



BioSolveIT
expect actives!

SeeSAR

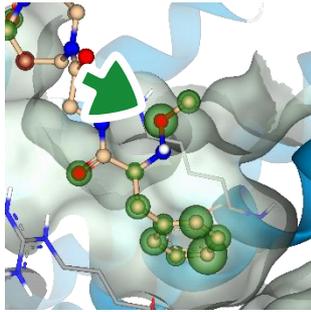
Beginner's Guide
Version 15 - Apollo



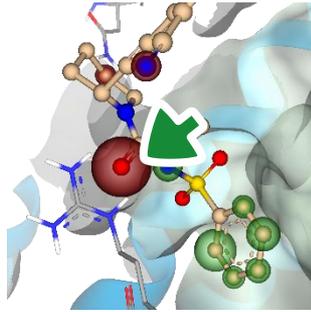
**Time to start an interactive dialog with
your compound!**

SeeSAR's Visual Elements

HYDE Spheres

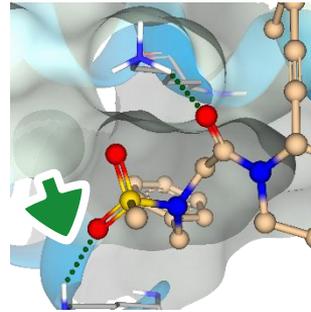


Green sphere: beneficial contribution to the binding affinity. Happy atom.

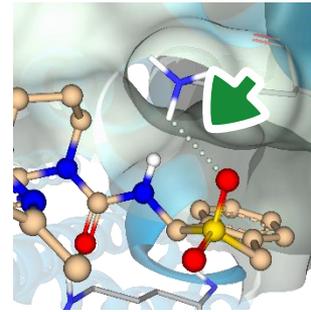


Red sphere: negative contribution to the binding affinity. Unhappy atom.

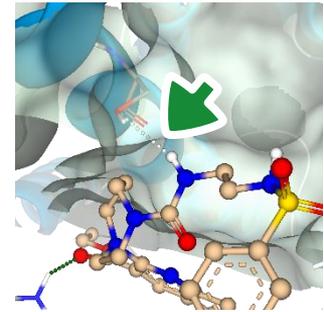
H-Bond Geometry



Dark green: Good geometry for H-bond interactions.

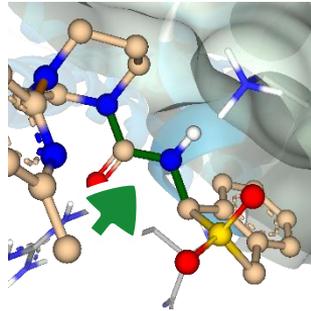


Light green: Moderate geometry for H-bond interactions.

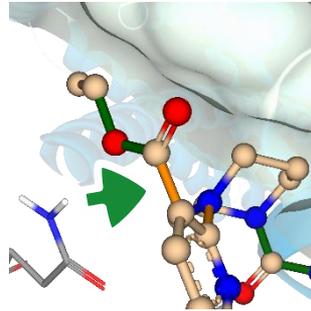


White: Poor geometry for H-bond interactions.

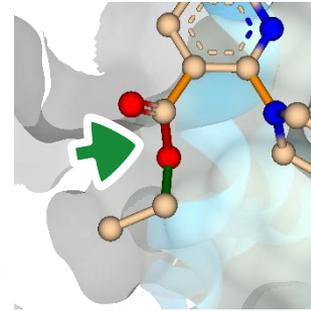
Torsions



Green: Frequent occurrence in PDB structures.



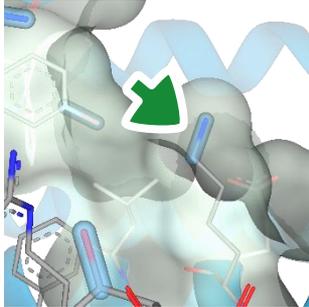
Orange: Occasional occurrence in PDB structures.



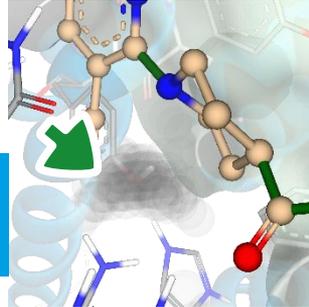
Red: Rare/no occurrence in PDB structures.

SeeSAR's Visual Elements

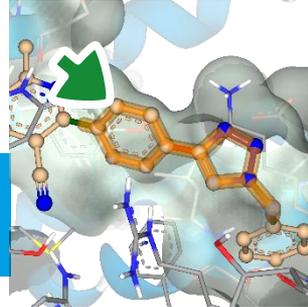
Visual Indicators



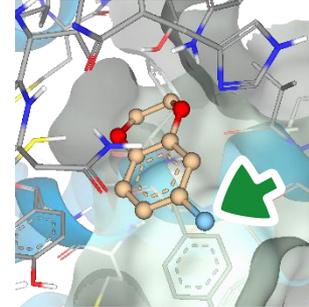
Blue tube: Potential target residue for covalent docking.



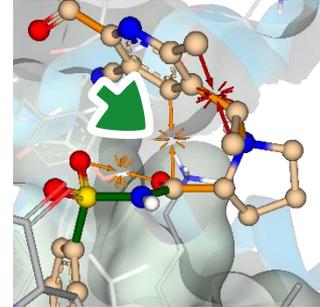
Unoccupied Space: Each sphere can host a fluorine atom.



Orange: Area replaced/added in the Inspirator Mode.



Blue atom: Linker atom. Extension point in Chemical Space Docking®.



Clashes: Intra- and intermolecular clashes of the ligand.

Table View

LLE	Tor.	Intra-clash	Inter-clash	MPO [Radar]

Lipophilic Ligand Efficiency (LLE):



Torsions: **green:** At most two tolerable bonds, **orange:**

More than two tolerable bonds or one strained bond and at most 2 tolerable bonds, **red:** Anything else.

Clashes: **green:** Distance of all evaluated atom pairs > 0.89 Å than the sum of their van der Waals radii,

orange: Distance > 0.85 Å, **red:** At least one atom pair has a distance < 0.85 Å or less of the sum of their van der Waals radii, or three orange clashes.

Multi-parameter Optimization (MPO): Gradient from no violations (**green**), half of the parameters violated (**yellow**), all parameters violated (**red**).

Hot Keys

General Viewing

right-click	rotate*
left-click	select
[Ctrl]+right-click middle-click	translate
[Shift]+right-click	z-rotation
[Ctrl]+[Shift]+ right-click mouse-wheel	zoom
[Del]	delete table entries
[Up] and [Down] arrows	move to the respective next table entry
[Space]	center view on selected pose

*If you click on an object, this is taken as the center of rotation. Otherwise, the rotation is – depending on the viewing mode – either around the center of the entire protein or around the center of the binding site. So don't just click anywhere but close to a ligand atom of interest to rotate around it.

3D Actions

[D]+left-clicks	measure distances
[L]+left-click	label items
[A]+left-clicks	measure angle
[T]+left-clicks	measure torsion

Molecule Table

[Alt+C]	check molecule
[Alt+V]	toggle visibility
[Alt+F]	favorite
[Alt+A]	set activity (twice for 'inactive')

Editing

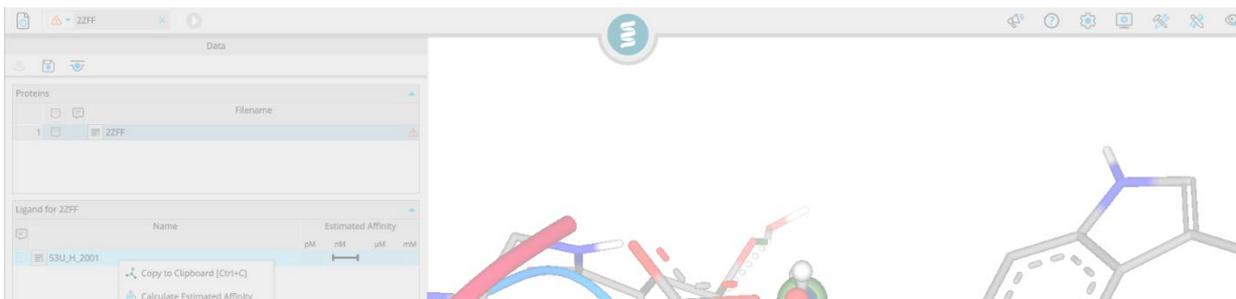
[Esc]	exit the editor
[Ctrl+S]	save the current project
[Ctrl+E]	save the current molecule in the Molecule Editor Mode
left-click: hold & drag	select all atoms and bonds in a box
[Del]	delete the current selection
[Ctrl+Z]	undo
[Ctrl+Shift+Z]	redo
right-click	context menu to add atom, resp. change bond type
left-click+ [C,B,O,S,P,F,I,1,2,3]	change element, resp. change bond type

Some keyboards will have [Strg] instead of a [Ctrl] button.
For the Mac, replace [Ctrl] by the Apple key. Also [fn]+[back] equals [del] on the Mac keyboard.

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Click on the section
you are interested in 



0. Before you start

Before diving into the individual workflows, it is worth taking a moment to get familiar with the basic concepts and interface elements of SeeSAR. This section introduces the essential setup steps, navigation principles, and display controls that will help you work efficiently and confidently throughout the program.

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Mode Overview

Welcome to SeeSAR 15.0

fast • visual • easy Apollo



Continue your last project.

Start a new drug discovery project.

Take a tour of the SeeSAR interface.

Table of Content

Mode Overview

The screenshot displays the SeeSAR software interface. On the left, a sidebar contains a 'Data' panel with a 'Proteins' list showing 'ZZFF' and a 'Ligand for ZZFF' list showing '53U_H_200'. A red box highlights a context menu for the ligand, listing various modes: Copy to Clipboard (Ctrl+C), Calculate Estimated Affinity, Add Molecule to, Add Complex to Protein Editor, Use as Reference In, Binding Site Mode, Analyzer, Molecule Editor, Inspirator, Local Docking Mode, Remote Docking Mode, Similarity Scanner, and Activity Spotter. The main window shows a 3D molecular model of a protein (blue) with a ligand (red and white) docked in its binding site. A 2D chemical structure of the ligand is shown in the bottom left. The bottom of the interface features a 'Target View Control' panel with a sequence viewer showing residues 1 to 30, including GLU12, ALA18, ASP14, CYS1, GLY1, LEU16, ARG4, PRO5, LEU16, PHE7, GLU18, LYS10, LYS10, SER11, LEU12, GLU13, ASP14, LYS14A, THR14B, GLU14C, ARG14D, GLU14E, LEU14F, LEU14G, GLU14H, SER14I, THR14J, SER14K, SER14L, VAL17, GLU18, GLY19, SER20, and ASP21.

How SeeSAR works

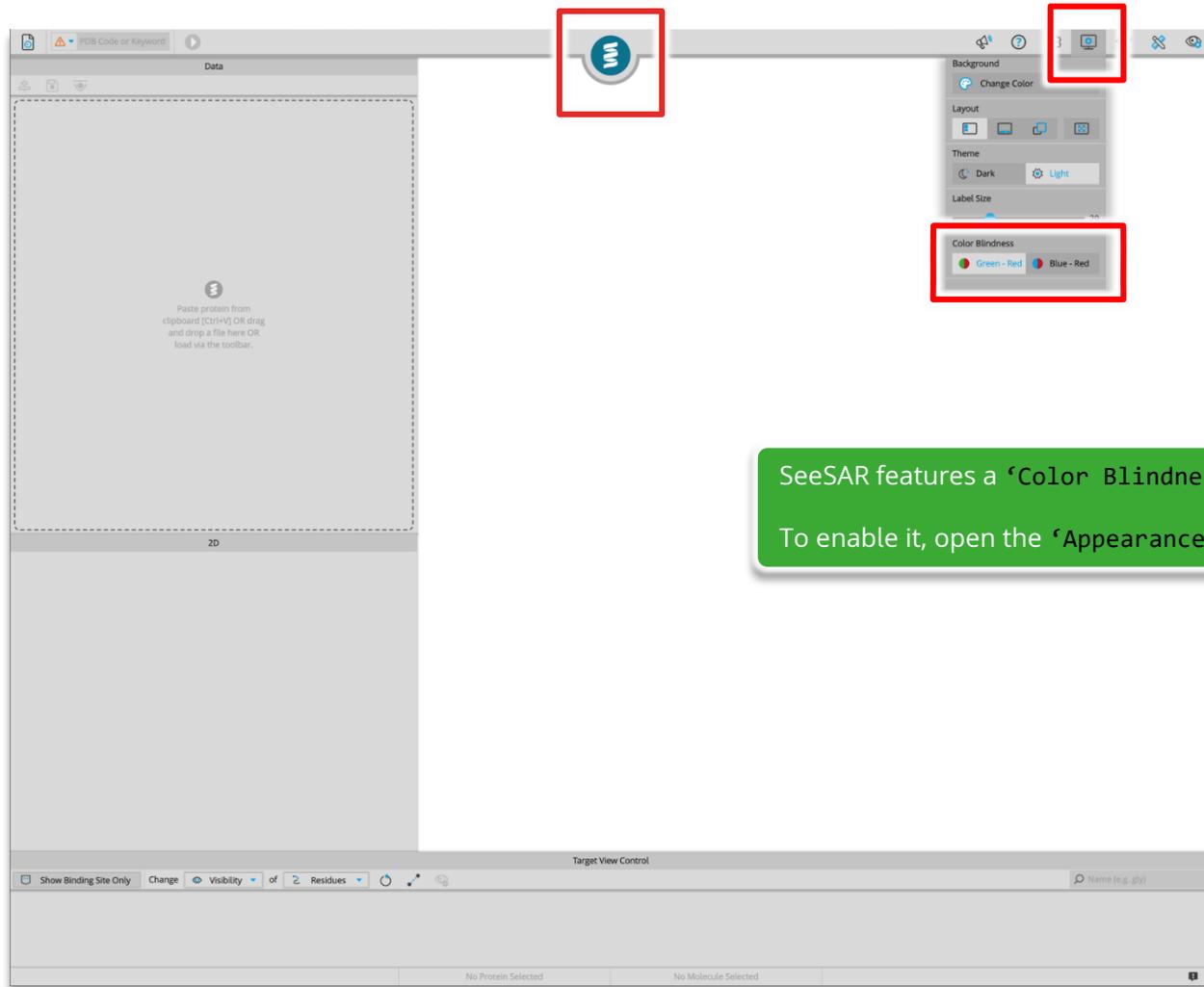
SeeSAR always works with one active binding site and one active ligand.

Before a ligand can be used for a specific task, it must be loaded into the appropriate **Mode**.

To load it, **right-click** the ligand and send it to the desired mode.

Table of Content

Mode Overview



SeeSAR features a 'Color Blindness' support.
To enable it, open the 'Appearance' menu.

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Mode Overview

Proteins

Filename
Z2FF

Ligand for Z2FF

Name	Estimated Affinity
53U_H_2001	1 nM

2D
53U_H_2001

C1CCN(C1)C(=O)N(Cc2ccccc2)C(=O)C(N)Cc3ccccc3

Target View Control

Show Binding Site Only Change Visibility of Residues

1	5	10	15	20	25	30																											
GLUE	ALAI	ASPI	CYST	GLYZ	LEUS	ARR4	PRCS	LEI6	PHF7	GLI9	LYS9	LYS10	SER11	LEU12	GLU13	ASP14	LYS14A	THR14B	GLU14C	ARG14D	GLU14E	LEU14F	LEU14G	GLU14H	SER14I	THR14J	LEU14K	LEU14L	VAL17	GLU18	GLY19	SER20	ASP

Z2FF 53U_H_2001

Lost your compound?
Zoomed out too far?

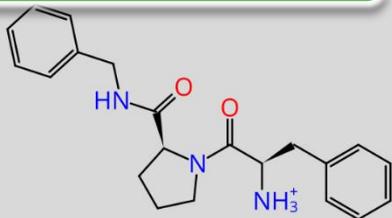
Press 'Space' key to center the view on the compound again.

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Mode Overview

Press 'L' to toggle labels on and off.

SeeSAR can label multiple molecules, helping you inspect individual atomic contributions to binding affinity, molecular torsions, and more.



Data

Proteins

Filename
1 Z2FF

Ligand for Z2FF

Name	Estimated Affinity			
	pM	nM	µM	mM
53U_H_2001				

N1, 53U_H_2001

Hyde: -2.5 kJ/mol

	Lig	Rec
Desolvation	10.4	9.5
Interaction	-12.1	-10.3

C3 - N2, 53U_H_2001

Torsion: 0°

Target View Control

Show Binding Site Only Change Visibility of 2 Residues

1 5 10 15 20 25 30

GLU1C ALA1B ASP1A CYS1 GLY2 LEU3 ARG4 PRO5 LEU6 PHE7 GLU8 LYS9 LYS10 SER11 LEU12 GLU13 ASP14 LYS14A THR14B GLU14C ARG14D GLU14E LEU14F LEU14G GLU14H SER14I THR14J LEU14K SER14L VAL14M VAL17 NGL19 GLY19 SER20 ASP

Z2FF 53U_H_2001

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Mode Overview

To save computational time and resources, you can choose which parameters are calculated when a molecule is added to one of SeeSAR's Modes.

Go to 'System' and select 'Calculation'.

The screenshot displays the SeeSAR software interface. On the left, a 'Data' panel shows a list of proteins and ligands. The main window shows a 3D molecular model of a protein (blue) with a ligand (green) bound to it. A 'System' menu is open, with the 'Calculation' option highlighted by a red box. Other options include Remote, Inspirator, License, Proxy, RCSB PDB, RCSB PDB, Readme, Systemlog, StarDrop, and YASARA. A tooltip for 'N1, 53U_H_2001' is visible, showing 'Hyde: -2.5 kJ/mol' and a table of 'Desolvation' and 'Interaction' values. Another tooltip for 'C3 - N2, 53U_H_2001' shows 'Torsion: 0°' and a bar chart. At the bottom, a 'Target View Control' panel shows a sequence of residues from 1 to 30, with '22FF' and '53U_H_2001' highlighted.

Parameter	Lig	Rec
Desolvation	10.4	9.5
Interaction	-12.1	-10.3

Torsion	Count
-180	1
-90	2
0	3
90	2
180	1

Table of Content

Mode Overview

In the table, select which parameters are to be calculated for the respective Modes.

