SeeSAR

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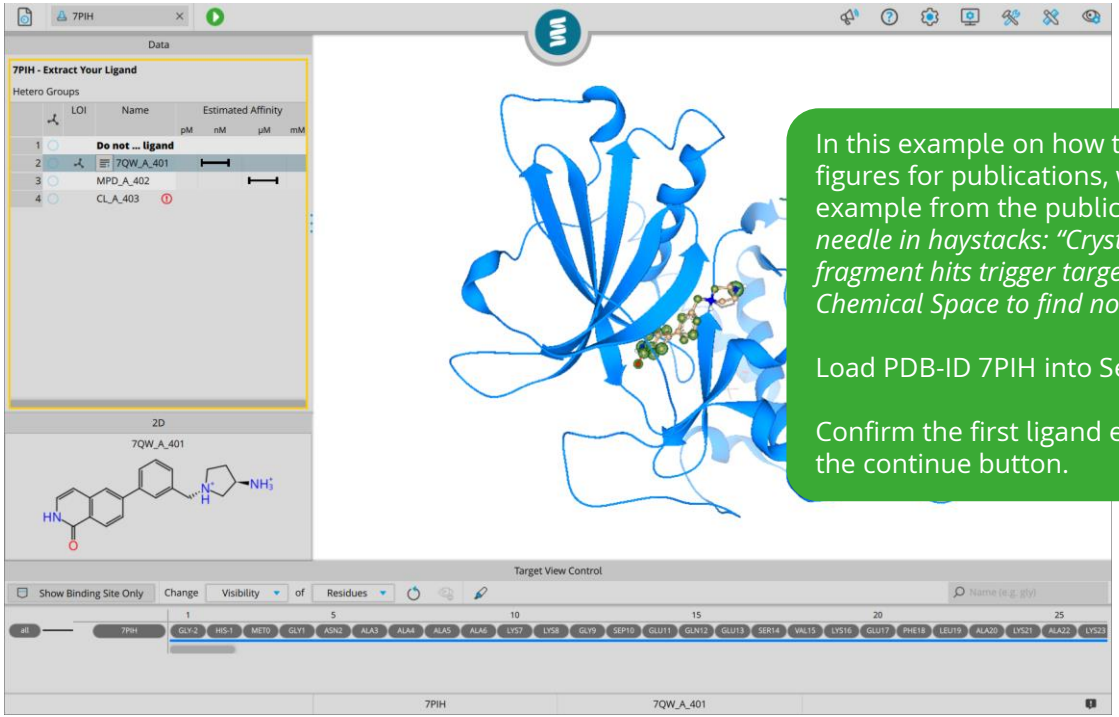
Publishing with SeeSAR

