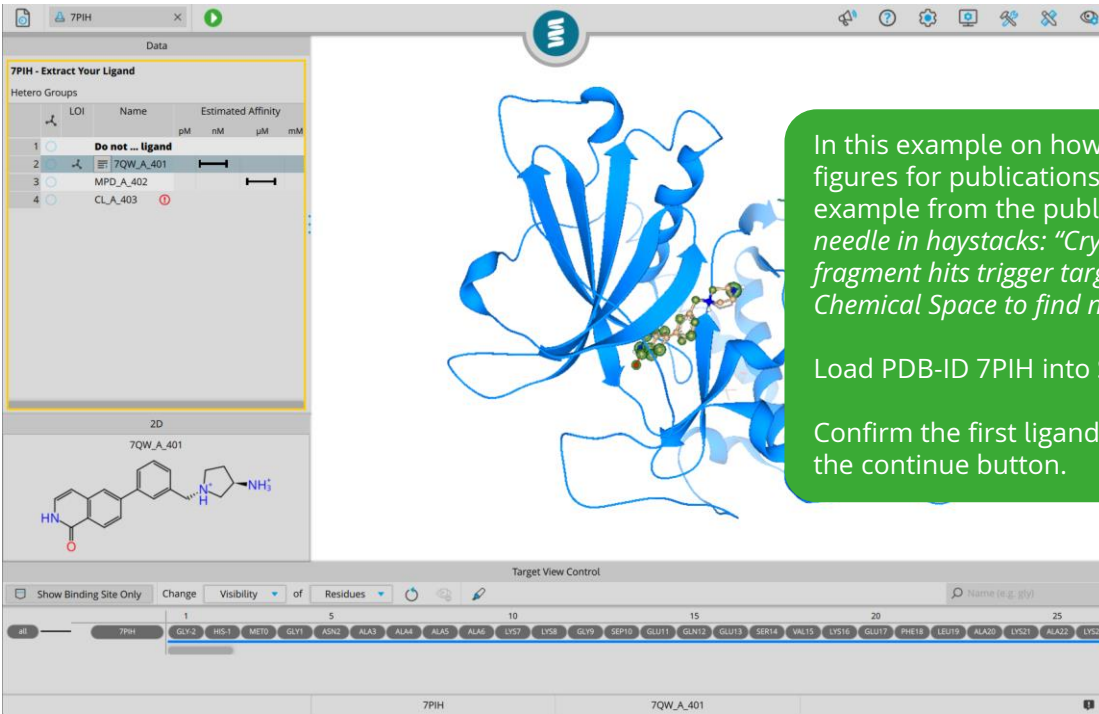


# Publishing with SeeSAR

How to generate high quality images

# Example PDB: 7PIH



The screenshot displays the SeeSAR interface for PDB entry 7PIH. The main window shows a blue ribbon representation of the protein structure with a green and blue ligand molecule bound to it. On the left, a 'Data' panel titled '7PIH - Extract Your Ligand' contains a table of hetero groups. Below the table is a 2D chemical structure of the selected ligand, 7QW\_A\_401. At the bottom, a 'Target View Control' panel shows a sequence of residues from 1 to 25, with the ligand's position indicated by a blue bar.

Hetero Groups	LOI	Name	Estimated Affinity
			pM nM $\mu$ M mM
1	<input type="radio"/>	Do not ... ligand	
2	<input checked="" type="radio"/>	7QW_A_401	██████████
3	<input type="radio"/>	MPD_A_402	██████████
4	<input type="radio"/>	CLA_403	○

2D  
7QW\_A\_401

Target View Control  
Show Binding Site Only Change Visibility of Residues of 1 5 10 15 20 25  
all 7PIH GLY2 HIS1 MET9 GLY1 ASN2 ALA3 ALA4 ALA5 ALA6 LYS7 LYS8 GLY9 SER10 GLU11 GLN12 GLU13 SER14 NLE15 LYS16 GLU17 PHE18 LEU19 ALA20 LYS21 ALA22 LYS23

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 screenshot shows the top portion of the 7PIH software interface. On the left, a 'Data' panel displays a table of 'Hetero Groups'. The main area shows a 3D ribbon representation of a protein structure in blue.