The screenshot displays a molecular docking software interface. The main window shows a protein structure (blue) with a ligand (green) docked. A 'System' configuration window is open, showing a table of calculation parameters. The table is as follows:

Calculation	Mode 1	Mode 2	Mode 3	Mode 4
Load Molecules from File	✓	✓	✓	✗
Load Proteins	✓	✓	✓	✗
Save Editor Molecules to Table	✓	✓	✓	✗
Save Inspirator Molecules to Table	✓	✓	✓	✗
Generate Local Docking Poses	✓	✓	✓	✗
Generate Remote Docking Poses	✓	✓	✓	✗
Generate Similarity Scanner Poses	✓	✓	✓	✗

Other panels include a 'Data' panel with 'Proteins' and 'Ligand for Z2FF' sections, a 'Target View Control' at the bottom, and two data windows: 'N1, 53U_H_2001' showing 'Hyde: -2.5 kJ/mol' and 'C3 - N2, 53U_H_2001' showing 'Torsion: 0°' with a histogram.

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Mode Overview

To clean up your project, you can choose between two options:

- ◆ 'New' (Ctrl + N): Clears the entire project, removing all structures and ligands from all Modes.
- ◆ 'Clear [Mode]' (e.g., Clear Inspirator): Removes only the molecules listed in the table of the current Mode.

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Mode Overview

	1	5	10	15	20	25	30																											
2ZF	GLU1C	ALA1B	ASP1A	CYS1	GLY2	LEU3	ARG4	PRO5	LEU6	PHI7	GLU8	LYS9	LYS10	SER11	LEU12	GLU13	ASP14	LYS14C	THR14B	GLU14C	ARG14D	GLU14E	LEU14F	LEU14G	GLU14H	SER14	THR14	LEU14	LEU14	VAL17	GLU18	GLY19	SER20	ASP

The screenshot displays the SeeSAR software interface. On the left, a 'Data' panel shows a table of molecules. The main area features a 3D molecular model of a protein-ligand complex. At the bottom left, a 2D chemical structure is shown. A green callout box is overlaid on the 3D model.

Current Edit State (# 1)					
S3U_H_2001_3					
Molecule editing is paused. Click here to resume.					
Molecules (# 3)					
	Name	Estimated Affinity	LLE	Tor.	
		μM	mM	mM	
1	S3U_H_2001	---	---	---	---
2	S3U_H_2001_1	---	---	---	---
3	S3U_H_01_2	---	---	---	---

2D
S3U_H_2001_2

Target View Control

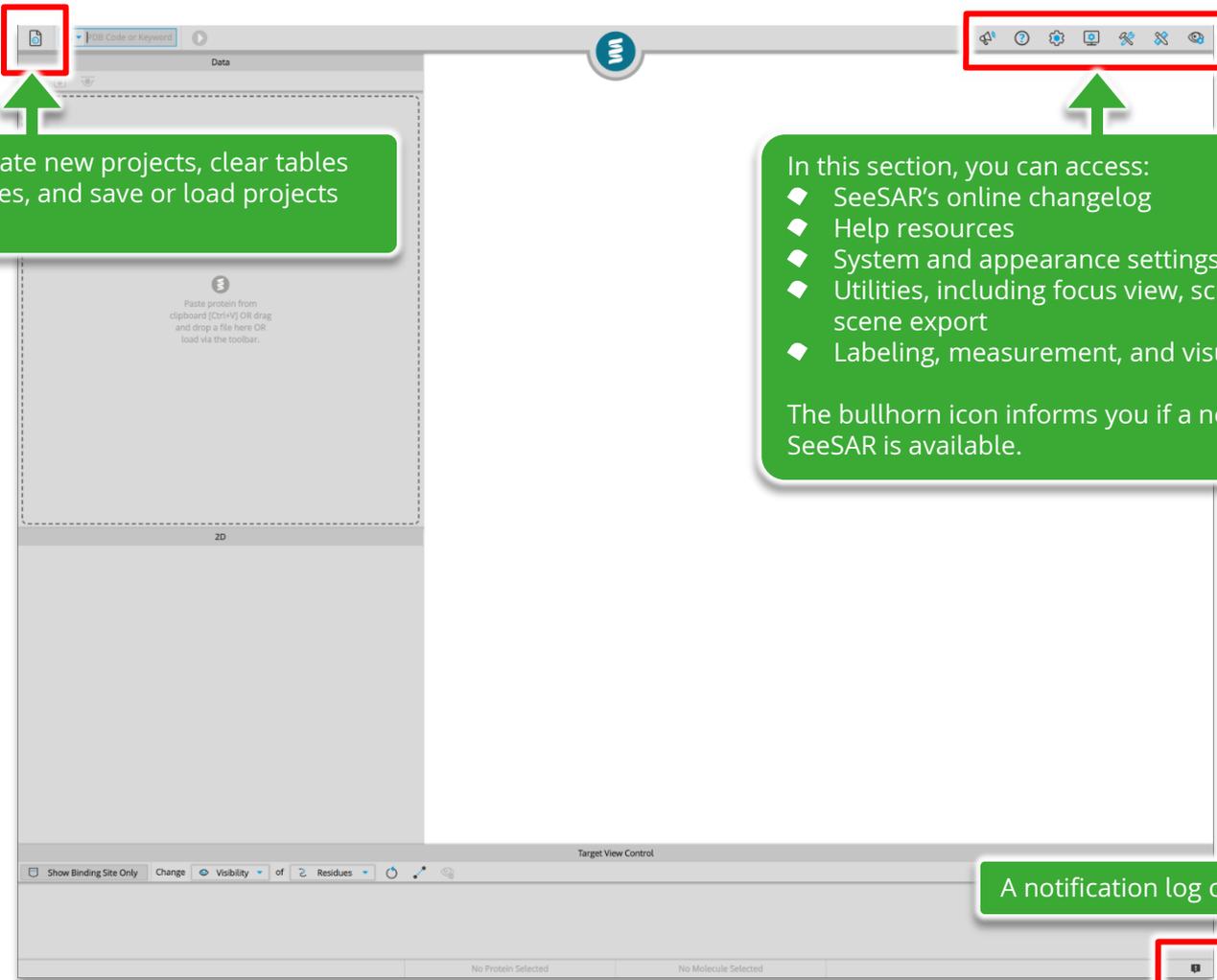
22FF S3U_H_2001_2

1. Basics

This section introduces the fundamental concepts and core functions of SeeSAR. It provides an overview of the interface, key controls, and essential principles that will help you understand how the software is organized and how to work with it effectively.

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Mode Overview



Here, you can create new projects, clear tables in individual Modes, and save or load projects and molecules.

In this section, you can access:

- ◆ SeeSAR's online changelog
- ◆ Help resources
- ◆ System and appearance settings
- ◆ Utilities, including focus view, screenshots, and 3D scene export
- ◆ Labeling, measurement, and visualization tools

The bullhorn icon informs you if a new version of SeeSAR is available.

A notification log can be found here.

Table of Content

Mode Overview

To download a structure directly from the RCSB PDB, enter a PDB code or protein name in the search box and press Enter.

For this exercise, we will use 2ZFF as example.

Note:
You can also load your protein from a file, via the file menu button.

2D

Target View Control

Show Binding Site Only Change Color of Chains Name (e.g. gly)

No Protein Selected No Molecule Selected 1 message

Table of Content

Mode Overview

1.

2.

How SeeSAR works

Once the protein is loaded, all molecules, buffers, cofactors, and other components are listed.

1. Select the ligand.
2. Press the 'Apply' button.

Note:
If you are not sure what name contains which molecule, click on the name and have a look at the 2D structure below.

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Mode Overview

ZZFF - Extract Your Ligand

Hetero Groups

	Name	Estimated Affinity
		pM nM μ M mM
1	Do not extract a ligand	
2	53U_H_2001	

Target View Control

Show Binding Site Only Change Visibility of Residues

1 5 10 15 20 25 30

all GLU1C ALA1B ASP1A CYS1 GLY2 LEU3 ARG4 PRO5 LEU6 PHE7 GLU8 LYS9 LYS10 SER11 LEU12 GLU13 ASP14 LYS16A THR16B GLU16C ARG16D GLU16E LEU16F LEU16G GLU16H SER16I THR16J SER16K SER16L VAL17 GLU18 GLY19 SER20 ASP21

ZZFF 53U_H_2001

A warning icon appears if the structure contains missing segments. These are visualized in 3D as yellow/black lines, or as red/black lines if they occur within a binding site.

Click on the ligand. Its structure will be presented in the 2D window.

How SeeSAR works

After ligand selection, all residues within a 6.5 Å radius around it are automatically selected and presented in the model.

The screenshot displays the SeeSAR software interface. At the top, a 'Proteins' panel shows 'ZZFF' selected. Below it, a 'Ligand for ZZFF' panel lists '53U_H_2001', which is highlighted with a red box. The main 3D view shows a blue ribbon protein structure with a ligand (53U_H_2001) bound in the center. A yellow and black dashed line indicates a missing segment. A green arrow points from the text box above to this segment. Another green arrow points from the text box below to the 2D chemical structure of the ligand. The 2D structure is a complex molecule with a benzamide group, a pyrrolidine ring, and a protonated amine group. At the bottom, a 'Target View Control' panel shows a sequence of residues from 1 to 30, with 'ZZFF' and '53U_H_2001' highlighted.

Table of Content

Mode Overview

Data

Proteins	
Filename	
ZZFF	

Ligand for ZZFF			
Name	Estimated At		
	pM	nM	μ M mM
S3U_H_2001			

3D viewer:

- ◆ Right-click to rotate.
- ◆ Mouse-wheel to zoom.
- ◆ Middle-click to shift.

Target View Control

Show Binding Site Only | Change | Visibility | of | Residues |

1 5 10 15 20 25 30

GLU1E ALA1B ASP1A CYS1 GLY2 LEU1B ARG14 PRO1 LEU16 PHE7 GLU18 LYS10 LYS10 SER11 LEU12 GLU13 ASP14 LYS14A THR14B GLU14C ARG14D GLU14E LEU14F LEU14G GLU14H SER14I THR14J SER14K SER14L VAL17 GLU18 GLY19 SER20

ZZFF | No Molecule Selected | 1 message

Tables:

- ◆ Collapse and re-open
- ◆ Drag rim to re-size
- ◆ Click entries to select

3D viewer:

- ◆ Right-click to rotate.
- ◆ Mouse-wheel to zoom.
- ◆ Middle-click to shift.

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Mode Overview

The screenshot displays the SeeSAR software interface. On the left, there are panels for 'Data' (listing proteins like ZZFF) and 'Ligand for ZZFF' (listing ligands like 53U_H_2001). The central area shows a 3D ribbon representation of a protein structure in blue, with a red ligand molecule bound to it. On the right, a 'Change Color' settings menu is open, highlighted with a red box. This menu includes options for 'Layout', 'Theme' (Dark/Light), 'Label Size' (a slider), and 'Color Blindness' (Green-Red/Blue-Red). At the bottom, there is a 'Target View Control' panel with a sequence viewer showing residues from 1 to 30.

Change the table layout

Adjust label size

Adjust background color

Switch between dark and light theme

Switch to color blindness mode

If you want to customize the layout of SeeSAR, click on the 'Appearance' button in the top right toolbar.

For this guide will use the light one, but feel free to use whatever you prefer!

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Mode Overview

The screenshot displays a software interface for molecular docking. On the left, a 'Data' panel shows a table of proteins and a table of ligands. The protein table has columns for 'Proteins' and 'Filename', with one entry '1' and 'ZZFF'. The ligand table has columns for 'Ligand for ZZFF', 'Name', and 'Estimated Affinity' (with sub-columns for pM, nM, μM, mM), with one entry '53U_H_2001'. The main window shows a 3D ribbon representation of a protein structure in blue, with a red stick model of a ligand bound to it. A yellow and black striped warning sign is positioned near the ligand. At the top right of the window, a circular button with '100' inside is highlighted by a red square. At the bottom, a 'Target View Control' panel shows a sequence of residues from 1 to 30, with 'ZZFF' selected at position 1. The status bar at the bottom indicates 'ZZFF' and 'No Molecule Selected'.

Proteins	Filename
1	ZZFF

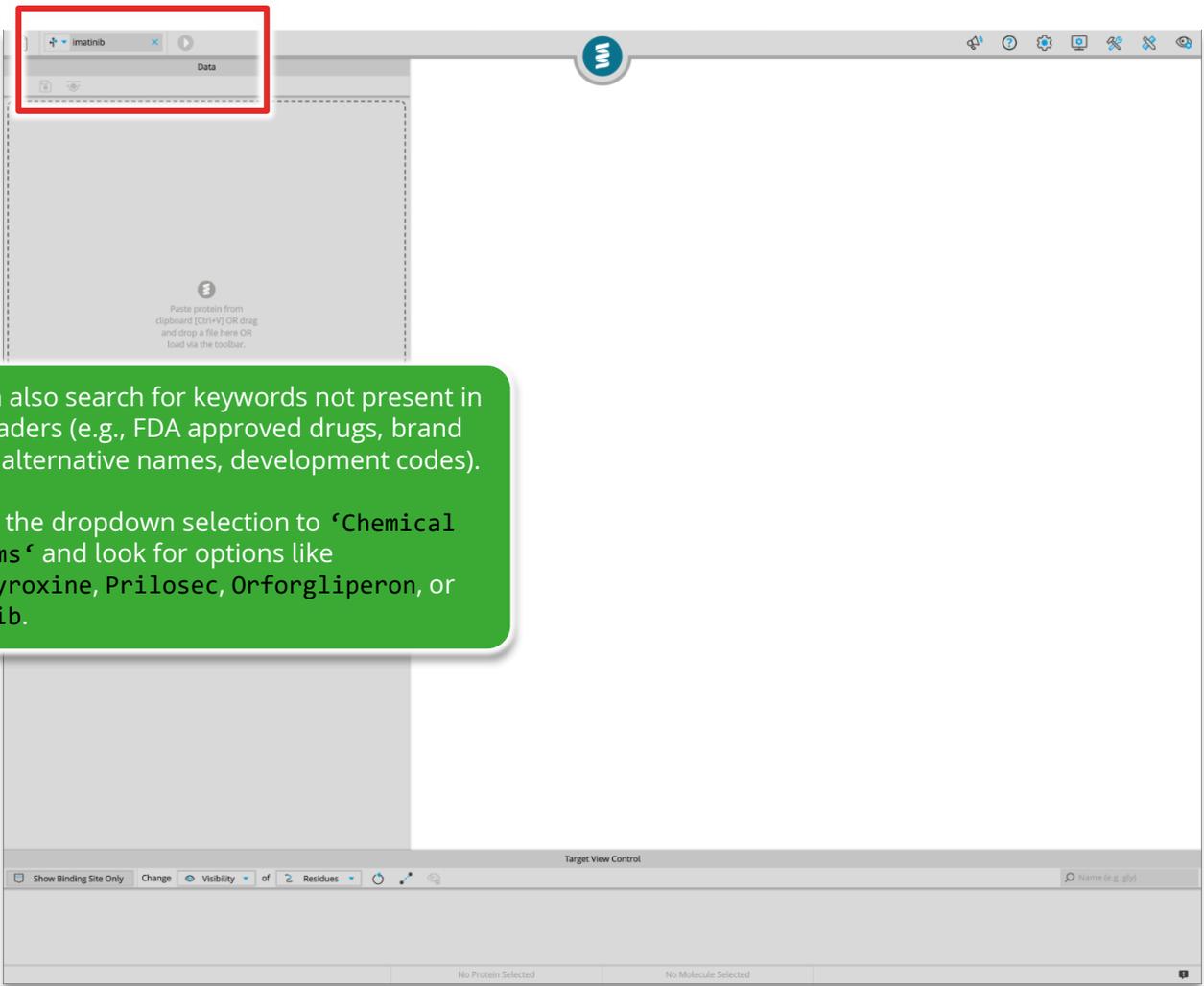
Ligand for ZZFF	Name	Estimated Affinity
		pM nM μM mM
<input type="checkbox"/>	53U_H_2001	

Note: You are currently in **Proteins Mode**.

The 'Mode Switch' button shows your active mode and lets you change it. Hover over it to see available options.