How to generate high quality images

Example PDB: 7PIH

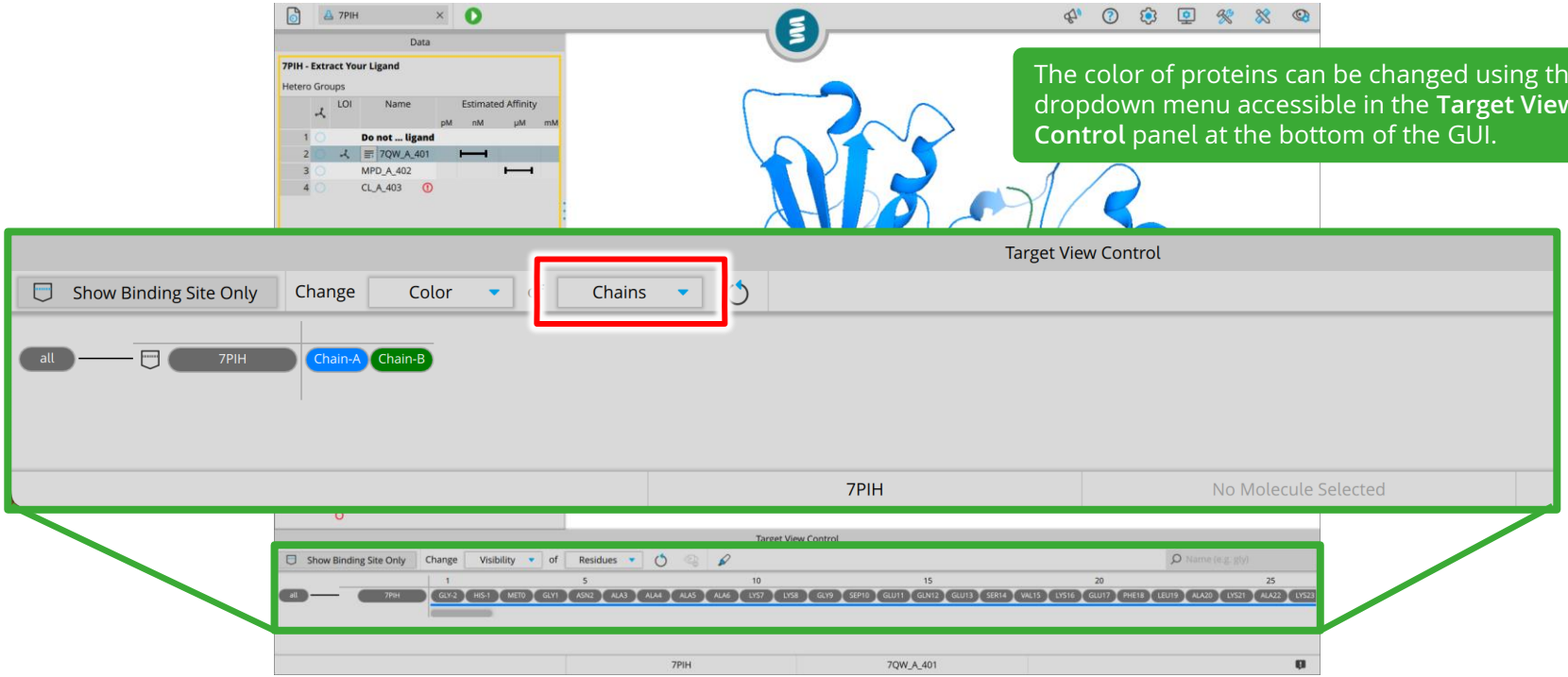


In this example on how to generate high quality figures for publications, we will work with an example from the publication *"A magnet for the needle in haystacks: "Crystal structure first" fragment hits trigger targeted exploration of the Chemical Space to find novel active matter"*.

Load PDB-ID 7PIH into SeeSAR.

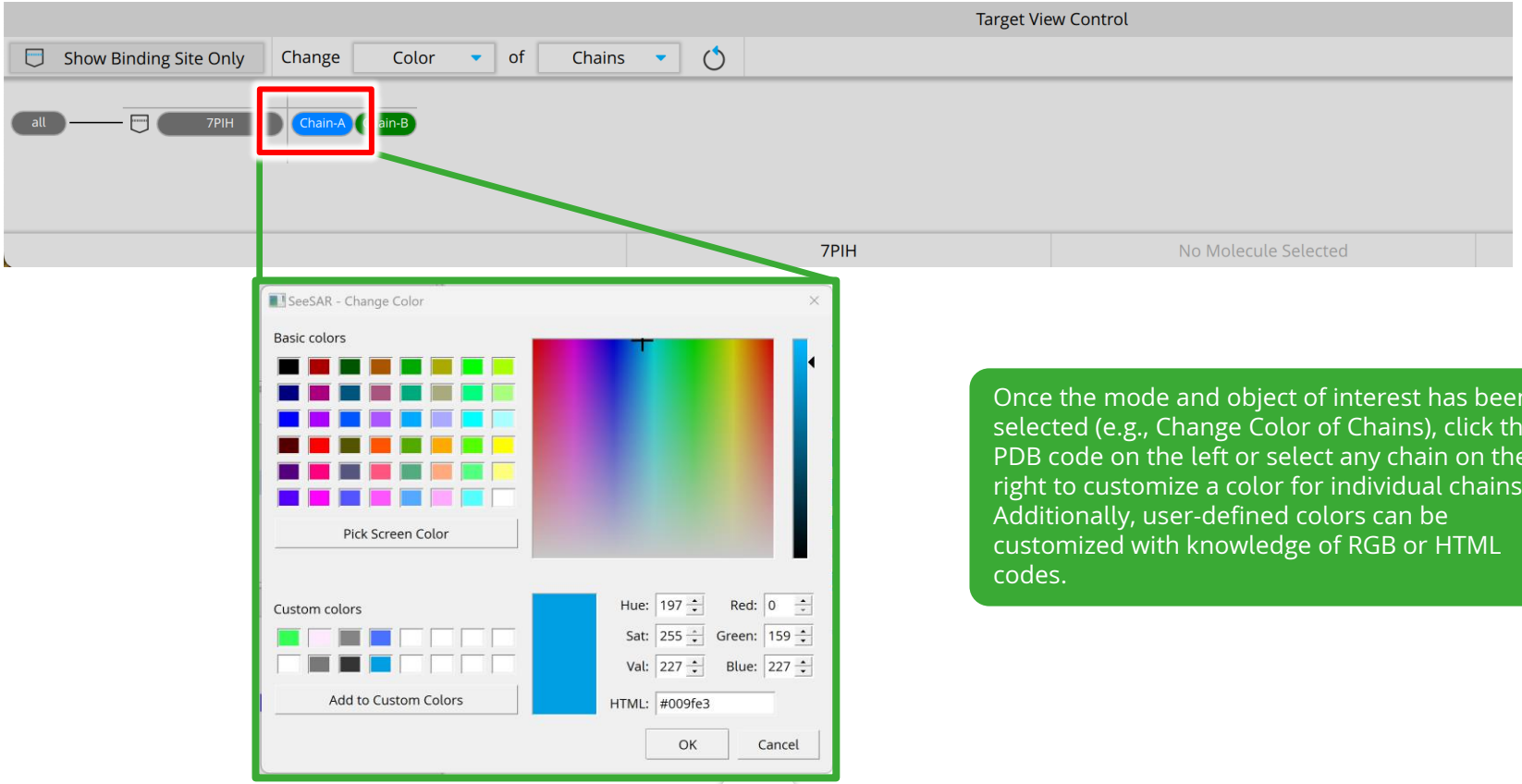
Confirm the first ligand entry and confirm with the continue button.