LOI	Name	Estimated Affinity
		pM nM $\mu$ M mM
1	Do not ... ligand	
2	7QW_A_401	
3	MFD_A_402	
4	CLA_403	

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

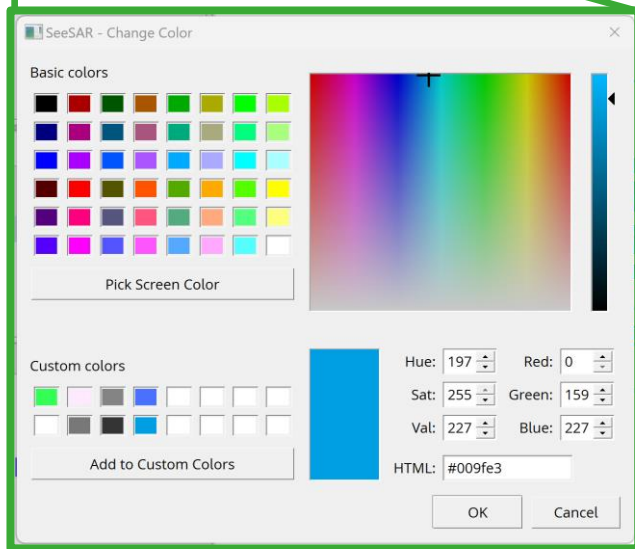
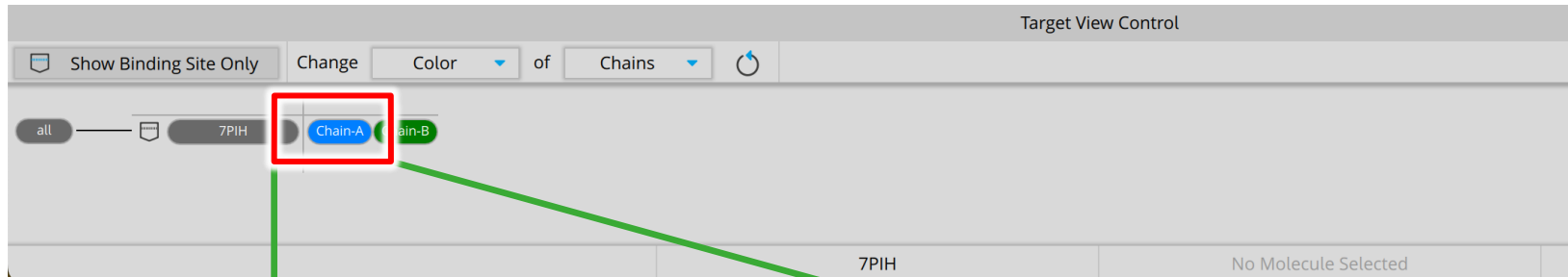
This panel, titled 'Target View Control', contains several interactive elements. A red box highlights the 'Chains' dropdown menu. Below it, there are buttons for 'Chain-A' and 'Chain-B'. The panel also includes a 'Show Binding Site Only' button, a 'Change' button, and a 'Color' dropdown menu.

This panel shows a detailed view of the residue list for the protein. It includes a search bar for 'Name (e.g. gly)' and a list of residues with their positions and names. The residues are color-coded by chain.

1	5	10	15	20	25
GLN2	HS-1	MET9	GLY1	ASN2	ALA3
ALA4	ALA5	ALA6	LYS7	LYS8	GLY9
SEP10	GLU11	GLN12	GLU13	SER14	VAL15
LYS16	GLU17	PHE18	LEU19	ALA20	LYS21
ALA22	LYS23				