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Mode Overview

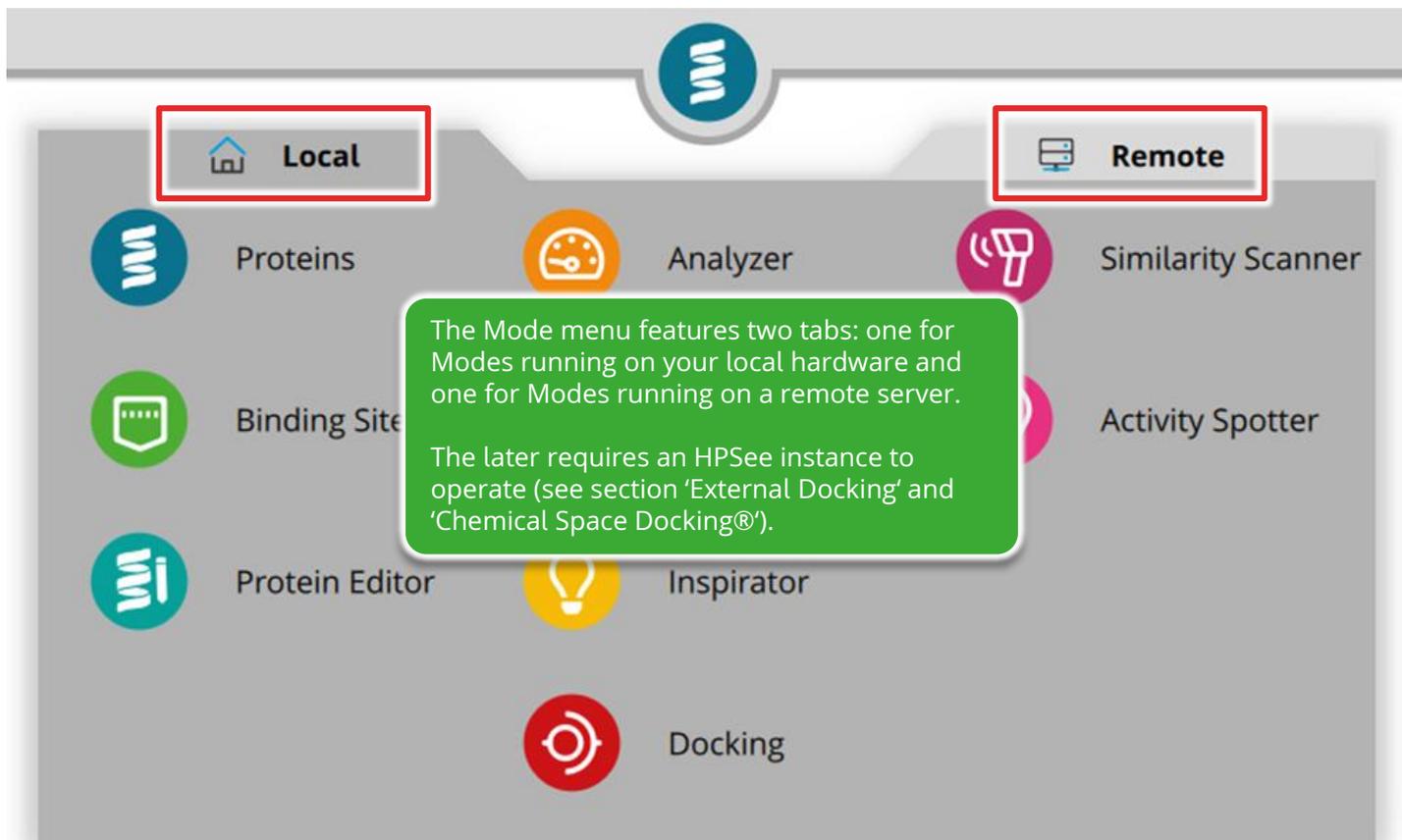


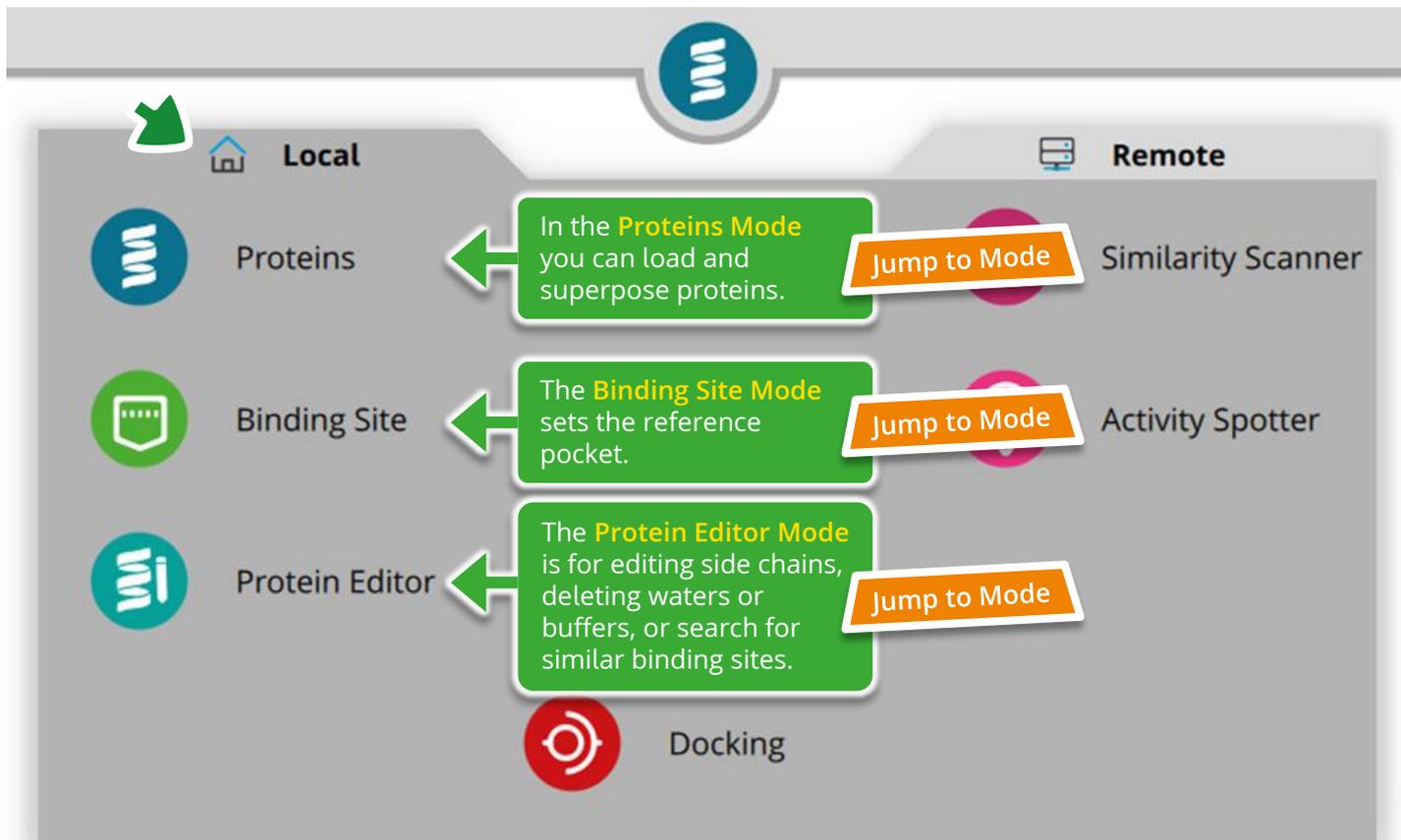
You can also search for keywords not present in PDB headers (e.g., FDA approved drugs, brand names, alternative names, development codes).

Change the dropdown selection to 'Chemical Synonyms' and look for options like Levothyroxine, Prilosec, Orforglipron, or Imatinib.

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Mode Overview







 **Local**

 **Remote**

Jump to Mode

The **Analyzer Mode** is for filtering molecule sets, grouping poses, and more.



Analyzer



Similarity Scanner

Jump to Mode

The **Molecule Editor Mode** is for designing new molecules in 3D.



Molecule Editor



Activity Spotter



Protein Editor



Inspirator

The **Inspirator Mode** helps you to generate new compound ideas.

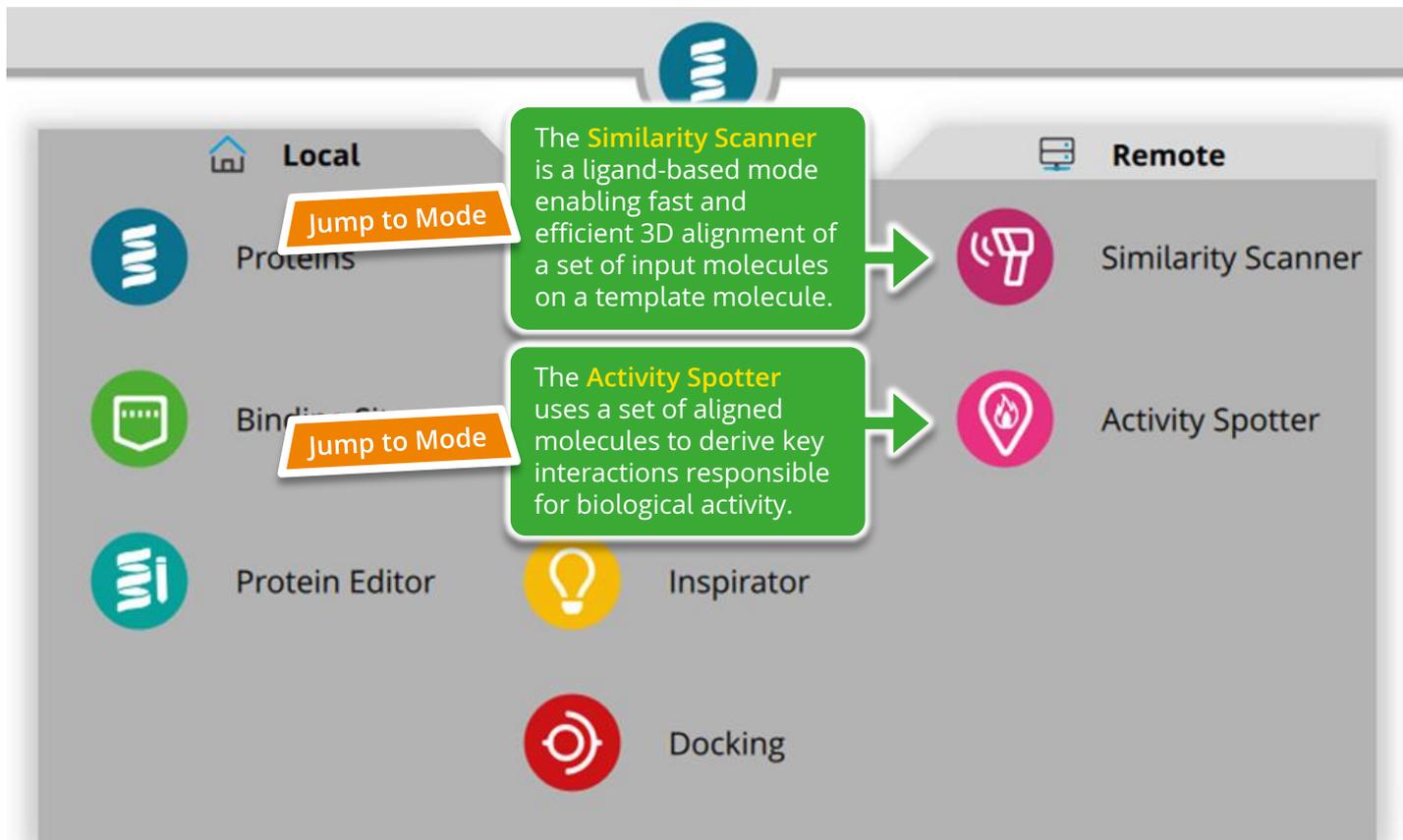
Jump to Mode

Jump to Mode

In the **Local Docking Mode**, you can generate ligand poses through molecular docking.



Docking





 **Local**

 **Remote**

Jump to Mode

The **Remote Docking Mode** initiates the docking calculation on the external server.



Docking

Jump to Mode

The **Space Docking® Mode** performs virtual screening with ultra-large Chemical Spaces.



Space Docking®

Important note:
All remote Modes require a connection to HPSee.

The screenshot displays a molecular docking software interface. On the left, a 'Data' panel shows a list of proteins with 'Z2FF' selected. Below it, the 'Ligand for Z2FF' section lists '53U_H_2001' with an estimated affinity of 1 nM. At the bottom left, a 2D chemical structure of the ligand is shown, featuring a benzamide group, a pyrrolidine ring, and a benzylammonium group. The main 3D view shows the protein structure in blue ribbons and the ligand in stick representation, with a yellow dashed line indicating a specific interaction. A green callout box points to the 3D view with the text: 'As the 3D view can easily get busy, let's customize the visualization in the 'Target View Control' window.' At the bottom, a 'Target View Control' panel is highlighted with a red border, showing a sequence viewer for the protein 53U_H_2001 with residues 1 through 30 displayed. The panel includes controls for 'Show Binding Site Only', 'Change', 'Visibility', and 'Residues'.

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Mode Overview

Choose one of the options to display

Show Whole Protein OR Show Binding Site Only

Change Visibility of Residues

- Targets
- Residues
- Molecules
- Metals
- Waters
- Chains
- Surfaces

Reset user settings

Show only interacting components

all — ZZFF

1 5

GLU1C ALA1B ASP1A CYS1 GLY2 LEU3 ARG4 PRO5

Identify the components that are most similar or different from each other, when multiple structures are loaded.

similar — 0.0 Å — different

The view controls let you toggle on/off. All buttons are clickable, so that you can hide all parts of one protein in one click

Example:
 To visualize surface, select Change 'Visibility' of 'Surfaces' and toggle on the PDB code. To adjust this surface visibility, set Change 'Color' of 'Surfaces' and right-click on PDB code to explore the options.

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Mode Overview

The screenshot displays the BioSolveIT software interface. On the left, the 'Data' panel shows a list of proteins with 'Z2FF' selected. Below it, the 'Ligand for Z2FF' section lists '53U_H_2001'. A red box highlights the 'Add Molecule to' button, which has a dropdown menu open showing 'Binding Site Mode' as the selected option. Other options in the menu include 'Molecule Editor', 'Inspirator', 'Local Docking Mode', 'Remote Docking Mode', 'Similarity Scanner', and 'Activity Spotter'. Below the menu is a 2D chemical structure of the ligand, 53U_H_2001. The main window shows a 3D ribbon representation of the protein structure in blue, with the ligand docked in the binding site. A yellow and black striped warning sign is positioned near the ligand. At the bottom, the 'Target View Control' panel shows a sequence viewer with residue numbers 1 to 30 and a search bar.

If you want to add or remove individual amino acids after the automatic selection of residues for the binding site, right click your ligand and add it to **Binding Site Mode**.

Table of Content

Mode Overview

2ZFF - Define Your Binding Site

30 residues are currently selected for the binding site.
You can modify the binding site selection, or **confirm with the green button above.**

Molecules	
Name	# Residues
53U_H_2001	30

Unoccupied Pockets				
Pocket ID	# Residues	DoGSiteScore	# Donors	# Acceptors

2D

Target View Control

Show Binding Site Only Change Visibility of Residues

1 5 10 15 20 25 30

2ZFF GLU1E ALA1B ASP1A CYS1 GLY2 LEU3 ARG4 PRO5 LEU6 PHE7 GLU8 LYS9 LYS10 SER11 LEU12 GLU13 ASP14 LYS14A THR14B GLU14C ARG14D GLU14E LEU14F LEU14G GLU14H SER14I THR14J SER14K SER14L VAL17 LEU18 GLY19 SER20 ASP21

2ZFF No Molecule Selected 1 message

You are now in the **Binding Site Mode**.
Residues already included in the binding site are highlighted in pink.

Table of Content

Mode Overview

The screenshot displays the BioSolveIT software interface. On the left, a data panel titled "Data" contains a section "2ZFF - Define Your Binding Site" with a yellow border. Below this is a table for "Molecules" and a section for "Unoccupied Pockets". The main area shows a 3D ribbon representation of a protein structure in blue, with a yellow and black striped hazard sign pointing to a specific region. A green callout box on the right contains the text: "Use this section to search for druggable binding pockets." The bottom of the interface features a "Target View Control" bar with a sequence viewer showing residues from 1 to 30, including 2ZFF and various amino acids like GLU1E, ALA1B, ASP1A, etc.

2ZFF - Define Your Binding Site

30 residues are currently selected for the binding site.
You can modify the binding site selection, or **confirm with the green button above.**

Name	# Residues
53U_H_2001	30

Pocket ID	# Residues	DoGSiteScore	# Donors	# Acceptors	Hydrophobic
-----------	------------	--------------	----------	-------------	-------------

Target View Control

Show Binding Site Only Change Visibility of Residues

1 5 10 15 20 25 30

2ZFF GLU1E ALA1B ASP1A CYS1 GLY2 LEU3 ARG4 PRO5 LEU6 PHE7 GLU8 LYS9 LYS10 SER11 LEU12 GLU13 ASP14 LYS14A THR14B GLU14C ARG14D GLU14E LEU14F LEU14G LEU14H SER14I THR14J SER14K SER14L VAL17 LEU18 GLY19 SER20 ASP21

2ZFF No Molecule Selected 1 message

Table of Content

Mode Overview

2ZFF - Binding Site is Defined
The binding site contains 30 residues and is ready to use in all other modes.

Molecules

Name	# Residues
53U_H_2001	30

Unoccupied Pockets

Pocket ID	# Residues	DoGSiteScore	# Donors	# Acceptors	Hydrophobic
1	56	0.53	39	45	
2	19	0.28	11	8	
3	16	0.20	7	10	
4	12	0.12	7	10	

Target View Control

1 5 10 15 20 25 30

GLU1E ALA1B ASP1A CYS1 GLY2 LEU3 ARG4 PRO5 LEU6 PHE7 GLY8 LYS14A THR14B GLU14C ARG14D GLU14E LEU14F LEU14G GLU14H SER14I THR14J SER14K SER14L VAL17 GLU18 GLY19 SER20 ASP

0 Molecule Selected 1 message

Unoccupied pockets are listed and presented with their respective color in 3D.

You can select desired binding pockets by clicking on the colored pockets on 3D or right-click on the table entry.

To add residues: in 3D, use 'Ctrl+left-click' to select. In the sequence view, right-click on a residue to access the option.

Finally, confirm your selection by clicking on the top green play button.

Table of Content

Mode Overview

To adjust the view, click on 'Show Binding Site Only'. Make sure to set the selection at Change to 'Visibility' of 'Residues'.

Now toggle your cursor and click on the PDB code below.

Go back to the **Proteins Mode** to inspect the binding mode of the ligand inside the binding site.

Target View Control

Show Whole Protein Change Visibility of Residues

2ZF

Table of Content

Mode Overview

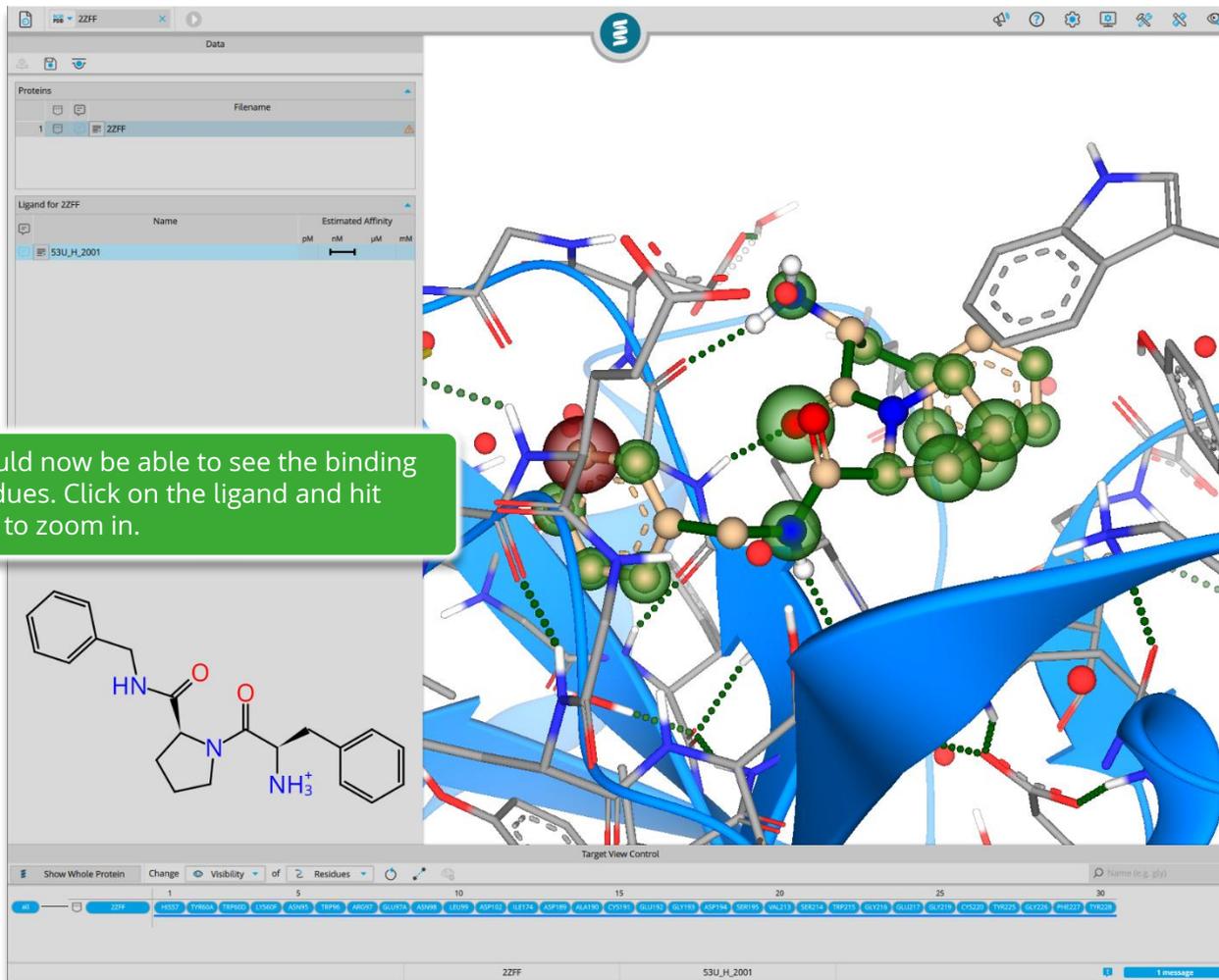


Table of Content

Mode Overview

Click on the 'Visualization' menu. Make sure the 'HYDE Coloring' is selected. Additionally, hydrogen bonds (H-bonds), Torsion Coloring, Molecular Clashes can also be kept on.