Set Colors – Protein



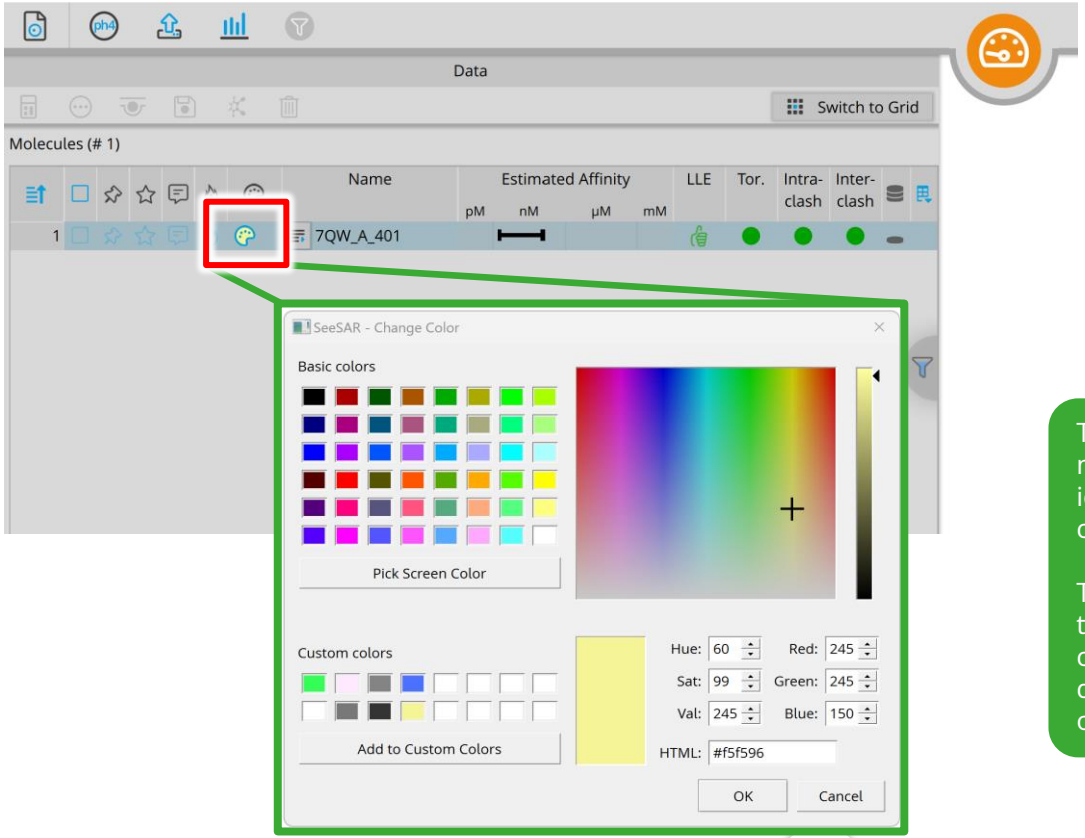
The color of proteins can be changed using the dropdown menu accessible in the **Target View Control** panel at the bottom of the GUI.

Set Colors – Protein



Once the mode and object of interest has been selected (e.g., Change Color of Chains), click the PDB code on the left or select any chain on the right to customize a color for individual chains. Additionally, user-defined colors can be customized with knowledge of RGB or HTML codes.