# 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

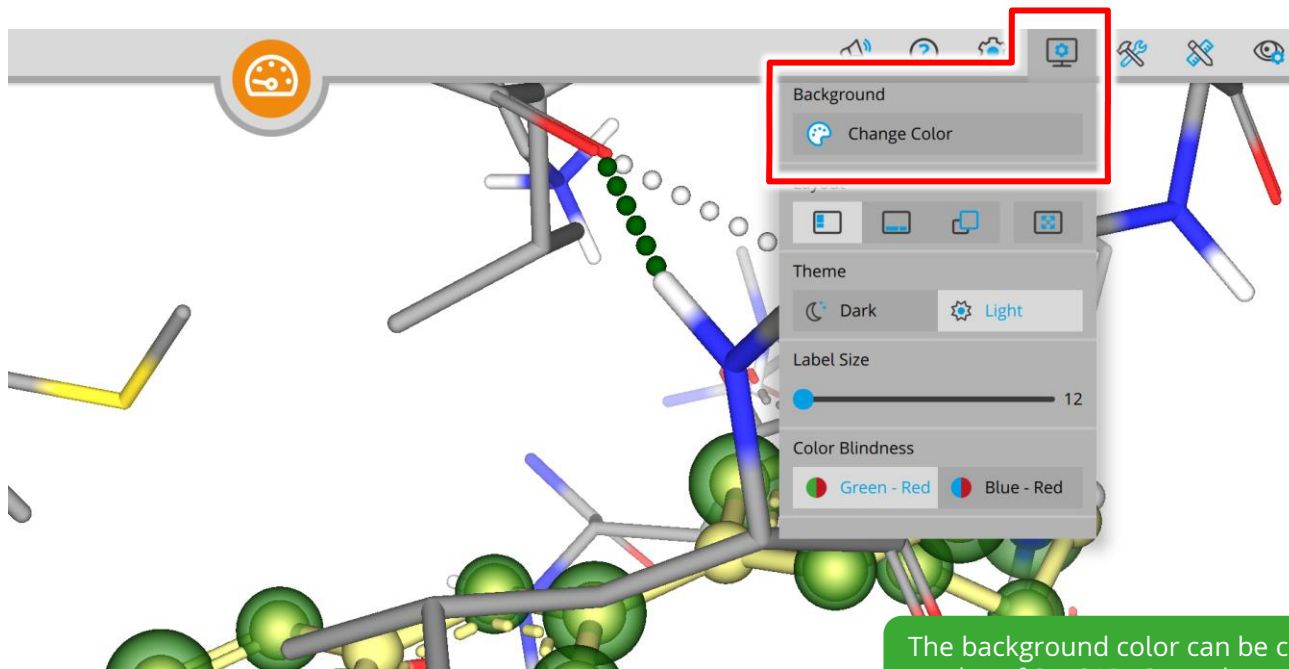
The screenshot displays the SeeSAR software interface. At the top, there is a toolbar with various icons. Below it is a 'Data' table with columns for Name, Estimated Affinity (pM, nM, μM, mM), LLE, Tor., Intra-clash, and Inter-clash. The first row shows a molecule named '7QW\_A\_401'. A red box highlights a palette icon in the table's toolbar. A green callout box points to a 'SeeSAR - Change Color' dialog box. This dialog box features a 'Basic colors' palette, a color wheel, a 'Pick Screen Color' button, and a 'Custom colors' section with a color picker and RGB/HTML input fields. The color picker shows a light yellow color with RGB values of 245, 245, 150 and HTML code #f5f596.

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

Label Size 12  
GLU\_A\_121 x

Label Size 20  
GLU\_A\_121 x

Background  
Change Color

Layout

Theme  
Dark Light

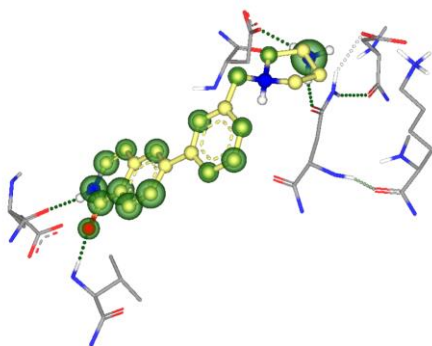
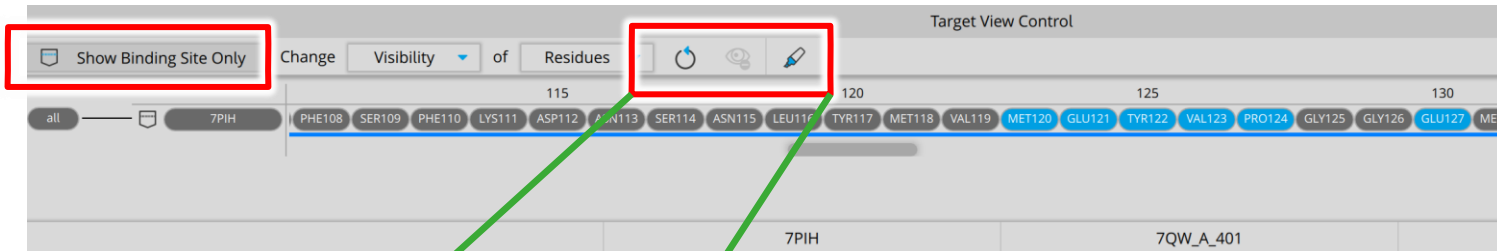
Label Size  
12

