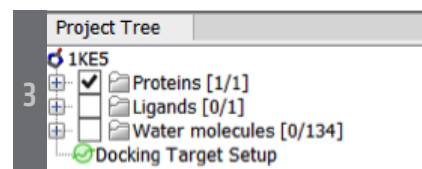
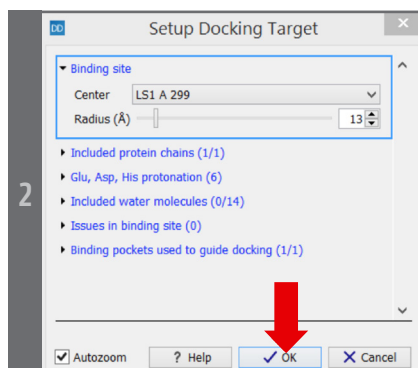


A Molecule Project is created with the content of the PDB file. The molecules are automatically sorted in categories in the Project Tree. From the Project Tree, molecules can be hidden or displayed, and their visual representation customized via quick-style buttons.

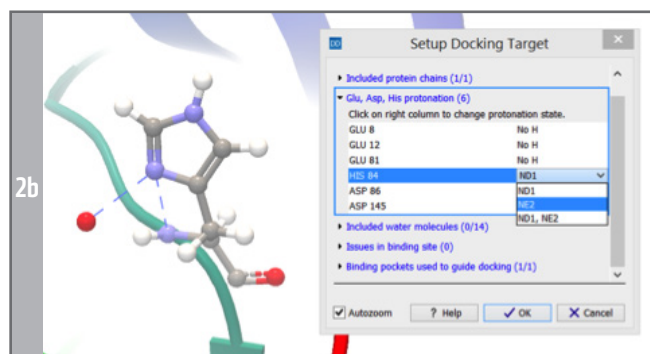
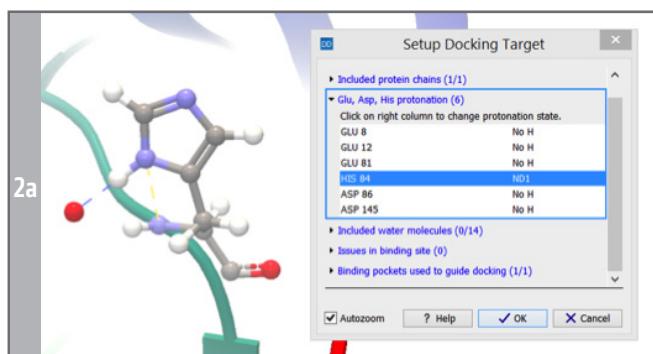
Setup Docking Target



The imported protein structure can be setup as a docking target in just two clicks.

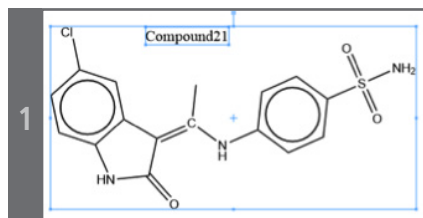


The Molecule Project now contains a Docking Target Setup



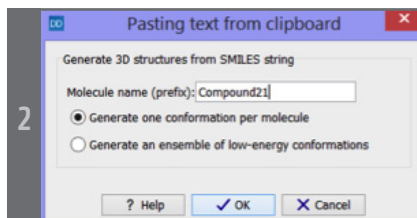
The Setup Docking Target dialog box is interactive, and the relevant molecules, residues, and interactions will automatically be displayed for easy inspection. The view is immediately updated when changes are made.

Copy-Paste Molecules from 2D Sketcher

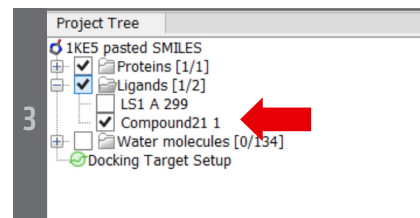


Use your favorite 2D molecule sketcher software to sketch up the molecules you wish to see binding to the target protein.

Select the molecule in the sketcher and use the Copy as SMILES option.
(ChemDraw: Alt+Ctrl+C, MarvinSketch: Ctrl+L).



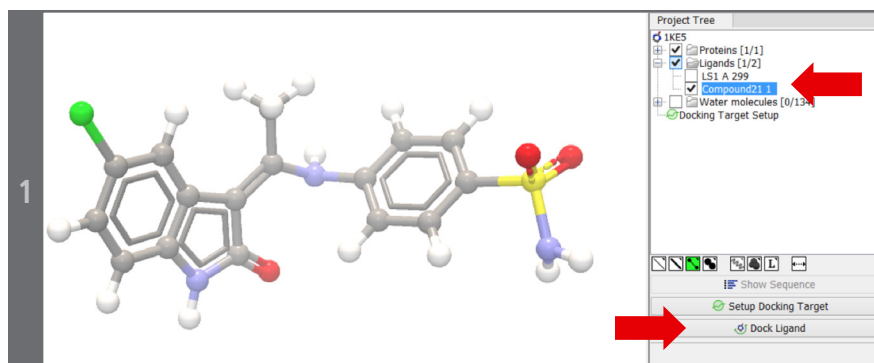
Paste the molecule to the Molecule Project using Ctrl-V.