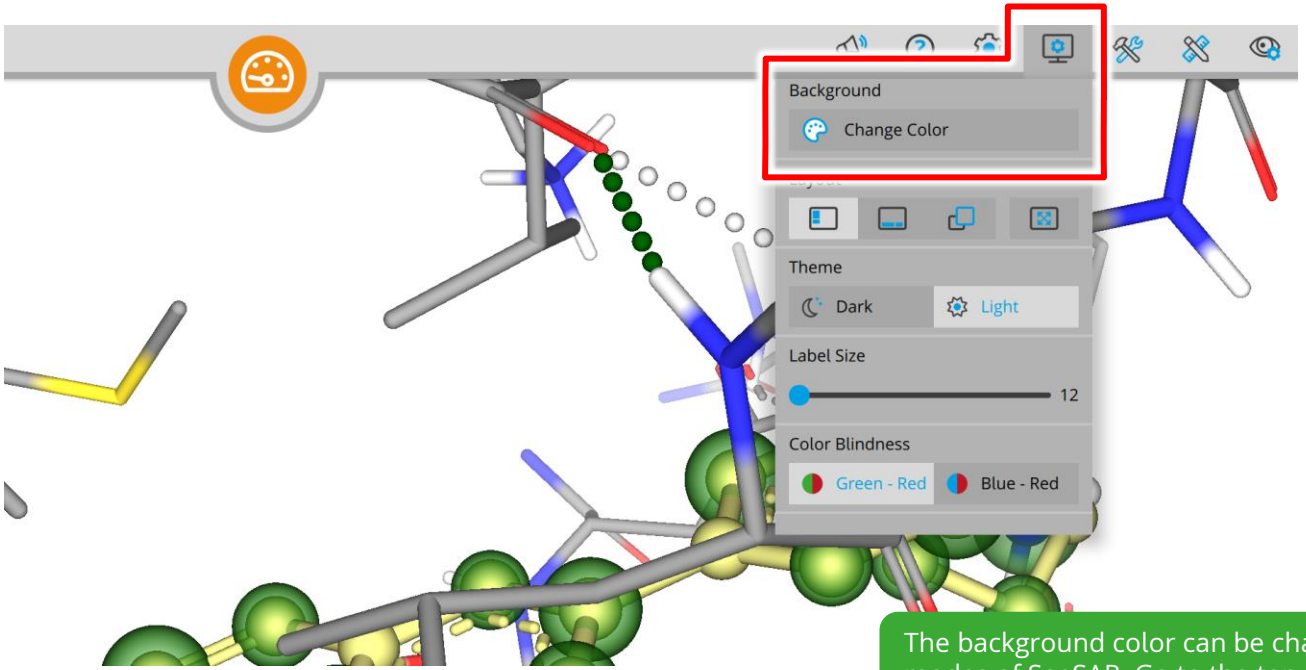
Set Colors – Ligand



The color of ligands can be changed in several modes, including the Analyzer Mode. A palette icon is present in each mode where a ligand can be colored.

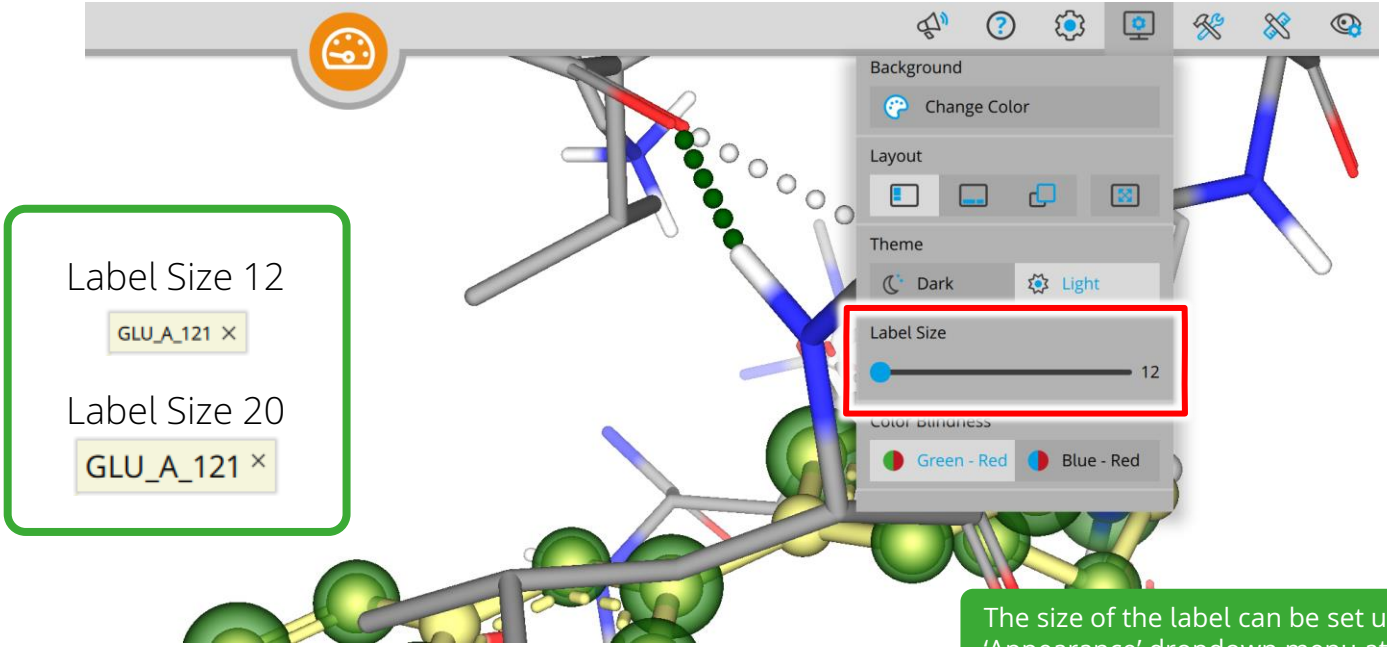
The color panel which is accessible via the data table enables the use of basic colors. A light color (RGB 245/245/150) was selected to easily differentiate from SeeSAR's red/green coloring of HYDE spheres and torsion angles.