Color Blindness  
Green - Red Blue - Red

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.

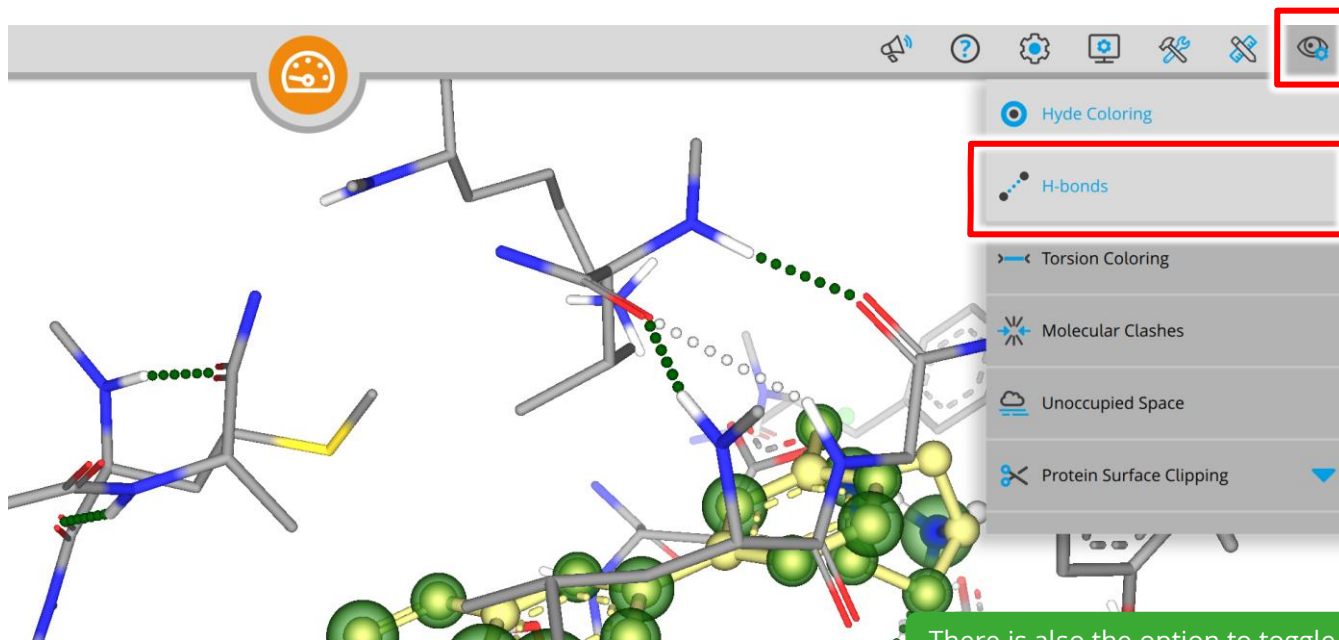
To achieve this, toggle on Show Binding Site Only in the Target View Control panel. This will display interactions that are part of a protein-ligand interaction (highlighted in blue).