Unresolved segments display parts of the structure where no 3D information is available.

Table of Content

Mode Overview

Target View Control

1 5 10 15 20 25 30

22FF 53U_H_2001

Colored spheres represent each atom's contribution to the estimated binding affinity.

- ◆ Red indicates an unfavorable contribution
- ◆ Green indicates a favorable contribution
- ◆ Larger spheres represent stronger effects
- ◆ No sphere means the atom is not expected to significantly affect binding affinity

To learn more about a specific HYDE sphere, enable the label function and click on an atom.

Note:
You can use the shortcut key 'L+left-click' to label your atoms.

Target View Control

N3, 53U_H_2001		Lig	Rec
Hyde: -3.6 kJ/mol			
Desolvation	6.8	8.4	
Interaction	-8.4	-10.4	

1 2ZFF

Proteins

Filename
2ZFF

Ligand for 2ZFF

Name	Estimated Affinity

Show Label

Measure Atom Distance

Measure Angle

Measure Torsion

Clear All Labels

Show Whole Protein

Change Visibility of Residues

1 2ZFF 4557 TYR66A TRP60D LYS60P ASN65 TRP6A ARG67 GLU74 ASN8 LEU91 ASP103 LEU74 ASP109 ALA130 CYS131 GLU132 GLY133 ASP134 SER135 VAL137 SER138 TRP139 GLY139 GLU137 GLY139 CYS220 TRG225 GLY228 PHE227 TRG228

2ZFF 53U_H_2001

1 message

Table of Content

Mode Overview

The screenshot displays a molecular docking software interface. The main window shows a 3D model of a protein (blue ribbon) with a ligand (green and red spheres) docked in its binding pocket. A red box highlights a menu with the following options: Show Label, Measure Atom Distance, Measure Angle, Measure Torsion, and Clear All Labels. On the left, a 'Data' panel shows 'Proteins' with 'ZZFF' and 'Ligand for ZZFF' with '53U_H_2001'. Below the protein view, a chemical structure of the ligand is shown with the label '53U_H_2001'. At the bottom, a 'Target View Control' panel shows a sequence of residues from 1 to 30, with 'ZZFF' and '53U_H_2001' highlighted.

Check-out the other analysis options!

Table of Content

Mode Overview

The screenshot displays the Molecule Editor software interface. The main window shows a 3D molecular model of a protein (blue ribbon) with a ligand (green and red spheres) docked in its binding site. The sidebar on the left contains a 'Data' panel with a 'Proteins' list and a 'Ligand for Z2FF' section. The 'Ligand for Z2FF' section lists the molecule '53U_H_2001' and provides options for adding it to different modes. The 'Molecule Editor' mode is highlighted with a red box. Below the sidebar, a 2D chemical structure of the ligand is shown. At the bottom, a 'Target View Control' panel displays a sequence of residues from 1 to 30, with the current residue '22FF' highlighted.

Table of Contents

Mode Overview

‘Add Molecule to’ → ‘Molecule Editor’ is accessible with a right-click on the table entry.

This copies the molecule into the mode and automatically switches to that Mode.

The editor-menu will appear on the top left.
There you can:

Add atoms
or rings

Change
charge

Adjust
torsion

Remove
atoms

Store the new molecule to the table
after a template-based docking



Create a new
molecule

Change atom
type

Change bond
type

Undo/redo

Store the current
molecule to the table

To edit a molecule ALWAYS:

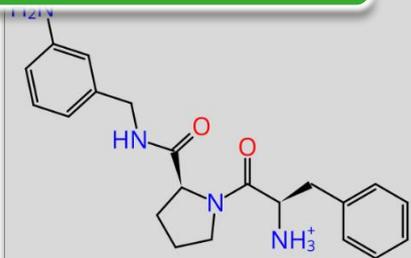
1. **Select** (atoms or bonds)
2. **Modify** (using the function of choice from above)

Note that many editor functions have shortcut-keys. E.g. select a bond and type '1', '2' or, '3' on the keyboard, or select an atom and type the element ('C', 'N', 'O', ...).

Table of Content

Mode Overview

1. As an exercise, we add an amino group to the ring by selecting the hydrogen in *meta* position and changing its element type to nitrogen with 'N'.



A screenshot of the software interface showing a control panel at the bottom. A red box highlights the 'Chains' visibility control, which includes a dropdown menu and a 'Change' button. The 'Chains' dropdown is currently set to 'All'.

Additionally toggle off visibility of chains to avoid clutter.

2.

2. Click this button to save the edited molecule.

The image shows a 3D ball-and-stick model of a protein-ligand complex. A red dashed box highlights a specific atom in the ligand, with a red arrow pointing to it. A green box with the number '2' and the text 'Click this button to save the edited molecule.' points to a green circular button with a white 'S' icon in the top toolbar of the software interface.

Table of Content

Mode Overview

The screenshot shows a molecular docking software interface. At the top, a 'Data' panel displays the 'Current Edit State (# 1)' as 'S3U_H_2001_4'. Below this is a 'Molecules (# 2)' table with two entries. The second entry is highlighted with a green background. The main window shows a 3D ball-and-stick model of a protein-ligand complex. A callout box on the right provides instructions on how to add new entries to the table.

	Name	Estimated Affinity			LLE	Tor.
		pM	nM	µM		
1	S3U_H_2001					
2	S3U_H_2001_3					

Note:
During editing, all hydrogen atoms are visible, but no estimated affinity or HYDE spheres are shown.

To view these:

1. Add the edited ligand to the table using the **green button**.
2. Then select the new entry in the table.

New entries are added to the 'Molecules' table.

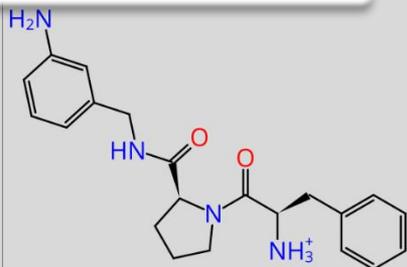


Table of Content

Mode Overview

The screenshot displays a molecular docking software interface. On the left, a 'Data' panel shows the 'Current Edit State (# 1)' as 'S3U_H_2001_4'. Below it, a 'Molecules (# 2)' table lists two molecules, both named 'S3U_H_200'. A red box highlights the 'Estimated Affinity' section, which includes columns for 'pM', 'nM', 'uM', and 'mM', and a 'Tor.' column. The main window shows a 3D ball-and-stick model of a protein-ligand complex. At the bottom left, a 2D chemical structure of the ligand is shown, featuring a benzamide group, a pyrrolidine ring, and a benzylammonium group. The interface also includes a 'Target View Control' bar at the bottom with 'Show Binding Site Only' and 'Change Visibility' options.

If the respective calculation setting is turned on, the affinity of your created compound will be displayed.

Table of Content

Mode Overview

The screenshot displays a molecular docking software interface. A red box highlights a notification bar at the top left that reads: "Current Edit State (# 1) 53U_H_2001_2" and "Molecule editing is paused. Click here to resume." Below this is a table with columns for Name, Estimated Affinity (pM, nM, μM, mM), LLE, and Tor. The table lists two entries: 1. 53U_H_2001 and 2. 53U_H_01_1. The main view shows a 3D molecular model of a protein-ligand complex. A 2D chemical structure of the ligand is shown in the bottom left corner. The interface includes various toolbars and a "Target View Control" section at the bottom.

Name	Estimated Affinity	LLE	Tor			
	pM	nM	μM	mM		
1						
2						

Once you browse through your created molecules, the editing process stops.

To resume from your last edit, click on the highlighted button.

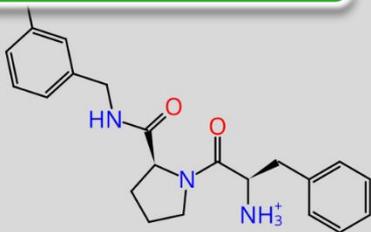


Table of Content

Mode Overview

The screenshot displays a molecular docking software interface. On the left, a 'Data' panel shows a table of molecules and their estimated affinity. A red box highlights the 'Estimated Affinity' section of the table. The main window shows a 3D ball-and-stick model of a protein-ligand complex, with a red dashed box highlighting a specific region of the ligand. At the bottom left, a 2D chemical structure of the ligand is shown, featuring a benzamide core with a hydroxyl group and a primary amine group.

Molecules (# 3)		Estimated Affinity				Tor.
	Name	pM	nM	µM	mM	
1	S3U_H_200					
2	S3U_H_200					
3	S3U_...					

Now let's add a hydroxy group to the other previous *meta* position. Again, storing this in the table, we see another change in affinity estimate.

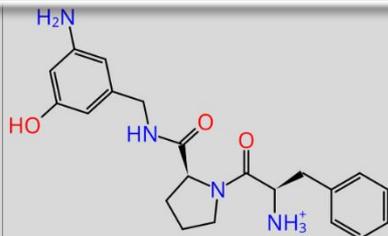


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Mode Overview

The screenshot displays a molecular docking software interface. On the left, a 'Data' panel shows a table of molecules and their estimated affinities. The main window shows a 3D molecular model of a protein-ligand complex. A green callout box provides instructions on how to use the 'Inspirator Mode'.

Current Edit State (# 1)					
S3U_H_2001_3					
Molecule editing is paused. Click here to resume.					
Molecules (# 3)					
	Name	Estimated Affinity	LLE	Tor.	
		pM	µM	mM	
1	S3U_H_2001				●
2	S3U_H_2001_1				●
3	S3U_01_2				●

Jump to Mode

HO

NH₃⁺

Target View Control

Show Binding Site Only Change Visibility of Chains

all 22FF Chains Chains Chains

22FF S3U_H_2001_2

If you are running out of ideas: try the **Inspirator Mode**.

To get your molecule there, select it with the checkbox at the front of every row and add it to the **Inspirator Mode**.

It will help you to replace parts of the molecule, further grow the molecule or merge molecules.

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Mode Overview

2. Visualization

This section introduces the visualization options available in SeeSAR and shows how to control the display of targets, ligands, surfaces, and other structural elements. Understanding these settings will help you tailor the view to your needs and interpret molecular interactions more clearly.

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Mode Overview

The screenshot displays the SeeSAR software interface. On the left, a 'Data' panel shows a table of proteins with columns for 'Filename' and 'Ligand for ZZFF'. The main window shows a 3D protein structure with a binding site highlighted in green and a yellow stick model of a ligand. A 'Target View Control' panel at the bottom contains a 'Show Binding Site Only' checkbox, a 'Change' button, a 'Visibility' dropdown menu, and a 'Surfaces' dropdown menu. A red box highlights the 'Show Binding Site Only' checkbox and the 'Change' button. Below the 'Change' button, a 'ZZFF' label is visible. The status bar at the bottom shows 'ZZFF' and 'No Molecule Selected'.

SeeSAR offers a wide range of options for controlling the target display. The key element here is the 'Target View Control'.

- ◆ 'Change' defines what you want to modify: 'Visibility' or 'Color'.
- ◆ In addition, the display always refers to one of the following options: 'Targets', 'Residues', 'Molecules', 'Metals', 'Waters', 'Chains', 'Surfaces'.
- ◆ 'Show Binding Site Only' is the switch for enabling the option to visualize only the binding site. Accordingly, all actions currently affect the entire structure.
- ◆ 'Show Whole Protein' is available as a button when we are currently working only with the binding site.

Table of Content

Mode Overview

The screenshot displays a molecular modeling software interface. On the left, the 'Data' panel shows a list of proteins with 'ZZFF' selected. Below it, the 'Ligand for ZZFF' section lists '53U_H_2001' with an estimated affinity range from pM to mM. The main window shows a 3D model of a protein structure with a white surface and a pink outline. At the bottom, the 'Target View Control' panel has a 'Visibility' dropdown set to 'Surfaces' and a 'ZZFF' button highlighted with a red box and arrow.

To display the surface of the target structure, go to 'Target View Control' and set 'Visibility' → 'Surfaces'. Click on the target button to show the surface.

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Mode Overview

The screenshot displays a molecular docking software interface. On the left, there are panels for 'Data', 'Proteins', and 'Ligand for ZZFF'. The 'Proteins' panel shows a table with one entry: 'ZZFF'. The 'Ligand for ZZFF' panel shows a table with one entry: '53U_H_2001'. The main window shows a 3D surface representation of a protein (ZZFF) with a binding site highlighted in green. A green callout box with a white border contains the text: 'Show Binding Site Only' will limit the surface display only to the defined binding site. At the bottom of the interface, there is a 'Target View Control' panel with a 'Show Binding Site Only' checkbox, which is highlighted with a red box. Other controls include 'Visibility', 'Surfaces', and a search field for 'Name (e.g. gly)'. The status bar at the bottom shows 'ZZFF' and 'No Molecule Selected'.

Proteins	Filename
1	ZZFF

Ligand for ZZFF	
Name	Estimated Affinity
53U_H_2001	pM nM μ M mM

Target View Control

ZZFF No Molecule Selected

'Show Binding Site Only' will limit the surface display only to the defined binding site.

Table of Content

Mode Overview

Data

Proteins	
Filename	
Z2FF	

Ligand for Z2FF		
Name	Estimated Affinity	
53U_H_2001		pM nM μ M mM

2D
53U_H_2001

C1CCN(C1)C(=O)N(Cc2ccccc2)C(=O)N(Cc3ccccc3)N

Target View Control

Show Whole Protein

22FF 53U_H_2001

You can switch back to the full protein display with the 'Show Whole Protein' button.

Table of Content

Mode Overview

The screenshot shows a molecular visualization software interface. On the left, there are panels for 'Data', 'Proteins', and 'Ligand for Z2FF'. The 'Proteins' panel lists a protein with ID '1' and filename 'Z2FF'. The 'Ligand for Z2FF' panel shows a ligand '53U_H_2001' with an estimated affinity range from pM to mM. The main window displays a 3D model of a protein structure with a blue ribbon and a semi-transparent grey surface. A context menu is open over the surface, with 'Toggle Transparency' highlighted in blue. A red box and arrow point to this option. Another red arrow points to the 'Z2FF' label in the 'Target View Control' panel at the bottom. A green callout box contains the following text:

To create transparent surfaces, set 'Color' → 'Surfaces'.
Right-click on the target and select 'Toggle Transparency'.

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Mode Overview

The screenshot displays a molecular visualization software interface. On the left, a 'Data' panel shows a table of proteins with columns for 'Proteins' and 'Filename'. Below it, a 'Ligand for Z2FF' panel lists a ligand '53U_H_2001' with an 'Estimated Affinity' column. The main window shows a 3D visualization of a protein-ligand complex. The protein surface is colored by chain, with one chain in red and others in blue and green. A context menu is open over the protein, with 'Set Chain Coloring' highlighted and a red arrow pointing to it. The interface also includes a '2D' panel at the bottom with various coloring options and a 'Target View Control' panel.

Proteins	Filename
1	Z2FF

Ligand for Z2FF	Name	Estimated Affinity
	53U_H_2001	pM nM μM mM

- 1- Set Standard Coloring
- 2- Set LogP-Based Coloring
- 3- Set Element Coloring
- 4- Set Chain Coloring
- 5- Set Residue Coloring
- 6- Toggle Transparency
- 7- Change Protein Surface Color
- 8- Change Binding Site Surface Color
- 9- Focus View on This Component

In the same menu it is also possible to color the surface in different styles. Here, the visualization based on the chain colors is presented.