Set Colors – Background



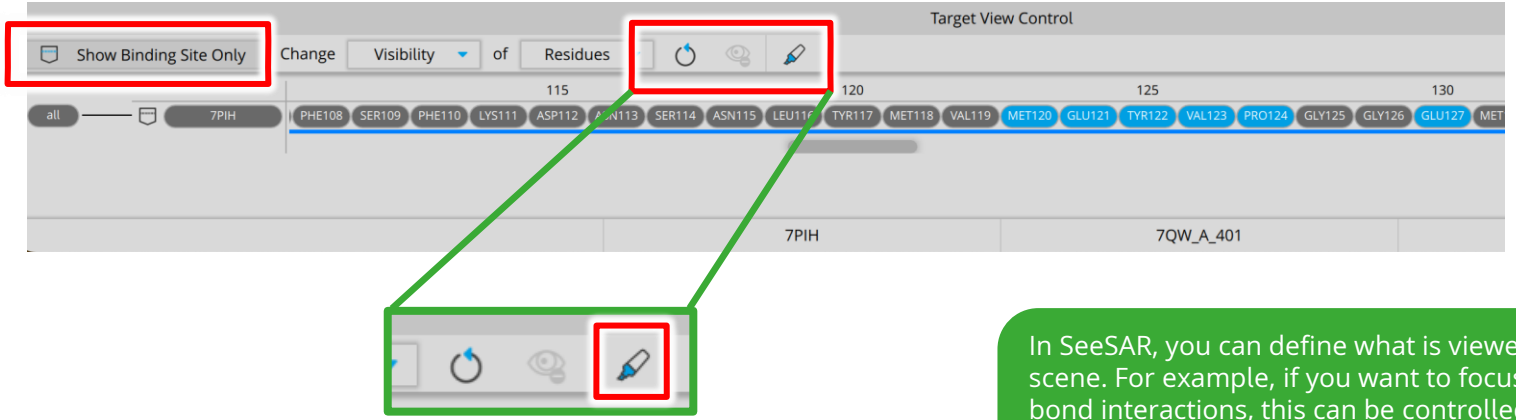
The background color can be changed in all modes of SeeSAR. Go to the top right toolbar ‘Appearance’ and open the Background color panel.
In publications the background is usually set to white.

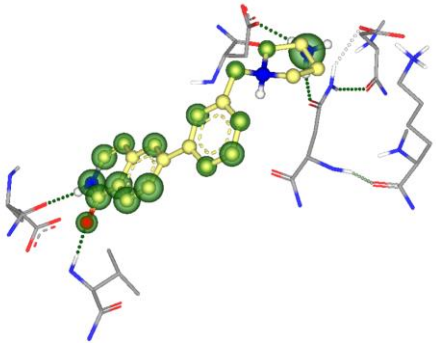
Set Label Size



The size of the label can be set under the 'Appearance' dropdown menu at the top right of the GUI. The size of the label will be adopted in the exported image.