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





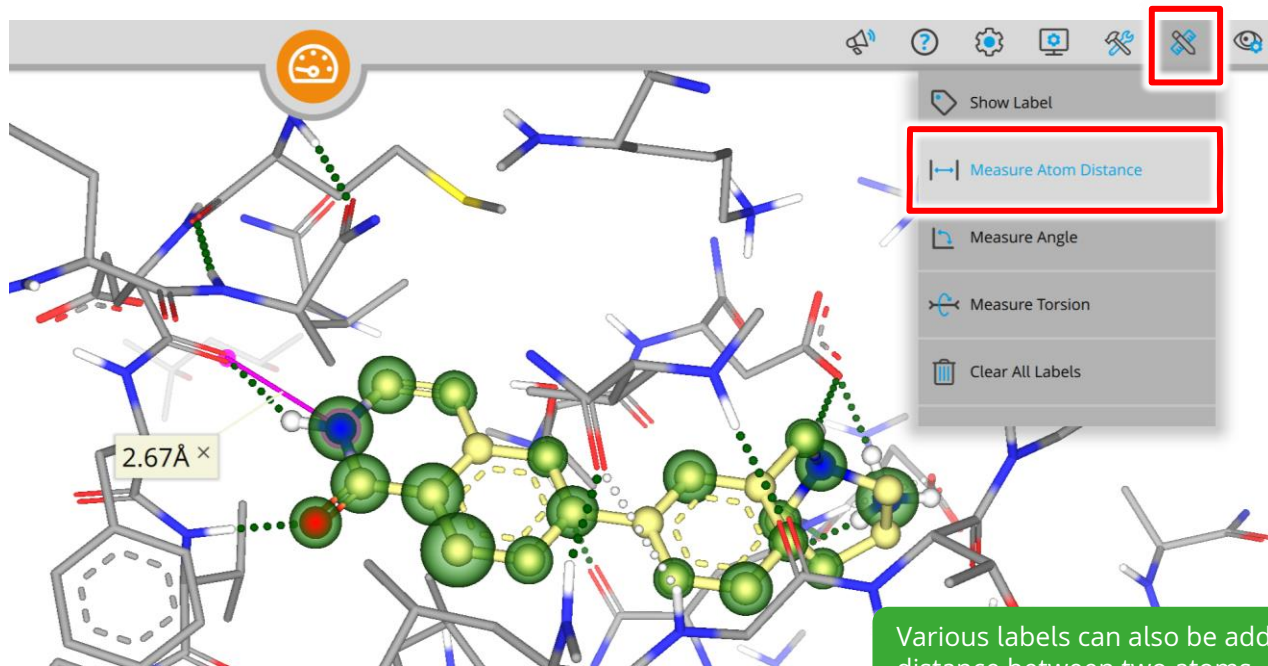
# Define Scene



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.



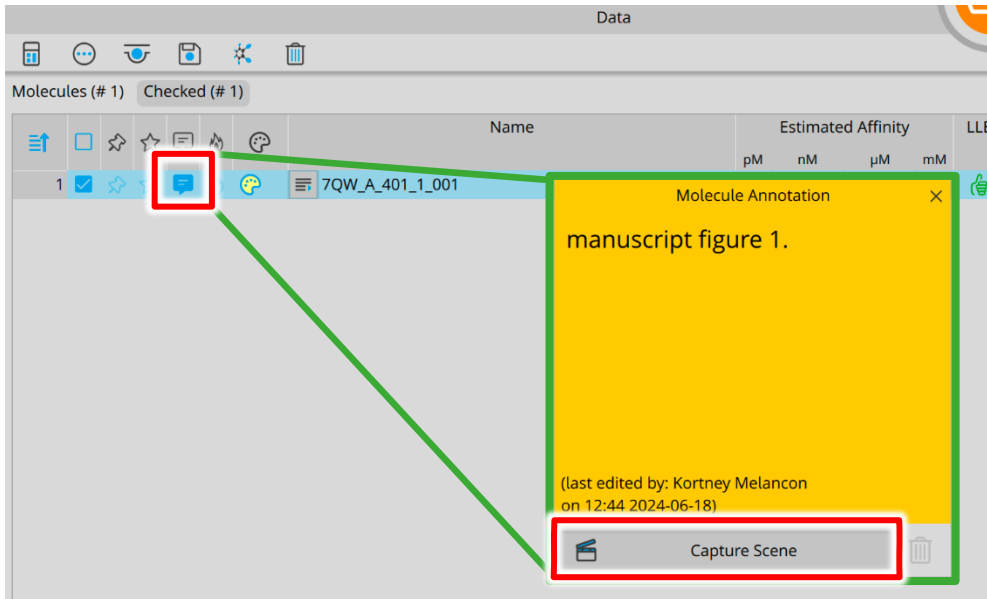
# Define Scene



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.