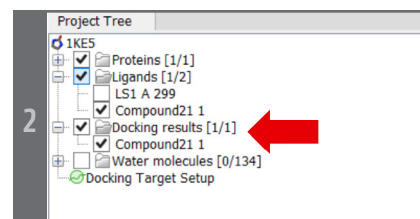
The molecule appears in the Ligands category in the Project Tree.

Double-click the entry in the Project Tree to zoom and fit the 3D view around the molecule.

One-click Docking



Select the pasted molecule in the Project Tree and click the Dock Ligand button.

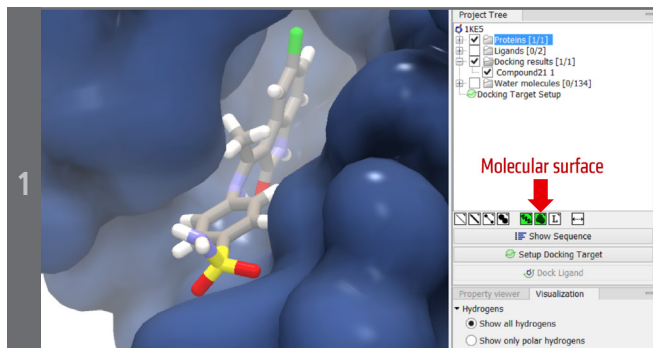


A new category appears in the Project Tree; Docking results.

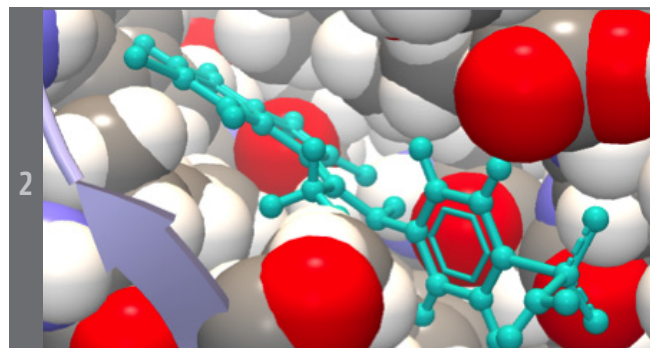
Double-click the docking result entry to center the 3D view on the docked ligand.



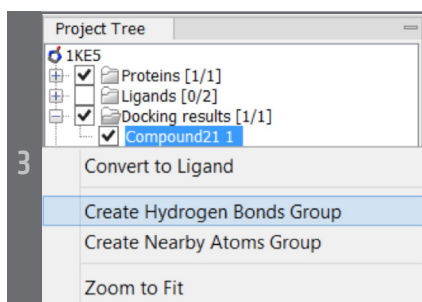
Inspect Interaction with Protein



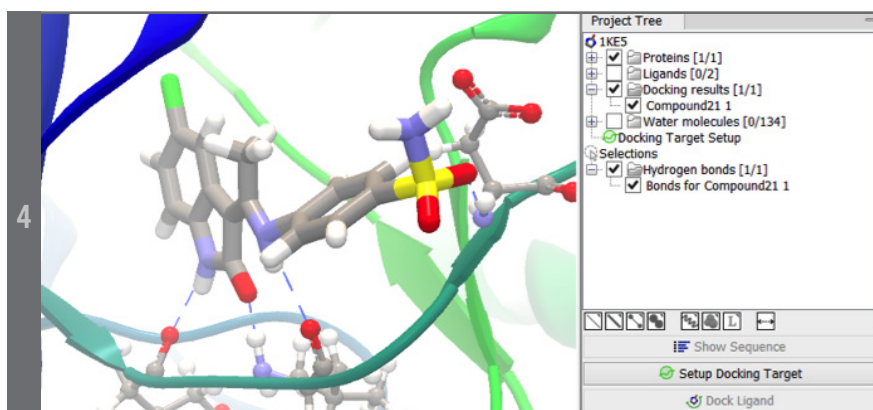
1 Show the molecular surface of the protein, to see how the molecule fills out the pocket...



2 ...or show the residues forming the binding pocket in space-filling. A selection of color schemes is available on the quick-style buttons.



3 Select the docking result in the Project Tree. From the context menu, generate atom groups showing hydrogen bonds specifically or showing all residues near the ligand.



4 The visual representation of created atom groups can be customized using the quick-style buttons.

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