Define Scene



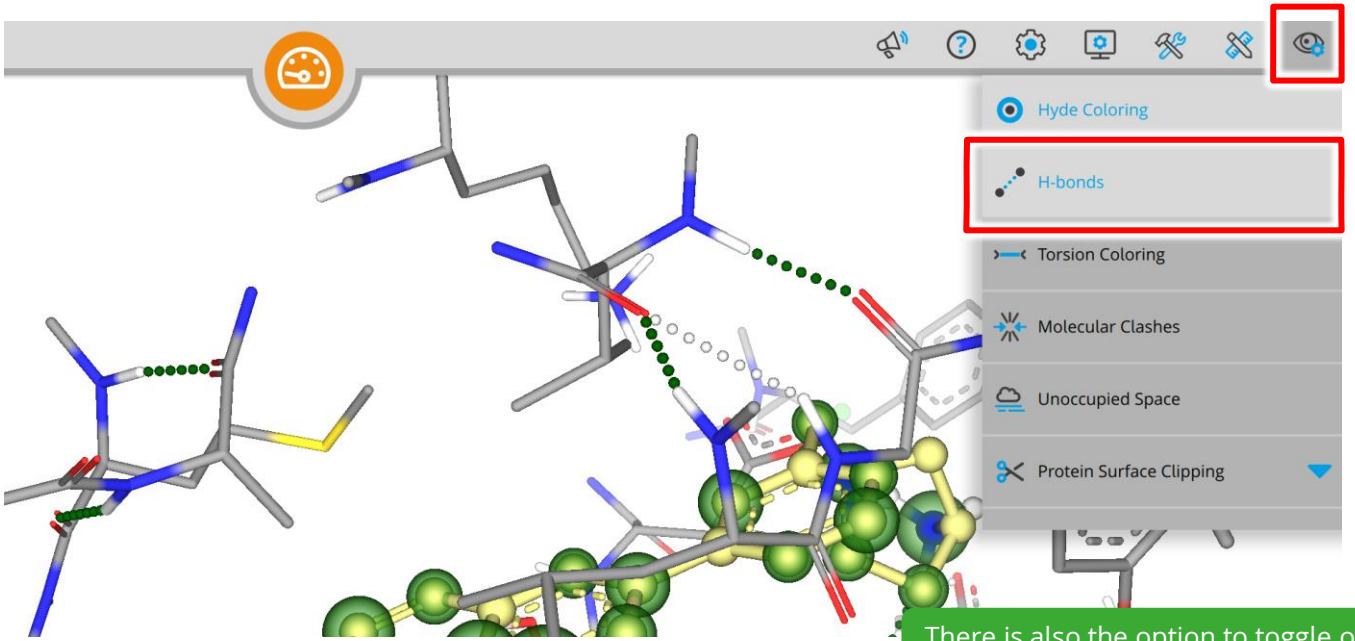


In SeeSAR, you can define what is viewed in the scene. For example, if you want to focus on H-bond interactions, this can be controlled in the Target View Control panel.

To achieve this, toggle on Show Binding Site Only in the Target View Control panel. This will display interactions that are part of a protein-ligand interaction (highlighted in blue).

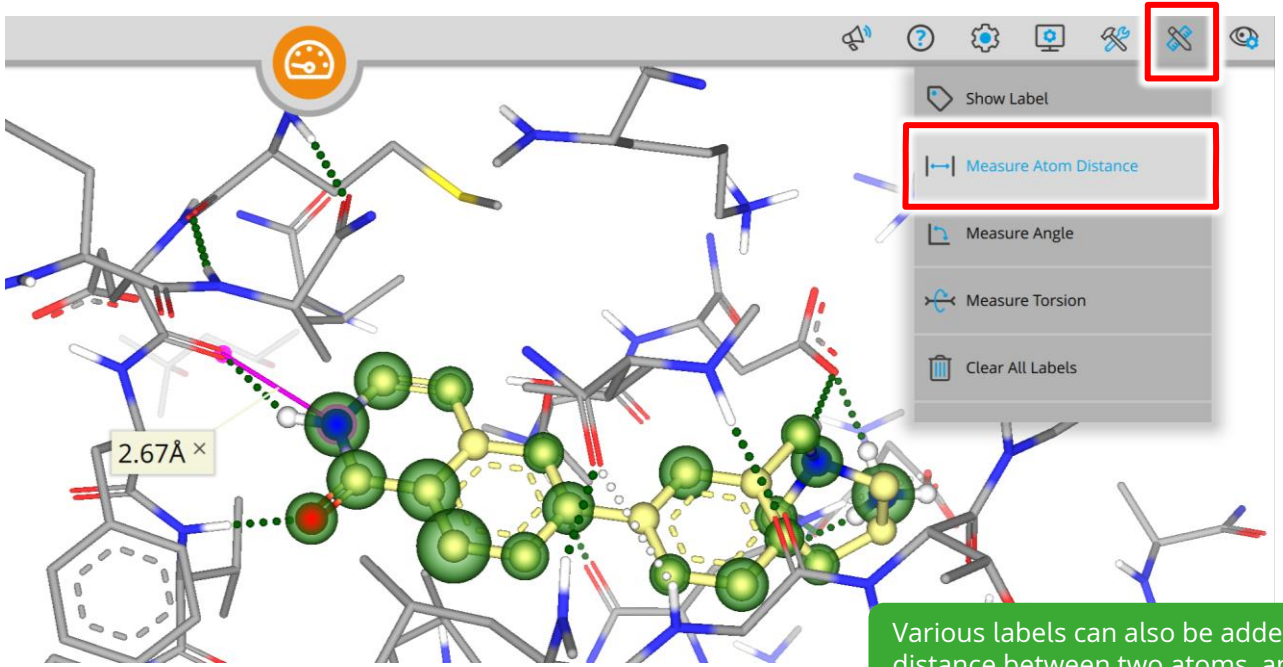
If all residues are hidden, you can use the 'Show all interacting components' to display only those forming H-bond interactions with the ligand.