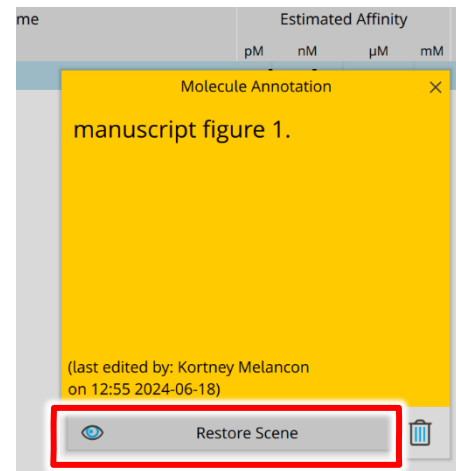
# Capture Scene



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

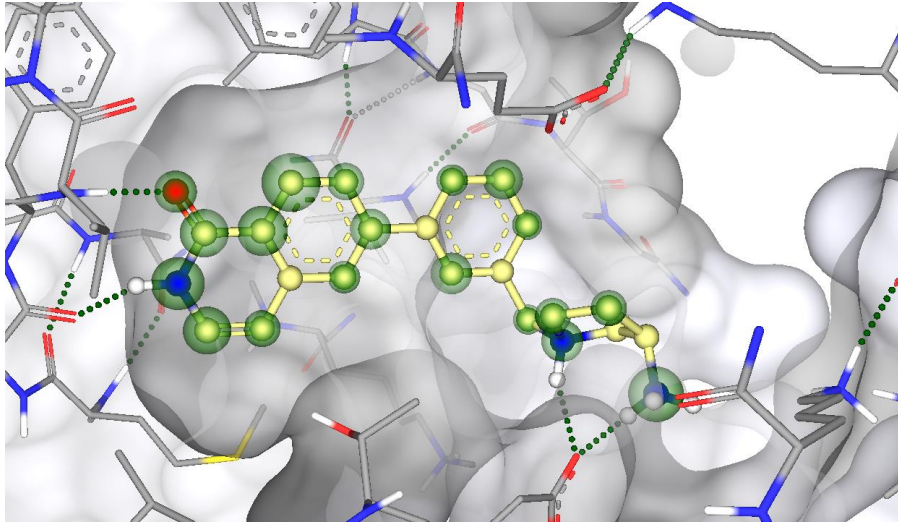
Poster: Use custom resolution and don't capture labels.

## Image Size

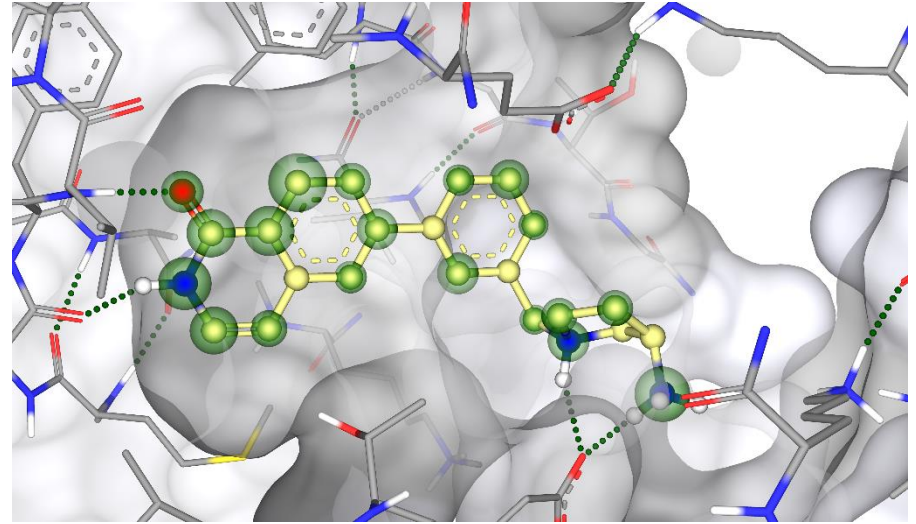
(see journal guidelines)  
 $\text{px} \cdot \text{dpi} = \text{mm}$



# Results of Poster Export



300 dpi  
1241px • 787px



300 dpi  
8000px • 5073px