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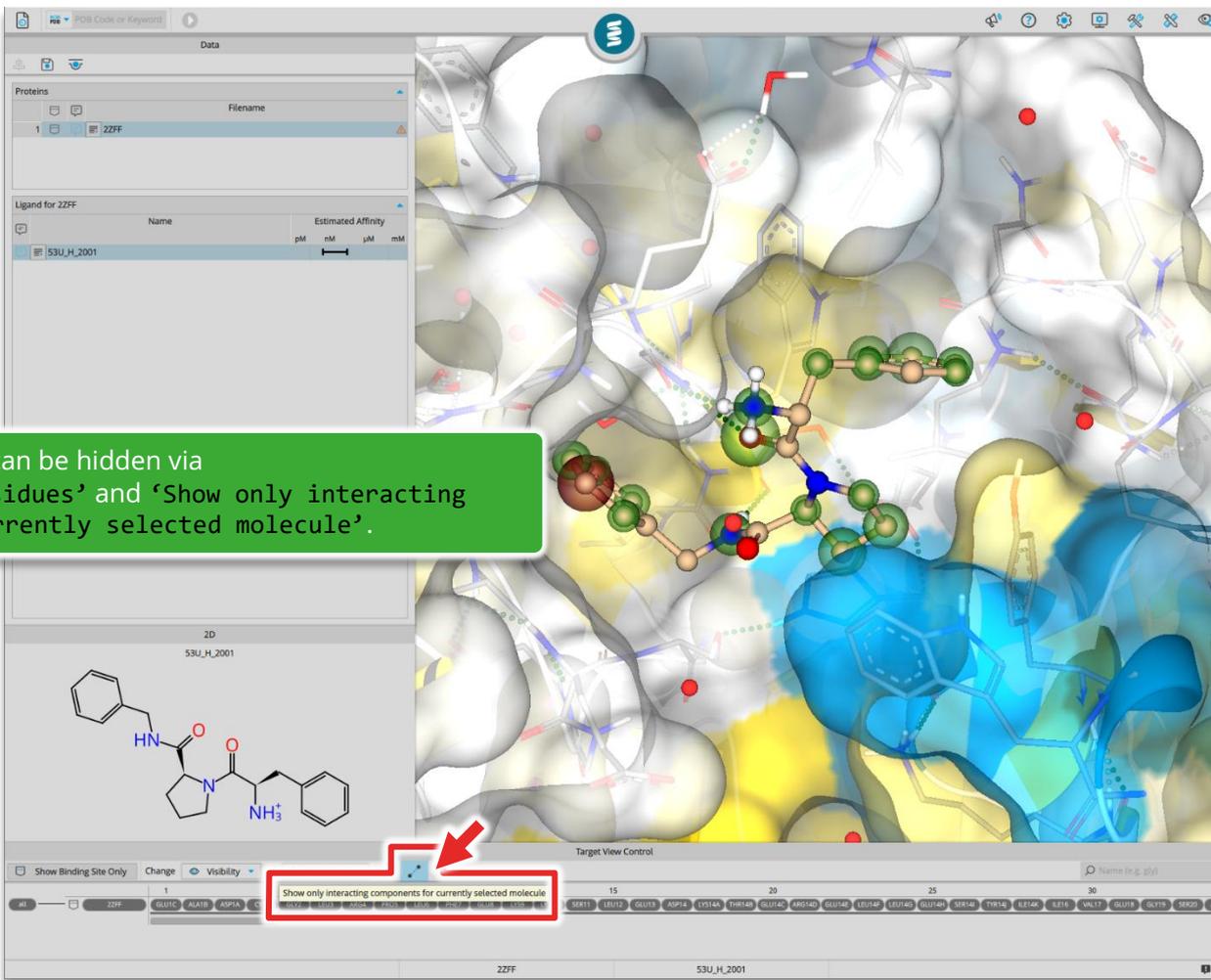
Mode Overview

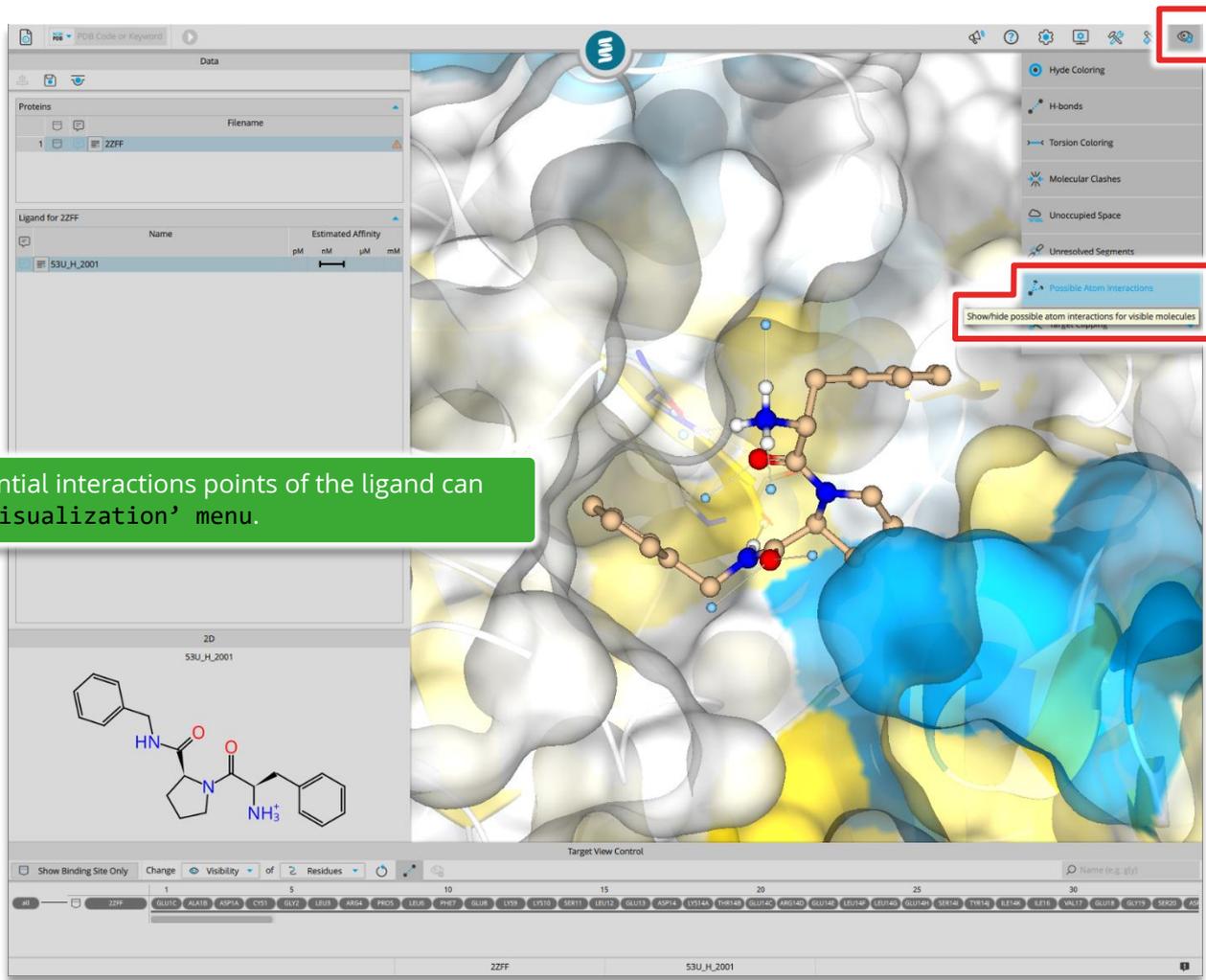
The screenshot displays a molecular visualization software interface. On the left, a 'Data' panel shows a table of proteins with columns for 'Proteins' and 'Filename'. Below it, a 'Ligand for Z2FF' panel shows a table with columns for 'Name' and 'Estimated Affinity'. The main window shows a 3D surface representation of a protein structure, colored by chain (white, yellow, and blue). A red arrow points to the 'Set Secondary Structure Coloring' option in the 'Target View Control' panel. The interface also includes a '2D' panel and a 'Show Binding Site' panel.

If the surface coloring is set to the chain colors, it will automatically reflect any changes you make. Select 'Color' → 'Chains' and right-click on the target to select 'Set Secondary Structure Coloring'. The surface will now adapt to the colors of the chains.

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Mode Overview





Complete parts of the target can be hidden with the 'Target Clipping' option. Extended options for visual refinement can be accessed by a click.

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Mode Overview

Target View Control

1	5	10	15	20	25	30
GLUE	ALAT	ASPA	CYST	GLY	LEU	ARG
PRO	LEU	PRO	GLU	LYS	LYS	SER
LEU	GLU	ASP	LYS	THR	GLU	ARG
GLU	LEU	SER	THR	SER	THR	LEU
SER	THR	LEU	SER	THR	LEU	SER
THR	LEU	SER	THR	LEU	SER	THR
THR	LEU	SER	THR	LEU	SER	THR
THR	LEU	SER	THR	LEU	SER	THR
THR	LEU	SER	THR	LEU	SER	THR

2D
53U_H_2001

C1CCN(C1)C(=O)Nc2ccccc2C(=O)N[C+]c3ccccc3

Target View Control

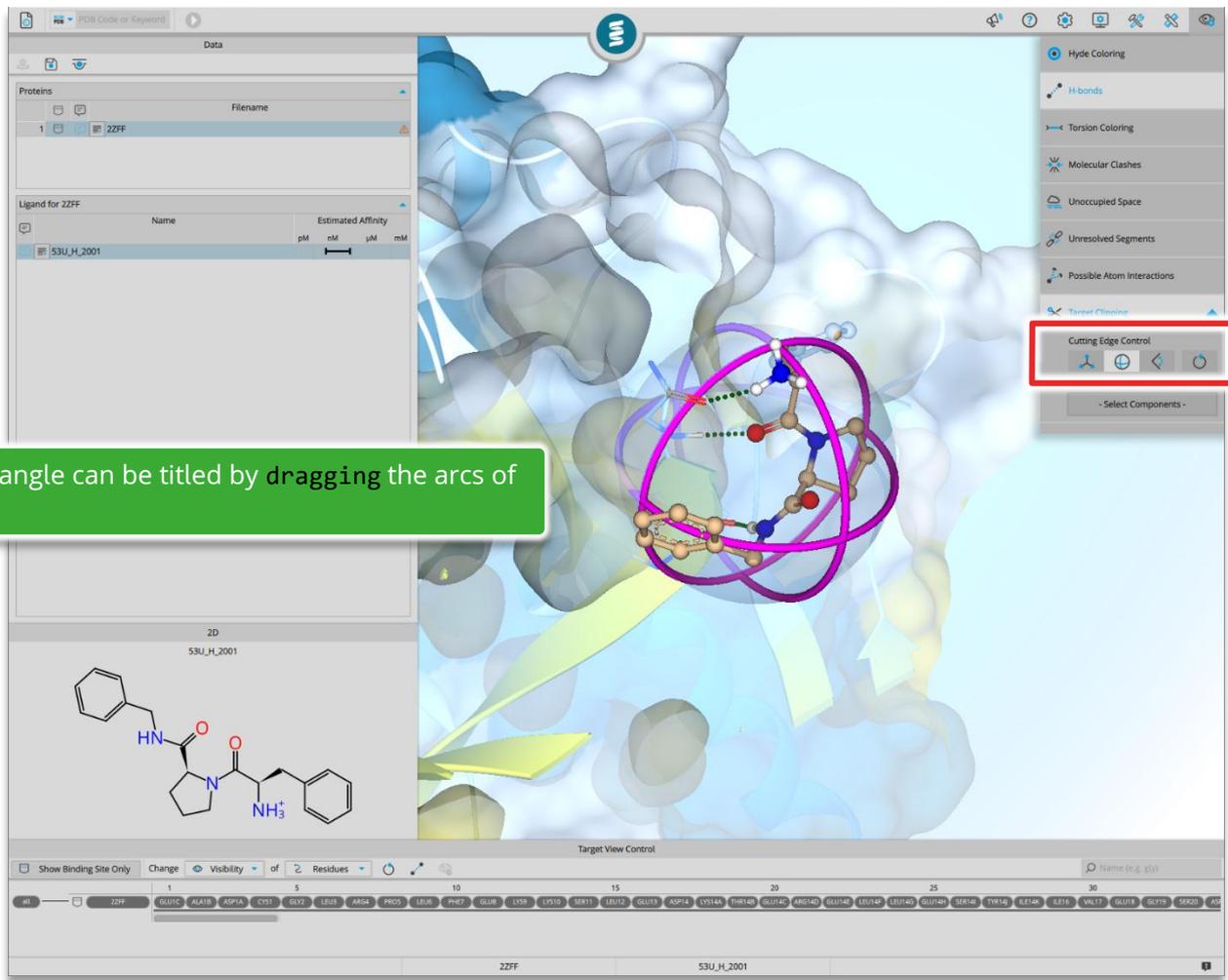
Show Binding Site Only Change Visibility of Residues

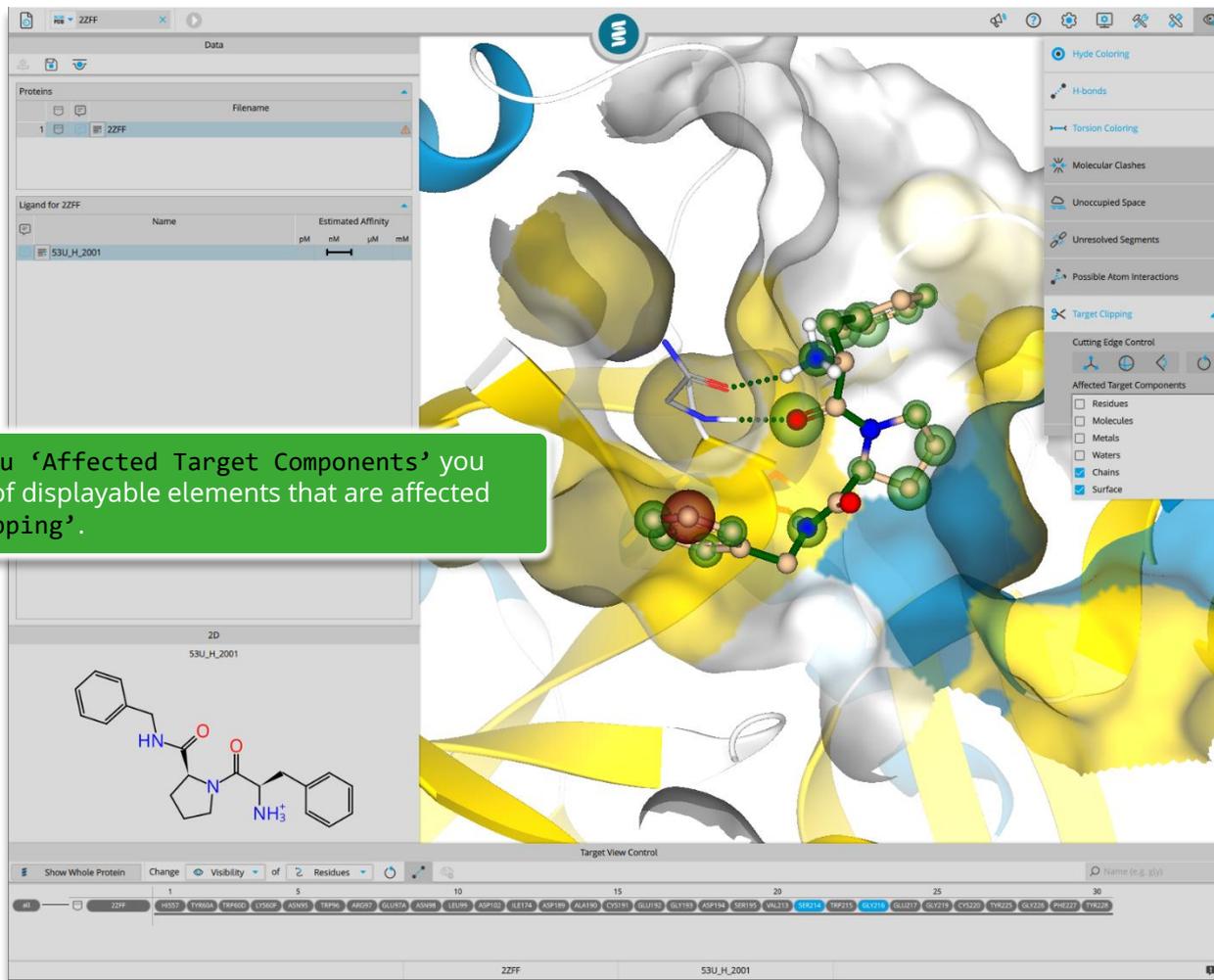
1	5	10	15	20	25	30																											
GLU12	ALA18	ASP14	CYS1	GLY2	LEU3	ARG4	PRO5	LEU6	PRO7	GLU8	LYS9	LYS10	SER11	LEU12	GLU13	ASP14	LYS14A	THR14B	GLU14C	ARG14D	GLU14E	LEU14F	LEU14G	GLU14H	SER14I	THR14J	LEU14K	SER14L	VAL17	GLU18	GLY19	SER20	ASP

Cut-off layer can be moved by dragging with a left-click to adjust the depth of the surface.

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Mode Overview





In the dropdown menu 'Affected Target Components' you will find a selection of displayable elements that are affected by the 'Target Clipping'.

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Mode Overview

Under the 'Utilities' menu, several export options for visual formats can be found. With the following settings 'Poster' → '300 dpi' → '(desired size)' → 'Transparent' publish-worthy images can be created (see next slide).

2D
53U_H_2001

C1CCN(C1)C(=O)NCC2=CC=CC=C2

Target View Control

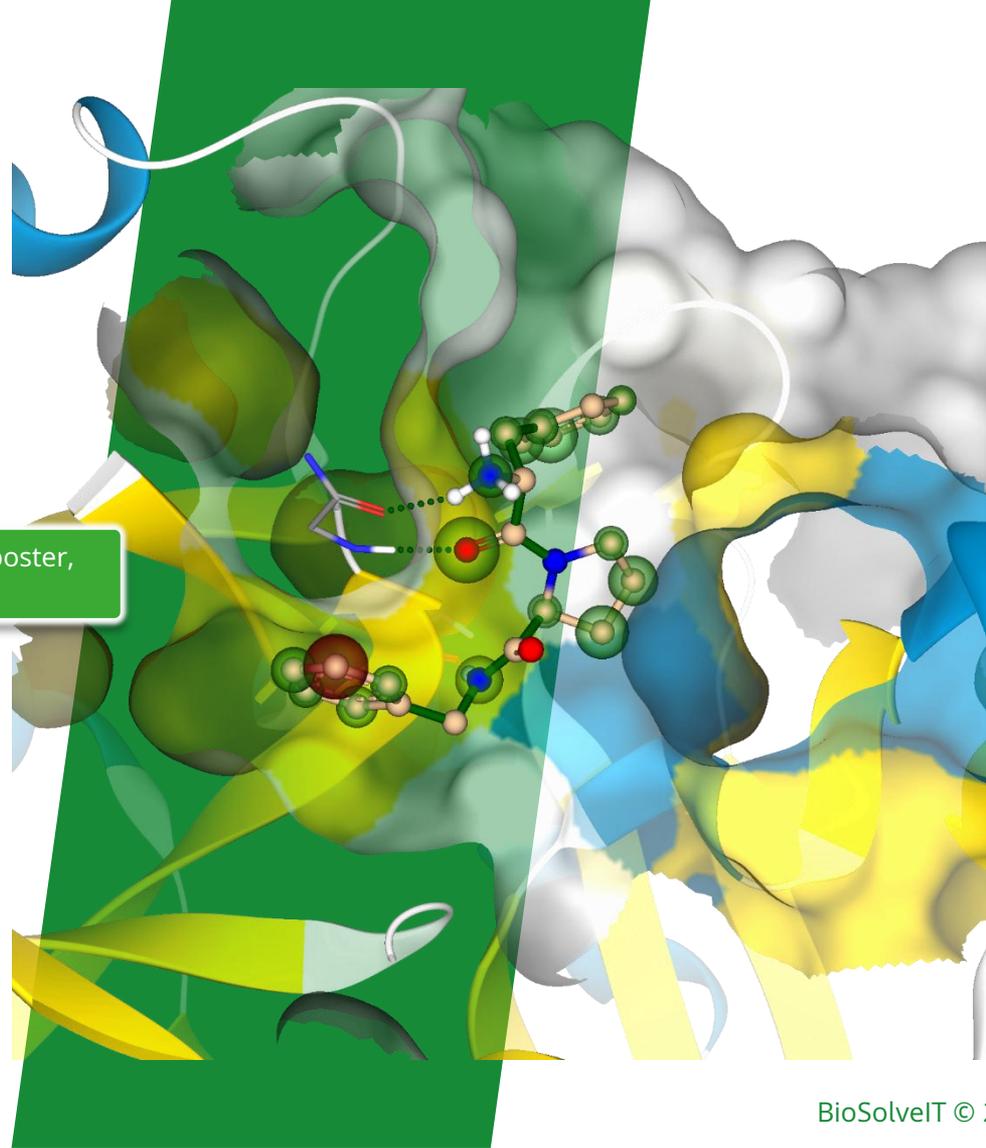
Show Whole Protein Change Visibility of Residues

1 5 10 15 20 25 30

22FF 53U_H_2001

Table of Content

Mode Overview



Transparency support helps to create great visuals for poster, presentations, reports, and more.