Define Scene



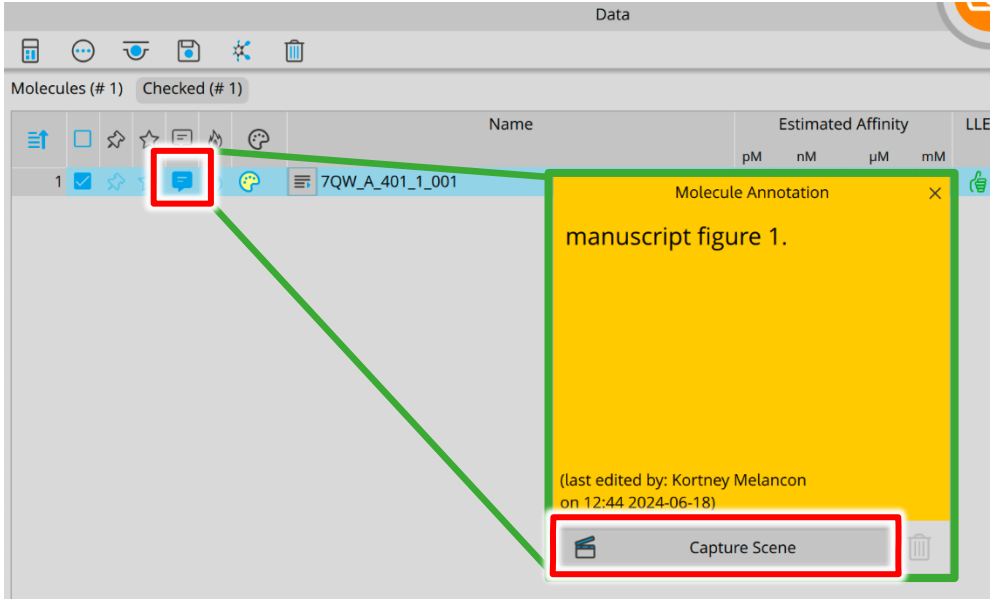
There is also the option to toggle off H-bonds by navigating to the top right of the GUI, selecting the 'Visualization' dropdown, and clicking H-bonds.

Define Scene



Various labels can also be added (e.g., the distance between two atoms, angles, or torsions) in the 3D Viewer by selecting the 'Label and measure' dropdown menu on the top right of the GUI.

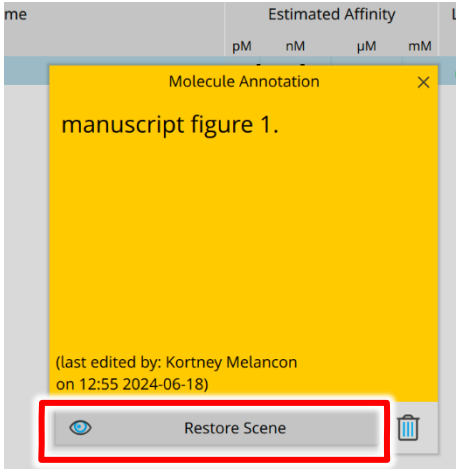
Capture Scene



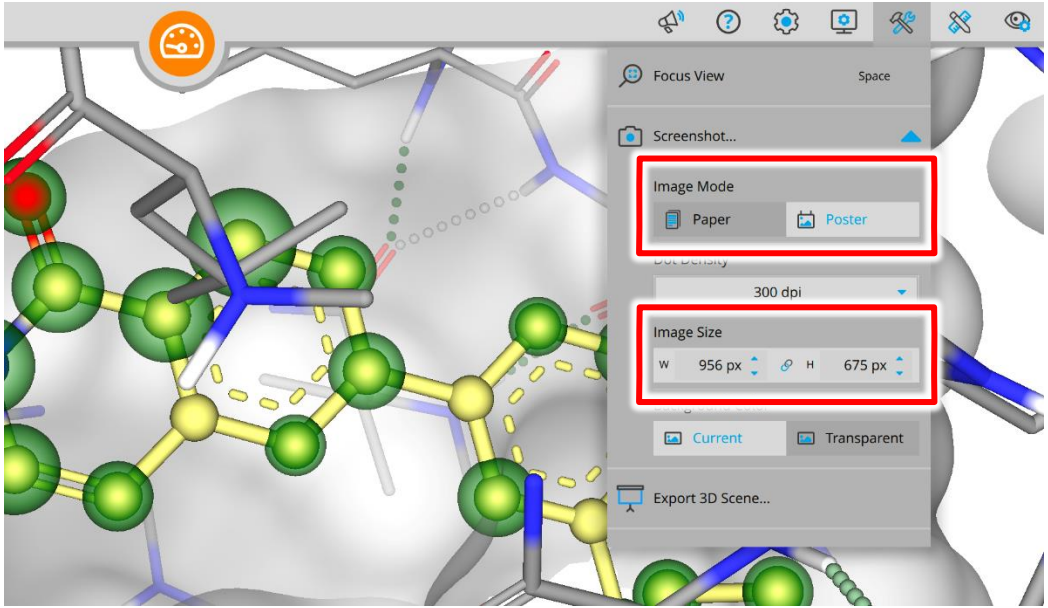
A specific scene can be captured within the 'Molecule Annotation' box.

A scene is the 3D view of the protein-ligand complex with options like colors, view of specific residues or chains, clipped binding sites, or surfaces toggled on/off, etc

Once the scene is captured, the view and settings can be restored.



Export Screenshot

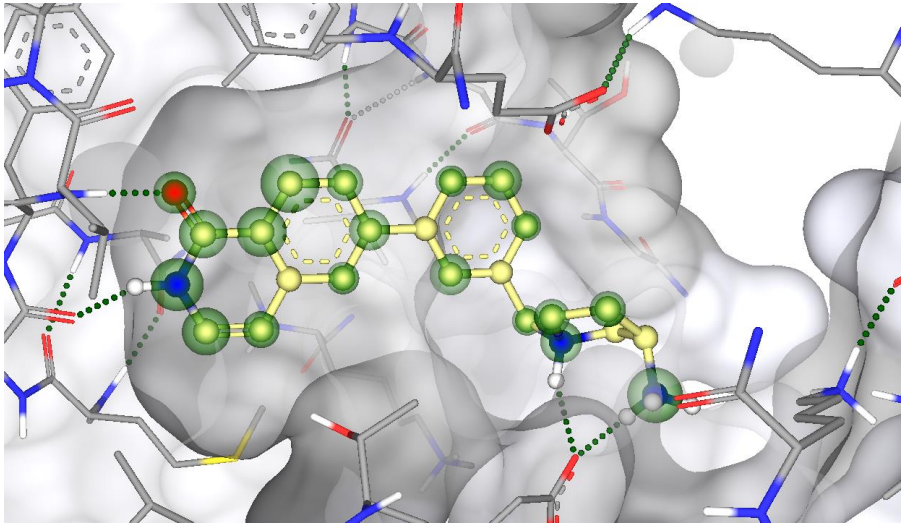


Screenshots of the scene can be exported as a PNG image file by clicking the 'Utilities' icon in the top right and selecting 'Screenshot'. Under the 'Screenshot' dropdown, the dot density and resolution can be adjusted as well as the transparency mode of the scene background.

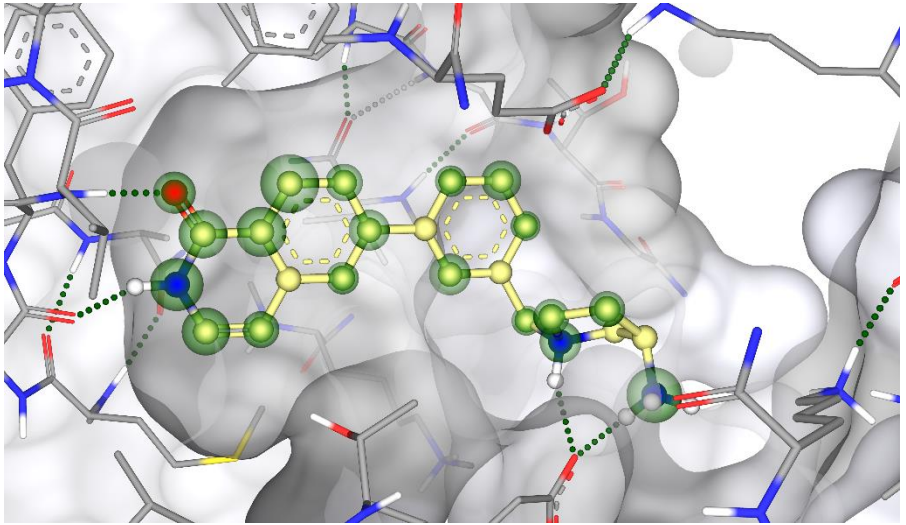
Image Mode
Paper: Use current resolution and capture labels
Poster: Use custom resolution and don't capture labels.

Image Size
(see journal guidelines)
px • dpi = mm

Results of Poster Export



300 dpi
1241px • 787px



300 dpi
8000px • 5073px