Table of Content

Mode Overview

Data

Proteins

Filename
1 Z2FF

Ligand for Z2FF

Name	Estimated Affinity			
	pM	nM	µM	mM
53U_H_2001				

Focus View

Space

Screenshot...

Image Mode

Paper

Poster

Dot Density

300 dpi

Image Size

W 1140 px H 1130 px

Background Color

Export 3D Scene...

Export 3D Scene...

2D

53U_H_2001

C1CCN(C1)C(=O)NCC2=CC=CC=C2

Target View Control

Show Whole Protein

Change Visibility of Residues

1 5 10 15 20 25 30

22FF 53U_H_2001

SeeSAR also supports the export of 3D files (*.glb) that can be used in various software, such as Powerpoint. 'Export 3D Scene...' captures whatever is currently set as visible in the Target View Control (including elements not shown on screen, as well as H-bonds, HYDE spheres, surface, and more.)

Table of Content

Mode Overview

A 3D molecular structure of a protein is shown, rendered in a ribbon style with various colors (white, yellow, blue, green). A ligand molecule is bound to the protein, shown in a stick representation with green, blue, red, and orange atoms. Dotted lines indicate interactions between the ligand and the protein. The background is a soft, abstract pattern of overlapping circles in shades of blue, green, and white.

The 3D format is great for impactful visualizations and can be used for smooth transitions. It supports motion on slides and be helpful to augment the understanding of the binding mode for the audience.

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Mode Overview

PowerPoint (Morph Transition)

It works also amazingly well with transitions from one slide to the next.

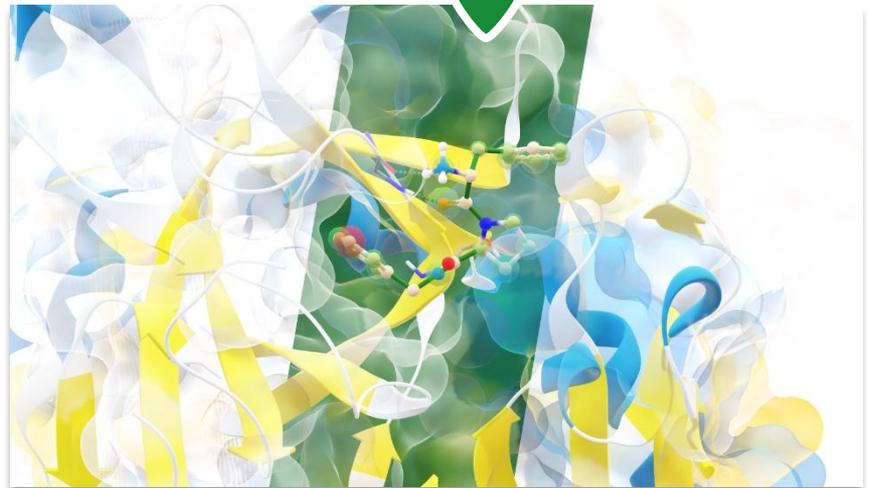
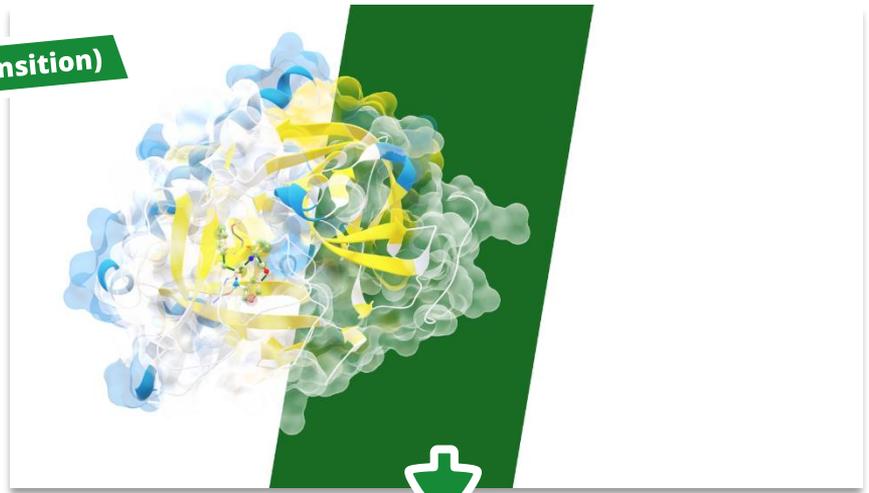


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Mode Overview

3. Proteins Mode

Proteins Mode provides the tools needed to load, explore, and manage protein structures in SeeSAR. This section gives an overview of its key functions and shows how to prepare targets for efficient downstream workflows.

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Mode Overview

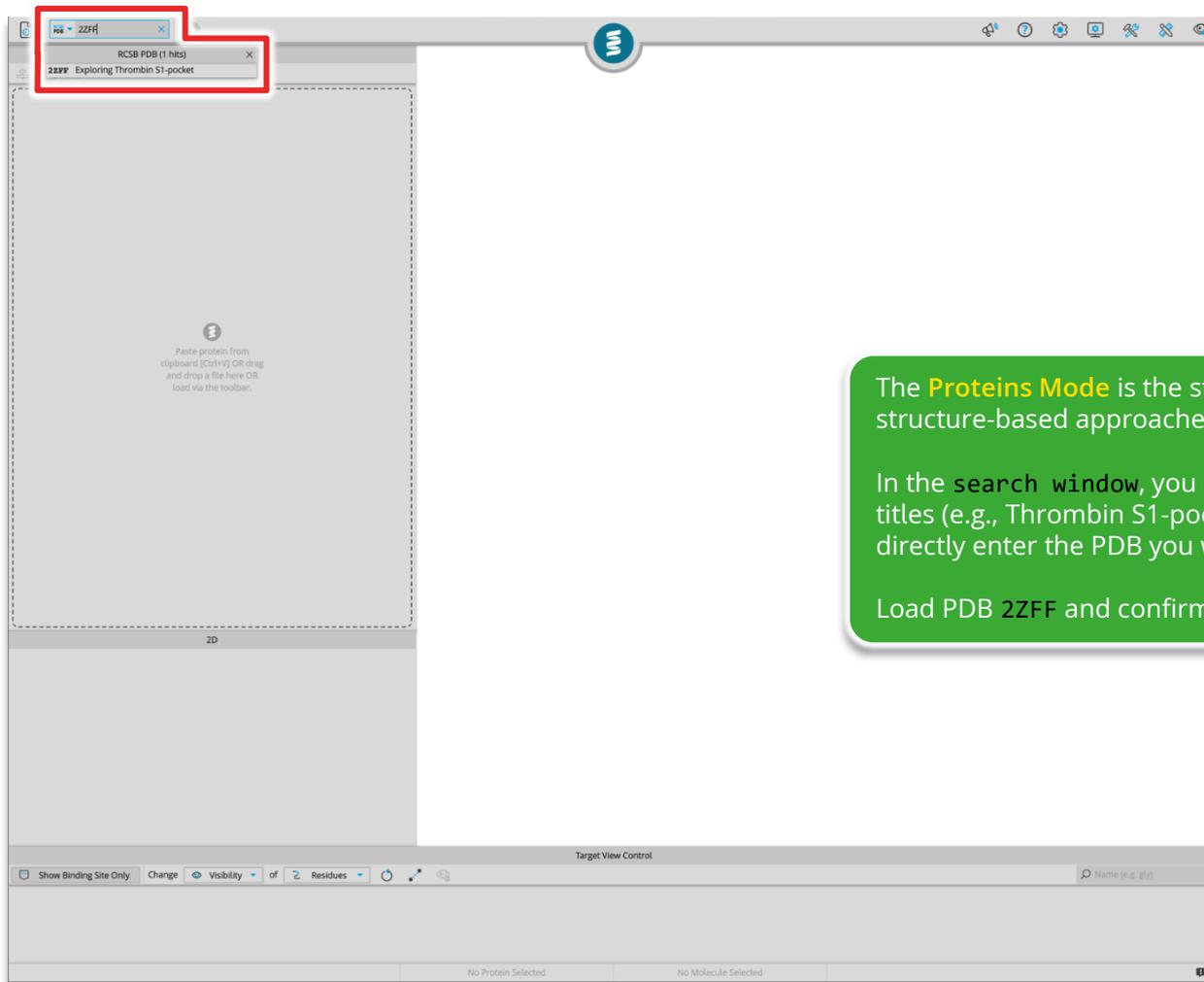
Protein	Filename
1	ZZFF
2	1A2C

Ligand for ZZFF	
Name	Estimated Affinity
53U_H_2001	pM nM μ M mM

Target View Control

1 5 10 15 20 25 30

ZZFF 53U_H_2001



The **Proteins Mode** is the starting point for structure-based approaches.

In the **search window**, you can look up PDB titles (e.g., Thrombin S1-pocket, ROCK1) or directly enter the PDB you want to access.

Load PDB 2ZFF and confirm with 'Enter' key.

Table of Content

Mode Overview

The screenshot displays the ZZFF software interface. At the top left, a green play button icon is highlighted with a red box. Below it, the 'ZZFF - Extract Your Ligand' panel is visible, containing a table of Hetero Groups. The table has columns for LOI, Name, and Estimated Affinity (pM, nM, μM, mM). A single entry is shown: 'Do not extract a ligand' with LOI '53U_H_2001'. A red box highlights a small blue square icon to the left of this entry. The main 3D view shows a protein structure in blue ribbon representation with a ligand molecule in stick representation. A green callout box points to the ligand with the text: 'Select ligand 53U_H_2001 and confirm your selection with 'Apply'. This step defines the binding site at your target structure.' At the bottom left, a 2D chemical structure of the ligand is shown. The bottom of the interface features a 'Target View Control' bar with a search field and a sequence of residues from 1 to 30, including GLU12, ALA18, ASP14, CYS1, GLY1, LEU18, ARG4, PRO5, LEU16, PHE7, GLU18, LYS10, LYS10, SER11, LEU12, GLU13, ASP14, LYS14A, THR14B, GLU14C, ARG14D, GLU14E, LEU14F, LEU14G, GLU14H, SER14I, THR14J, SER14K, SER14L, VAL17, GLU18, GLY19, SER20, ASP21.

Hetero Groups	LOI	Name	Estimated Affinity
			pM nM μM mM
Do not extract a ligand	53U_H_2001		

Table of Content

Mode Overview

Clicking on a ligand will make appear in the 2D window and in 3D.

Right-clicking in the 2D window allows you to copy the ligand for different purposes.

- Copy to clipboard as SMILES
- Copy to clipboard as svg
- Copy to clipboard as png

Table of Content

Mode Overview

The screenshot displays the BioSolveIT software interface. On the left, the 'Data' panel shows a list of proteins with '53U_H_2001' selected. A context menu is open over the protein entry, with the 'Change Ligand...' option highlighted in blue and a red arrow pointing to it. Below the protein list, the 'Ligand for Z2FF' section shows '53U_H_2001' with an 'Estimated Affinity' scale. At the bottom left, a 2D chemical structure of the ligand is shown. The main window displays a 3D ribbon representation of the protein (blue) with a ligand (red and yellow) bound to it. At the bottom, the 'Target View Control' panel shows a sequence of residues from 1 to 30, with 'Z2FF' and '53U_H_2001' highlighted.

It is also possible to change the active binding site within the **Proteins Mode**. Right-click on a target structure containing a ligand. Here, you will find the option 'Change Ligand...' to select a new molecule to define the binding site.

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Mode Overview

The screenshot displays a molecular docking software interface. The main window shows a protein structure in blue ribbon representation with a ligand (red sticks) bound to it. The interface includes a sidebar on the left with a search bar containing '1A2C' and a list of proteins. Below the search bar, there is a table for ligands. The bottom of the interface features a 'Target View Control' panel with a sequence viewer showing residues from 1 to 30.

1A2C RCSB PDB (1 hits)
1A2C Structure of thrombin inhibited by AERUGINOS

Proteins	
Filename	
ZZFF	

Ligand for ZZFF	
Name	Estimated Affinity
53U_H_2001	pM nM μM mM

Target View Control

Show Binding Site Only Change Visibility of Residues

1	5	10	15	20	25	30																									
GLUE	ALAT	ASPA	CYST	GLY	LEU	ARG	PRO	LEU	PRO	GLU	LYS	LYS	SER	LEU	GLU	ASP	LYS	THR	GLU	ARG	GLU	LEU	SER	THR	LEU	LEU	VAL	GLU	GLY	SER	ASP

ZZFF No Molecule Selected 2 messages

It is possible to perform binding site alignment in the **Proteins Mode**.

For this, load PDB 1A2C.

Table of Content

Mode Overview

1A2C - Extract Your Ligand

Hetero Groups	LOI	Name	Estimated Affinity
			pM nM μ M mM
<input checked="" type="checkbox"/>		Do not extract a ligand	
<input type="checkbox"/>		MOL_J_1	

2D
MOL_J_1

Target View Control

Show Binding Site Only Change Visibility of Residues

1 5 10 15 20 25 30

2ZFF ALA18 ASP14 CYS1 GLY2 LEU3 ARG4 PRO5 LEU6 PHE7 GLU8 LYS9 LYS10 SER11 LEU12 GLU13 ASP14 LYS15A THR16B GLU17C ARG18D GLU19E LEU20F SER14B THR15A LEU16B LEU17B VAL17D LEU18B GLY19B SER20B ASP

THR18B PHE19B GLY20B SER18B GLY21B GLU22B ALA23B ASP24B CYS1 GLY2 LEU3 ARG4 PRO5 LEU6 PHE7 GLU8 LYS9 LYS10 SER11 LEU12 GLU13 ASP14 LYS15A THR16B THR17B LEU18B LEU19B LEU20B LEU21B ASP

2ZFF MOL_J_1 2 messages

Select ligand MOL_J_1 and confirm your selection with 'Apply'.

Table of Content

Mode Overview

3D alignment of binding sites

Ligand for Z2FF	
Name	Estimated Affinity
53U_H_2001	pM nM μM mM

With the second structure loaded, '3D alignment of binding sites' becomes available. Use the button to align the binding sites.

Target View Control

1	5	10	15	20	25	30
Z2FF	GLUC ALAT ASPA CYS1 GLY2 LEU3 ARG4 PRO5 LEU6 PHE7 GLU8 LYS9 LYS10 SER11 LEU12 GLU13 ASP14 LYS14A THR14B GLU14C ARG14D GLU14E LEU14F LEU14G LEU14H VAL14I LEU14J LEU14K LEU14L LEU14M LEU14N LEU14O LEU14P LEU14Q LEU14R LEU14S LEU14T LEU14U LEU14V LEU14W LEU14X LEU14Y LEU14Z					
1A2C	THR1B PHE1D GLY1F SER1E GLY1D GLUC ALAT ASPA CYS1 GLY2 LEU3 ARG4 PRO5 LEU6 PHE7 GLU8 LYS9 LYS10 SER11 LEU12 GLU13 ASP14 LYS14A THR14B GLU14C ARG14D GLU14E LEU14F LEU14G LEU14H LEU14I LEU14J LEU14K LEU14L LEU14M LEU14N LEU14O LEU14P LEU14Q LEU14R LEU14S LEU14T LEU14U LEU14V LEU14W LEU14X LEU14Y LEU14Z					

Z2FF No Molecule Selected 2 messages

Table of Content

Mode Overview

The screenshot displays a molecular docking software interface. On the left, a 'Data' panel lists proteins (1: Z2FF, 2: 1A2C) and a ligand (53U_H_2001) with an estimated affinity of approximately 1 nM. Below this is a 2D chemical structure of the ligand. The main window shows a 3D ribbon representation of protein structures in blue and green, with the ligand in stick representation. A green callout box contains the following text:

The binding sites of all loaded structures will be aligned based on topology using the active binding site as guidance. All other binding sites will be aligned on the active pocket.

To highlight differences, switch to a binding site-focused view with 'Show Binding Site Only'.

At the bottom, a 'Target View Control' panel shows a sequence alignment of residues for Z2FF and 1A2C. A red box highlights the 'Show Binding Site Only' checkbox, which is currently checked.

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Mode Overview

The screenshot displays a molecular docking software interface. On the left, the 'Data' panel shows a list of proteins (1: Z2FF, 2: 1A2C) and a list of ligands for Z2FF (53U_H_2001). Below this is a 2D chemical structure of the ligand, 53U_H_2001. The main 3D view shows a blue protein ribbon structure with a red dashed box highlighting a specific region. At the bottom, the 'Target View Control' panel features a similarity slider set to 1.2 Å, with 'similar' and 'different' labels. Below the slider is a sequence alignment table with columns for protein residues and rows for different ligands.

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
Z2FF	1H557	TRP62	ASP102	ILE174	ASP180	ALA190	GLU192	GLY193	ASP194	SER195	VAL213	SER214	TRP215	GLU217	GLU217	GLU217	GLU217	CYS220	TRP225	GLY226	PRO227	TRP228							
1A2C	1H557	TRP62	ASP102	ILE174	ASP180	ALA190	CYS191	GLU193	GLY193	ASP194	SER195	VAL213	SER214	TRP215	GLU217	GLU217	GLU217	CYS220	TRP225	GLY226	PRO227	TRP228							

After zooming in on your ligand with 'Space' key, use the 'Hide components with similar conformation to binding site protein' to hide residues and components, that are too similar to the active binding site to spot differences.

Dissimilar residues will remain visible.

Table of Content

Mode Overview

Add ligands of all proteins to a different mode

You can also export all ligands from the loaded PDBs into another Mode with 'Add ligands of all proteins to a different mode'.

Change	Visibility	of	Residues
2ZFF			
1A2C			

1	5	10	15	20	25	30
TYR64	TRP62	LYS67	ASP152	GLU192	GLY216	TRG28
ASP154	ASP194	ASP199	ASP199	ASP199	ASP199	ASP199

Table of Content

Mode Overview

The screenshot displays the SeeSAR software interface. At the top, there is a toolbar with various icons for file operations and editing. Below the toolbar, a 'Data' panel shows the current edit state as 'CreatedMolecule_1'. The main workspace is divided into two views: a 3D view of a protein structure with a blue ribbon and a ball-and-stick model of a molecule, and a 2D view of a chemical structure (indole) with 'HN' labeled. A 'Target View Control' panel at the bottom shows a sequence of residues from 1 to 30, with a search bar for 'Name (e.g. glp)'. The interface is overlaid with a green banner and a text box.

4. Adding Molecules

This section introduces the different ways of adding molecules in SeeSAR and explains how they can be loaded, imported, and transferred between workflows. It provides the foundation for bringing new compounds into your project and preparing them for further analysis, design, and evaluation.

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Mode Overview

To add your own molecules to a SeeSAR session:
Use your preferred drawing tool and save the molecules as an SDF, SMILES, or MOL2 file.

Then switch to **Analyzer Mode** and either load the file via the 'Load Molecules...' option or copy/paste the structures into the Input Library field (see next slide).

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Mode Overview

Paste molecule from clipboard [Ctrl+V] OR drag and drop a file here OR load via the toolbar.

Alternatively, copy/paste (Ctrl+c/Ctrl+v) or drag your molecules (as smiles or sdf) here.

For example, add the following three molecules:

```
O=C(N1CCCC1)c2c3c(NC=C3)ccc2  
O=C(N1CCOCC1)c2c3c(NC=C3)ccc2  
O=C(N1c2c(c(N)ccc2)CC1)c3c4c(NC=C4)ccc3
```

Target View Control

Show Whole Protein Change Visibility of Residues

1 5 10 15 20 25 30

22FF No Molecule Selected

Table of Content

Mode Overview

The screenshot displays a molecular docking software interface. At the top left, a 'Data' table lists three entries, with the first entry highlighted in red:

	Name	Estimated Affinity	LLE	Tor.	in	
		pM	nM	µM	mM	d
1	no name					●
2	no name					●
3	no name					●

The central 3D view shows a protein structure in blue ribbon representation with a ligand molecule in stick representation. A green callout box provides instructions: "To change their names: Double-click on the molecule name ('no name' in this case) to change it. Confirm the change with the 'Enter' key."

The bottom left shows a 2D chemical structure of the ligand, which is a benzimidazole derivative with a pyrrolidine ring attached to the imidazole ring via a carbonyl group. The SMILES string for this structure is C1CCN1C(=O)c2c[nH]c3ccccc23.

The bottom right shows the 'Target View Control' panel, which includes a 'Show Whole Protein' checkbox, a 'Change' dropdown, a 'Visibility' dropdown, and a 'Residues' dropdown. A sequence bar at the bottom displays the protein sequence from residue 1 to 30, with the current view centered on residue 22 (22FF).

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Mode Overview

	Name	Estimated Affinity				LLE	Tor.	Inti cla
		pM	nM	µM	mM			
1	mol_e 1							
2	molecule 2							
3	molecule 3							



	Name	Estimated Affinity				LLE	Tor.	Inti cla
		pM	nM	µM	mM			
1	mol_e 1							
2	molecule 2							
3	molecule 3							

To transfer all your compounds to another Mode (e.g., to dock them in the Docking mode), click on the 'Checked' column and select 'Check all' to mark all molecules in the list.

If you want to transfer only some of the molecules, check them individually in the column.

Table of Content

Mode Overview

Click on 'Add checked molecules to mode' and select the Mode of your choice to work with the molecules. For example, if you want to dock them, select the **(Local) Docking Mode**.

The docking procedure is the dedicated section.

Jump to Mode

Table of Content

Mode Overview

Target View Control

2ZFF molecule 1

Current Edit State (# 0)

Edit state is empty. Add at least one molecule or create a new one.

Paste molecule from clipboard [Ctrl+V] OR drag and drop a file here OR load via the toolbar.

2D

Target View Control

Show Whole Protein Change Visibility of Residues

1 5 10 15 20 25 30

2ZF C4577 TYR60A TRP60D LYS60P ALA65S TRP66 ARG67 GLY74A ASN8 ADN8 LEU91 ASP103 LEU174 ASP188 ALA190 CYS191 GLU192 GLY193 ASP194 SER195 VAL213 SER214 TRP215 GLY219 GLU227 GLY228 CYS229 TYR229 GLY228 PHE227 THR226

2ZF No Molecule Selected

You can also create new molecules in the **Molecule Editor Mode**.
Click on 'Create a new molecule'.

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Mode Overview

The screenshot shows a software interface for molecular modeling. On the left, a panel titled 'Create New Ring' is open, listing options: Cyclopropane, Cyclobutane, Cyclopentane, Cyclohexadiene, and Benzene. The 'Benzene' option is highlighted with a red box. Below this panel, there is a text box: 'Paste molecule from clipboard [Ctrl+V] OR drag and drop a file here OR load via the toolbar.' The main window displays a protein structure in blue ribbon representation with a yellow and black dashed line indicating a path. At the bottom, a 'Target View Control' panel shows a sequence of residues from 1 to 30, with '2ZF' selected. The status bar at the bottom indicates 'No Molecule Selected'.

Going from 'Create New Ring', click on 'Benzene' to create the starting point.

Hint:

Once you started editing, you can always focus on the molecule with 'Space'.

Sometimes the starting fragment is created somewhere outside the screen, which makes this functionality extremely helpful.

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Mode Overview

The screenshot displays a molecular modeling software interface. At the top, a toolbar contains several icons, with a red box highlighting a group of icons including a percentage sign, a square with a circle, a blue circle, a blue square, and a blue circle with a square. Below the toolbar, the interface is split into two main panels. The left panel, labeled '2D', shows a 2D chemical structure of a benzene ring. The right panel, labeled '3D', shows a 3D ball-and-stick model of a molecule with orange carbon atoms, white hydrogen atoms, and a blue ribbon structure. At the bottom, there is a 'Target View Control' panel with a sequence of residues: 1 5 10 15 20 25 30. The residues are: 2ZF, 4357, TYR6A, TRP6D, LYS6P, ASN6, TRP6, ARG6, GLY1A, ASN6, LEU9, ASP10, LEU14, ASP18, ALA19, CYS19, GLU19, GLY19, ASP14, SER15, VAL11, SER14, TRP19, GLY19, GLY17, GLY19, CYS20, TRG20, GLY28, PHE27, THR28. The status bar at the bottom indicates '2ZF' and 'No Molecule Selected'.

You can modify your molecule in the 2D, and 3D window.

In 2D you can add rings and change the bond type.

In 3D it is also possible to select the hydrogen atoms and replace them with 'Change element' button. You can also use hot keys for elements, e.g., use 'C' to change an atom to a carbon or 'N' to change it to a nitrogen.

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Mode Overview

The screenshot displays a molecular modeling software interface. At the top, a toolbar contains several icons, with a red box highlighting the 'Data' section. The main workspace is split into two views: a 3D view on the right showing a protein structure with a stick model of a molecule, and a 2D view on the left showing a benzene ring with a highlighted bond. A context menu is open over the highlighted bond in the 3D view, offering options to 'Add Ring' or 'Change Bond' to various ring types: Cyclopropane, Cyclobutane, Cyclopentane, Cyclopentadiene, Cyclohexane, and Benzene. The bottom of the interface features a 'Target View Control' panel with a sequence of residues and a search bar.

Right-clicking on a bond or heavy atom in 2D or 3D with provides you with option on common decorations or the possibility to change the bond type.

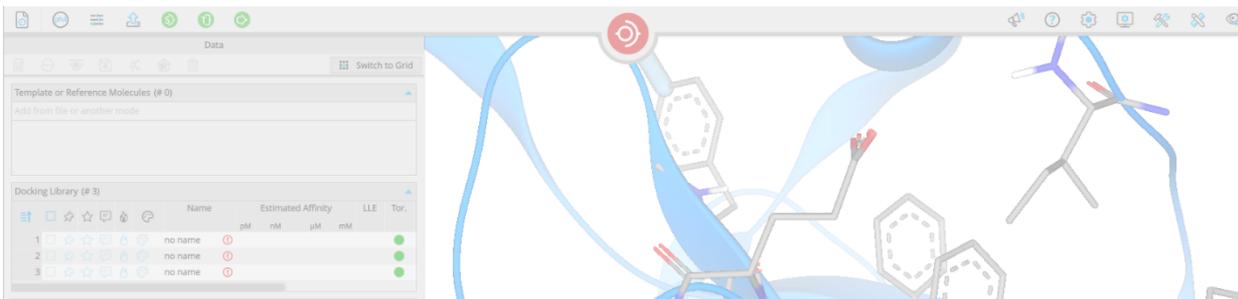
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Mode Overview

Once you are finished, export the molecule to the table with 'Save edited molecules to table' or 'Ctrl+E'.

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Mode Overview



5. Docking

This section introduces docking in SeeSAR and explains how candidate molecules can be placed into the binding site to explore possible binding modes. It outlines the key steps and settings needed to generate, inspect, and compare docking poses efficiently.

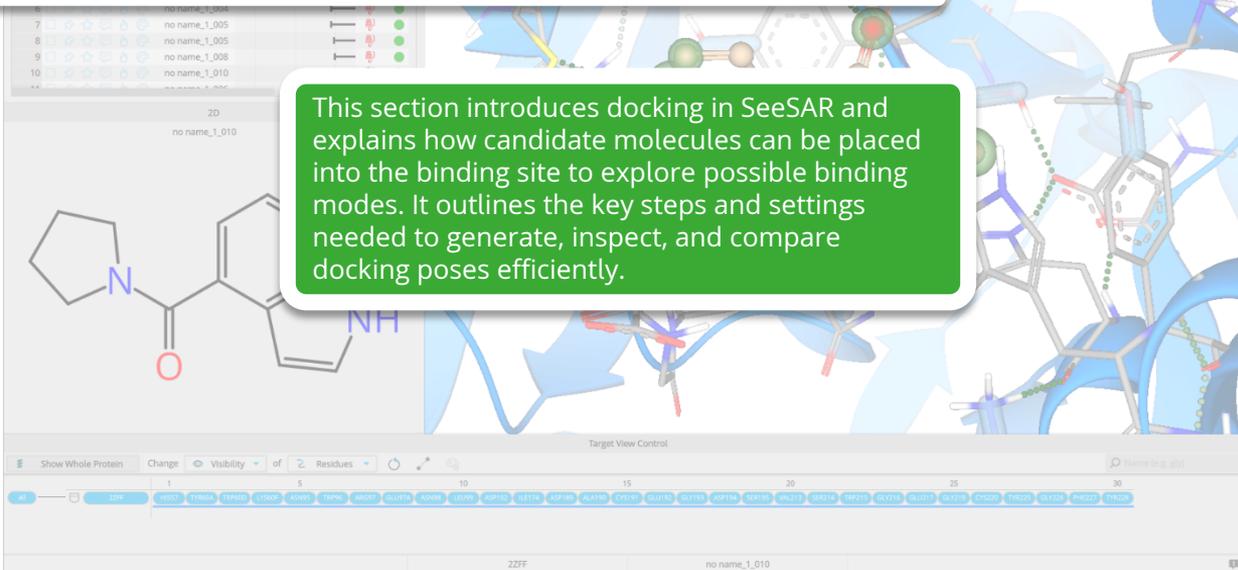


Table of Content

Mode Overview

Paste molecule from clipboard [Ctrl+V] OR drag and drop a file here OR load via the toolbar.

Target View Control

Show Whole Protein Change Visibility of Residues

1 5 10 15 20 25 30

22FF No Molecule Selected

If not already in use, we load the PDB 2ZFF and select 53U_H_2001 to define the binding site.

The **Docking Mode** is used to predict the binding modes of ligands.

You need ligands to dock them. See Section 'Adding Molecules' on how to add molecules to the docking library.

For this example, copy and paste (Ctrl+C/Ctrl+V) the following three molecules into SeeSAR:

```
O=C(N1CCCC1)c2c3c(NC=C3)ccc2
O=C(N1CCOCC1)c2c3c(NC=C3)ccc2
O=C(N1c2c(c(N)ccc2)CC1)c3c4c(NC=C4)ccc3
```

Note:
ALL molecules in the 'Docking Library' will be docked if they are added.

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Mode Overview

The screenshot displays a docking software interface. On the left, there is a sidebar with several panels: 'Template or Reference Molecules (# 0)', 'Docking Library (# 3)', and 'Generated Poses (# 0)'. The 'Docking Library' panel contains a table with the following data:

	Name	Estimated Affinity	LLE	Tor.		
		pM	nM	µM	mM	
1	no name	⊖	⊖	⊖	⊖	●
2	no name	⊖	⊖	⊖	⊖	●
3	no name	⊖	⊖	⊖	⊖	●

The main window shows a 3D visualization of a protein structure (blue ribbon) with a yellow and black striped cylinder and a red molecule docked. A green callout box on the right contains the following text:

To start docking, click 'Standard Docking: Generate Poses'.
By default, up to 10 poses per molecule are generated.
The next slide shows how to adjust the docking settings to refine the results.

At the bottom, there is a 'Target View Control' panel with a sequence viewer showing residues from 1 to 30. The sequence is: 22FF, 44577, TYR60A, TRP60D, LYS60P, ALA60S, TRP6L, ARG6T, GLU6A, ASP6A, LEU6I, ASP6L, LEU6L, ASP6R, ALA6R, CYS6I, GLU6D, GLY6S, ASP6A, SER6S, VAL6I, SER6L, TRP6I, GLY6I, GLU6I, GLY6I, CYS6D, TRP6D, GLY6D, PHE6D, TRP6D.

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Mode Overview

Maximum Number of Poses
10

Clash Tolerance
Standard Medium High

Allowed Ring Conformations
Off R/S E/Z Both

Allow Stereo Center Flipping
Off R/S E/Z Both

Flexible Covalent Attachment

‘Maximum Number of Poses’ sets the maximum number of poses generated per molecule. The default is 10.

‘Clash Tolerance’ controls how clashes between ligand and target are handled during docking. For tight binding sites, Medium or High may improve results.

‘Allowed Ring Conformations’ allows unfavorable ring conformations, such as twist and boat.

‘Allow Stereo Center Flipping’ allows automatic flipping of R/S, E/Z, or both during docking.

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Mode Overview

The screenshot displays a molecular docking software interface. On the left, there are panels for 'Template or Reference Molecules (# 0)', 'Docking Library (# 3)', and 'Generated Poses (# 30)'. The 'Generated Poses' table is highlighted with a red border. Below it, the chemical structure of a ligand is shown. The main window displays a 3D ribbon representation of a protein structure in blue, with a yellow and black striped ligand docked in the binding pocket. At the bottom, there is a 'Target View Control' panel showing a sequence of residues from 1 to 30.

Generated Poses (# 30)		Name	Estimated Affinity				LLE	Tor.
			pM	nM	µM	mM		
1	<input type="checkbox"/>	no name_1_001						●
2	<input type="checkbox"/>	no name_1_002						●
3	<input checked="" type="checkbox"/>	no name_1_003						●
4	<input type="checkbox"/>	no name_1_004						●
5	<input type="checkbox"/>	no name_1_005						●
6	<input type="checkbox"/>	no name_1_006						●
7	<input type="checkbox"/>	no name_1_007						●
8	<input type="checkbox"/>	no name_1_008						●
9	<input type="checkbox"/>	no name_1_009						●
10	<input type="checkbox"/>	no name_1_010						●

Chemical structure of the ligand: C1=CC=C2C(=C1)C(=O)N2C3CCOCC3

The 'Generated Poses' table will be populated with generated poses of the ligands from 'Docking Library'.

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Mode Overview

The screenshot displays a molecular docking software interface. On the left, there are three panels: 'Template or Reference Molecules (# 0)', 'Docking Library (# 3)', and 'Generated Poses (# 30)'. The 'Generated Poses' table is highlighted with a red box and a green arrow pointing to the 'Inter-clash' column. Below this table is a chemical structure of a ligand, which is a benzimidazole derivative with a morpholine ring attached to the imidazole ring.

Name	Estimated Affinity				LLE	Tor.	Intra-clash	Inter-clash
	pM	nM	µM	mM				
no name_1_001								
no name_1_002								
no name_1_003								
no name_1_004								
no name_1_005								
no name_1_006								
no name_1_007								
no name_1_008								
no name_1_009								

The chemical structure of the ligand is shown below the table:

C1=CN2C(=N1)C=CC=C2C(=O)N3CCOCC3

The 'Target View Control' at the bottom shows the protein sequence from residue 1 to 30, with the current view centered on residue 5.

Depending on your desktop setup, not all calculated properties may be displayed. You can always adjust the width of the windows by dragging the rim to resize or use the scroll bar to browse through the columns.

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Mode Overview

The screenshot displays the HYDE software interface. On the left, a sidebar contains a 'Data' panel with a red box highlighting the 'Estimated Affinity' section, which includes a 'Calculate estimated affinity for checked molecules' button. Below this are sections for 'Molecular Clashes' and 'Optimum Properties'. The main area shows a 3D ribbon representation of a protein (blue) with a ligand (grey sticks) bound to it. A yellow dashed line indicates a specific interaction. At the bottom, a 'Target View Control' panel shows a sequence of residues from 1 to 30, with the current view centered on residue 5.

Generated Poses (# 30)		Checked (# 30)		Estimated Affinity		LLE	Tor.	
				pM	nM	µM	mM	
1	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>
2	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>
3	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>
4	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>
5	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>
6	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>
7	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>
8	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>
9	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>
10	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>
11	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>

If your poses did not generate affinity automatically, check all poses with the 'Checked' column and 'Check all'. Then go to 'Calculations for checked molecules' and select 'Estimated Affinity'.

Note: You may restrict the HYDE calculation to a pre-selected set of checked molecules.

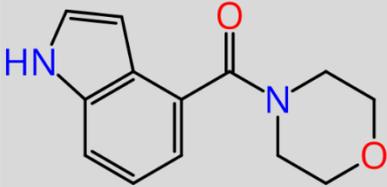


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Mode Overview

The screenshot displays a molecular docking software interface. On the left, there are panels for 'Data', 'Docking Library (# 3)', and 'Generated Poses (# 30)'. The 'Generated Poses' table is highlighted with a red box, showing columns for 'Name', 'Estimated Affinity' (with sub-columns for pM, nM, μM, mM), and 'Tor.'. A red arrow points to the 'Estimated Affinity' column headers. A green callout box on the right contains the text: 'Now the estimated affinities appear as a range on the logarithmic scale. Clicking on a column header sorts according to this value.' Below the tables, a 2D chemical structure of a ligand is shown. The main window displays a 3D molecular model of the protein-ligand complex. At the bottom, there is a 'Target View Control' panel with a sequence viewer showing residues 1 to 30.

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Mode Overview

The screenshot displays a molecular docking software interface. The main window shows a protein structure in blue ribbon representation with a ligand molecule docked in a binding pocket. The ligand is shown in a stick representation with a color scheme of green, blue, and red. The interface includes a 'Data' panel on the left with sections for 'Template or Reference Molecules (# 0)', 'Docking Library (# 3)', and 'Generated Poses (# 30)'. The 'Generated Poses' table lists 30 poses with columns for Name, Estimated Affinity (pM, nM, μM, mM), LLE, and Tor. The 10th pose, 'no name_1_010', is selected. Below the table is a 2D chemical structure of the active compound, which is a benzimidazole derivative with a pyrrolidine ring. At the bottom, a 'Target View Control' panel shows a sequence of residues from 1 to 30, with a red box highlighting a specific residue.

Generated Poses (# 30)		Estimated Affinity				LLE	Tor.
	Name	pM	nM	μM	mM		
1	no name_1_004						●
2	no name_1_001						●
3	no name_1_002						●
4	no name_1_007						●
5	no name_1_010						●
6	no name_1_004						●
7	no name_1_005						●
8	no name_1_008						●
9	no name_1_010						●
10	no name_1_010						●
11	no name_1_007						●

By activating 'Show only interacting components for currently selected molecule', only residues, waters, ions and other molecules forming interactions with the active compounds will be displayed. This keeps a clean interface for easy visual assessment and adapts to each new active ligand.

Table of Content
Mode Overview

The screenshot shows a molecular docking software interface. On the left, there are panels for 'Template or Reference Molecules (# 0)', 'Docking Library (# 3)', and 'Generated Poses (# 30)'. The 'Generated Poses' table has a red box around the 6th row, which is highlighted. A context menu is open over this row, with a red box around the 'Calculate Estimated Affinity' option. Below the menu, a chemical structure of a molecule is shown. The main view displays a protein structure in blue with a molecule docked in pink. At the bottom, there is a 'Target View Control' panel showing a sequence of residues.

Docking Library (# 3)	
Name	Estimated Affinity
	pM nM μM mM
1 no name	0
2 no name	0
3 no name	0

Generated Poses (# 30)	
Name	Estimated Affinity
	pM nM μM mM
1 no_name_1_004	0
2 no_name_1_001	0
3 no_name_1_002	0
4 no_name_1_007	0
5 no_name_1_010	0
6 no_name_1_004	0
7 no_name	0
8 no_name	0
9 no_name	0
10 no_name	0

Context Menu	
Calculate Estimated Affinity	
Calculate H-bond Network	
Calculate Torsion Quality	
Calculate Molecular Clashes	
Calculate Optibrium Properties	
Add Molecule to	
Add Complex to Protein Editor	
Use as Reference in	

To inspect multiple poses in comparison, toggle the permanent visibility by marking a molecule as reference.

The reference will now stay visible while you browse through the other poses. You can even color each molecule to differentiate them.

You can calculate more assessment parameters with a right-click on a molecule, or using the method describe in the previous slides to calculate them for all checked molecules.

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Mode Overview

The screenshot displays a molecular docking software interface. The main window shows a protein structure in blue ribbon representation with a ligand molecule docked in a binding pocket. The ligand is shown in a stick representation with green and brown spheres. A red box highlights a 'Properties' menu that is open, showing various options to be checked or unchecked. Below the main window, there is a 'Generated Poses (# 30)' table with columns for Estimated Affinity (pM, nM, μM, mM), LLE, Tor., Intra-clash, Inter-clash, MW, and LogP. A 2D chemical structure of the ligand is shown in the bottom left corner. The bottom of the interface features a 'Target View Control' bar with a sequence of residues from 1 to 30.

Generated Poses (# 30)

	Estimated Affinity				LLE	Tor.	Intra-clash	Inter-clash	MW	LogP
	pM	nM	μM	mM						
1									214.27	2.40
2									214.27	2.40
3									214.27	2.40
4									277.33	2.95
5									214.27	2.40
6									277.33	2.95
7									277.33	2.95
8									214.27	2.40
9									277.33	2.95
10									277.33	2.95
...									277.33	2.95

Properties

- Checked
- 3D Visibility
- Favorite
- Annotation
- Active Status
- Molecule Color
- Name
- Template Name
- Optimization State
- Src
- Estimated Affinity

2D Structure

Nc1ccc2c(c1)C(=O)N2C(=O)c3c[nH]c4ccccc34

Target View Control

1 5 10 15 20 25 30

22FF 4652 TYR60A TRP60D LYS60C ALA65S ALA65S TRP65E ARG67T GLU74A ALA76S LEU79P ASP70L LEU74A ASP78S ALA79S CYS131I GLU132E GLU133S ASP134I SER135S VAL213I SER214L TRP215S GLN219I GLU217T GLY219I CYS220S TRP225S GLY228S PHE227T THR228S

To change table properties, scroll horizontally to the last column header and click on it. This will provide options to choose which columns to display.

Table of Content

Mode Overview

The screenshot shows a molecular docking software interface. A red box highlights a toolbar with the following callouts:

- 3D visibility**: Callout pointing to the 3D view icon.
- Add annotation**: Callout pointing to the speech bubble icon.
- Molecule color**: Callout pointing to the palette icon.
- Mark as favorite**: Callout pointing to the star icon.
- Mark as active/inactive**: Callout pointing to the flame icon.

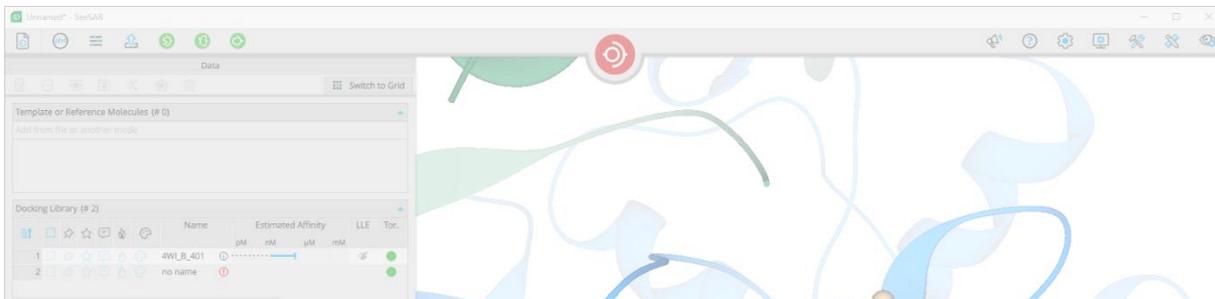
A green callout at the top right states: "You can add notes and descriptors to the table entries." A red arrow points from the toolbar to a table of entries in the Docking Library.

	Name	Estimated Affinity	LLE	Tor.		
1	no name	pM	nM	μM	mM	●
2	no name	●	●	●	●	●
3	no name	●	●	●	●	●
4	no name_1_001	●	●	●	●	●
5	no name_1_002	●	●	●	●	●
6	no name_1_007	●	●	●	●	●
7	no name_1_010	●	●	●	●	●
8	no name_1_004	●	●	●	●	●
9	no name_1_005	●	●	●	●	●
10	no name_1_008	●	●	●	●	●
11	no name_1_010	●	●	●	●	●
12	no name_1_007	●	●	●	●	●
13	no name_1_004	●	●	●	●	●

Below the table, a 2D chemical structure is shown with the label H_2N . The interface also features a "Molecule" label and a "EIO" logo.

Table of Content

Mode Overview



5.1. Pharmacophore Constraints

The screenshot shows a chemical structure of a molecule with a vinylamide group. The structure is labeled 'no name_Vinylamide_MichaelAddition...'. Below the structure is a 'Target View Control' panel with a sequence of residues: 1 5 10 15 20 25 30. The sequence is: 7TLL 1ST 2ND 3RD 4TH 5TH 6TH 7TH 8TH 9TH 10TH 11TH 12TH 13TH 14TH 15TH 16TH 17TH 18TH 19TH 20TH 21TH 22TH 23TH 24TH 25TH 26TH 27TH 28TH 29TH 30TH. The current view is centered on residue 7TLL. A green text box is overlaid on the image:

This section introduces pharmacophore constraints in SeeSAR and explains how they can be used to guide docking toward poses that satisfy defined interaction patterns. It shows how to set up and apply these constraints to focus the search on binding modes that match your structural hypotheses.

Table of Content

Mode Overview

Paste molecule from clipboard (Ctrl+V) OR drag and drop a file here OR load via the toolbar.

2D

Target View Control

Show Binding Site Only Change Color of Residues

1 5 10 15 20 25 30

2ZFF GLU16 ALA18 ASP14 CYS1 GLY2 LEU3 ARG4 PRO5 LEU6 PHE7 GLU8 LYS9 LYS10 SER11 LEU12 GLU13 ASP14 LYS14A THR14B GLU14C ARG14D GLU14E LEU14F LEU14G GLU14H SER14I THR14J SER14K LEU14L VAL17 GLU18 GLY19 SER20 ASP21

2ZFF No Molecule Selected 1 message

If not already in use, we load the PDB 2ZFF and select 53U_H_2001 to define the binding site and switch into the **Docking Mode**.

In this example, we will apply pharmacophore constraints during the docking process to guide our results.

Copy and paste (Ctrl+C/Ctrl +V) the following three molecules into SeeSAR:

O=C(N1CCCC1)c2c3c(NC=C3)ccc2

O=C(N1CCOCC1)c2c3c(NC=C3)ccc2

O=C(N1c2c(c(N)ccc2)CC1)c3c4c(NC=C4)ccc3

Table of Content

Mode Overview

The screenshot displays a molecular docking software interface. On the left, there is a 'Data' panel with a 'Switch to Grid' button. Below it is a 'Docking Library (# 3)' table with columns for Name, Estimated Affinity (pM, nM, μM, mM), LLE, and Tor. The table contains three entries, all named 'no name'. Below the docking library is a 'Generated Poses (# 0)' table. At the bottom left of the interface is a '2D' view showing a chemical structure of a ligand with an amino group (H₂N) and an NH group. The main window shows a blue ribbon representation of a protein structure with a yellow and black striped cylinder representing a binding site. A red stick model of a ligand is docked in the binding site. At the bottom, there is a 'Target View Control' bar with a 'Show Binding Site Only' button highlighted by a red box. The bar also includes a search field for 'Name (e.g. gly)' and a sequence of residues: 1 5 10 15 20 25 30. The residues listed are: 22FF, GLUT1E, ALA1B, ASP1A, CYS1, GLY2, LEU3, ARG4, PRO5, LEU6, PHE7, GLU8, LYS9, LYS10, SER11, LEU12, GLU13, ASP14, LYS14A, THR14B, GLU14C, ARG14D, GLU14E, LEU14F, SER14G, GLU14H, SER14I, THR14J, SER14K, SER14L, VAL17, GLU18, GLY19, SER20, ASP21.

Docking Library (# 3)						
	Name	Estimated Affinity			LLE	Tor.
		pM	nM	μM	mM	
1	no name	0				●●●
2	no name	0				●●●
3	no name	0				●●●

Generated Poses (# 0)						
	Name	Estimated Affinity			LLE	Tor.
		pM	nM	μM	mM	

2D
no name

Target View Control

Show Binding Site Only

1 5 10 15 20 25 30

22FF GLUT1E ALA1B ASP1A CYS1 GLY2 LEU3 ARG4 PRO5 LEU6 PHE7 GLU8 LYS9 LYS10 SER11 LEU12 GLU13 ASP14 LYS14A THR14B GLU14C ARG14D GLU14E LEU14F SER14G GLU14H SER14I THR14J SER14K SER14L VAL17 GLU18 GLY19 SER20 ASP21

22FF no name 1 message

If you cannot see any residues in the binding site, click on 'Show Binding Site Only'.
Skip this, if 'Show Whole Protein' is displayed; You are already seeing only the binding site.

Table of Content

Mode Overview

The screenshot displays a molecular docking software interface. On the left, the 'Data' panel shows a 'Docking Library' with three entries, all named 'no name', and a 'Generated Poses' section. Below this, a 2D chemical structure of the ligand is shown. The main window features a blue ribbon representation of a protein structure with a yellow and black striped cylinder docked into its binding site. At the bottom, the 'Target View Control' panel shows a sequence of amino acids: TYR59A, TRP50D, LYS50C, ALA55S, TRP56L, ARG57I, GLU57A, ASN58I, LEU59I, ASP60L, LEU74L, ASP139I, ALA139I, CYS151I, GLU152I, GLY153I, ASP154I, SER155I, VAL113I, SER214I, TRP215I, GLY217I, GLY219I, CYS220I, THR225I, PHE228I, THR229I. A red box highlights the 'Change', 'Visibility', and 'Residues' buttons, and a red arrow points to the 'Change' button.

To display all residues, be sure that 'Change' → 'Visibility' → 'Residues' is selected. Use the target button to show all residues within the binding site.

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Mode Overview

The screenshot displays a molecular docking software interface. On the left, there are panels for 'Template or Reference Molecules (# 0)', 'Docking Library (# 3)', and 'Generated Poses (# 0)'. The main window shows a blue ribbon representation of a protein structure with a grey stick model of a ligand. A search bar at the bottom right contains the text 'gly216' and '1/1'. A red box highlights the search bar, and another red box highlights the 'gly216' text. A green callout box with the text 'Search for Gly216.' points to the search bar. The bottom of the interface shows a 'Target View Control' bar with a sequence of residues from 1 to 25, including 2ZF, 4657, TYR6A, TRP6D, LYS6P, ASN6S, TRP6L, ARG6T, GLU7A, ASN6N, LEU6I, ASP6Q, LEU7A, ASP6R, ALA7B, CYS19, GLU19, GLY19, ASP14, SER19, VAL13, SER14, and GLY22. A red box highlights the 'gly216' text in the search bar.

Table of Content

Mode Overview

Data

Switch to Grid

Template or Reference Molecules (# 0)

Docking Library (# 3)

	Name	Estimated Affinity	LLE	Tor.	
		pM	nM	µM	mM
1	no name	⊖	⊖	⊖	⊖
2	no name	⊖	⊖	⊖	⊖
3	no name	⊖	⊖	⊖	⊖

Generated Poses (# 0)

Name

Estimated Affinity

LLE

Tor.

pM

nM

µM

mM

2D

Target View Control

Show Whole Protein

Change

Visibility

of

Residues

gly216

1/1

Hide Component in 3D

Focus View on This Component

22FF

No Molecule Selected

1 message

Adjust the visualization by right-clicking on Gly216 in the Target View Control and 'Focus View on This Component'.

Table of Content

Mode Overview

The screenshot displays a molecular docking software interface. On the left, a sidebar contains a 'Define pharmacophore' button, which is highlighted with a red rectangular box. Below this button are sections for 'Template or Reference Molecules (# 0)', 'Docking Library (# 3)', and 'Generated Poses (# 0)'. The 'Docking Library' section contains a table with the following data:

	Name	Estimated Affinity	LLE	Tor.
1	no name	µM nM µM mM	○	●
2	no name	µM nM µM mM	○	●
3	no name	µM nM µM mM	○	●

The main window shows a 3D visualization of a protein (blue) with a ligand (grey) docked in its binding pocket. A specific residue is labeled 'GLY_H_216'. At the bottom, a 'Target View Control' panel shows a sequence of residues from 1 to 30, with 'GLY216' highlighted in pink. The interface also includes a '2D' view section and a 'Show Whole Protein' button.

After setting up the visualization, we can start with defining the pharmacophore constraints. Click on the 'Define pharmacophore' button.

Table of Content

Mode Overview

The screenshot displays a molecular docking software interface. A dialog box titled "Define Pharmacophore" is open in the top-left corner, with a red border. The dialog contains the text "New spheres will be created in center of selected objects." and a "Define New Constraint" button. The main 3D view shows a protein structure in light blue and a ligand in stick representation. A label "GLY_H_216 x" is visible near the ligand. The bottom of the interface features a "Target View Control" panel with a sequence viewer showing residues from 1 to 30, with residue 25 highlighted in pink. The sequence includes: 1 2ZF, 44577 TYR6A, TRP6D, LYS6P, ASN6L, TRP6L, ARG6T, GLU7A, ASN6N, LEU6R, ASP6D, LEU7A, ASP6R, ALA7D, CYS1R, GLU1D, GLY1R, ASP14, SER1R, VAL1L, SER14, TRP2D, VAL2R, GLY2D, GLY2R, CYS2D, TRP2R, GLY2R, PHE2D, TRP2R.

Select 'Define New Constraint'.

Table of Content

Mode Overview

The screenshot displays the 'Define Pharmacophore' panel on the left, which includes a 'Show Possible Interactions' button highlighted by a red box and an arrow. The main 3D view shows a protein-ligand complex with a red box highlighting a purple sphere on a nitrogen atom of the Gly216 backbone, also indicated by a red arrow. A green callout box provides a detailed explanation of this feature.

Right-click on the nitrogen of the Gly216 backbone. In this case, a purple sphere will then pop up on the nitrogen. The option 'Show Possible Interactions' becomes available.

This feature displays the best geometry point for interactions with the selected heavy atom if it is eligible for H-bond interactions.

Click on it to calculate the interaction points.

Table of Content

Mode Overview

Define Pharmacophore

Include - Select constraint type -

in SMARTS

your Possible Interactions

Set Sphere to Center
Set sphere to center of selected obj

Cancel Apply

Generated Poses (# 0)

Name	Estimated Affinity	LLE	Top
------	--------------------	-----	-----

2D

Target View Control

Show Whole Protein Change Visibility of Residues gly216 1/1

1 5 10 15 20 25 30

2ZF 44577 TYR60A TRP60D LYS60P ASN65 TRP66 ARG67 GLU74 ASN8 ADP88 LEU99 ASP103 LEU14 ASP146 ALA130 CYS131 GLU132 GLY133 ASP134 SER135 VAL133 SER134 TRP135 VAL139 GLU137 GLY139 CYS220 TRG225 GLY228 PHE227 THR228

2ZF No Molecule Selected 1 message

GLY_H_216 x

Right-click on the now displayed interaction point. A purple highlight will pop up if it is selected. Center your pharmacophore constraint with 'Set Sphere to Center'.

Table of Content

Mode Overview

Define Pharmacophore

Include ▼

Radius 1.3 Å

- acceptor interaction contact
- acceptor interaction contact to metal
- acceptors
- acceptors or donors
- aliphatic
- any C
- any heavy atom
- any N
- any N or any O
- any O
- arom. CH
- aromatic
- bicyclic
- covalent warhead
- donor interaction contact
- donors
- halogens

Generated Poses (# 0)

2D

Target View Control

Show Whole Protein Change Visibility of Residues gly216 1/1

1 5 10 15 20 25 30

22FF No Molecule Selected 1 message

'Include' and 'Exclude' determine whether the constraint should be matched or avoided.

The 'Radius' option controls the size of the sphere.

Under 'Select Constraint Type', you can choose different chemical properties to match, or define your own SMARTS pattern.

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Mode Overview

Define Pharmacophore

Include: acceptor interaction contact

Template Radius: 1.3 Å

Docking: Set Sphere to Center

Generated Poses (# 0)

- acceptors
- aliphatic
- any C
- any heavy atom
- any N
- any N or any O
- any O
- arom. CH
- aromatic
- bicyclic
- covalent warhead
- donor interaction contact
- donors
- halogens

2D

Target View Control

Show Whole Protein Change Visibility of Residues gly216 1/1

1 5 10 15 20 25 30

22FF No Molecule Selected 1 message

Select 'acceptors': This means that all generated poses should contain an H-bond acceptor (N, O, S) within this sphere constraint.

Constraints are colored based on their chemical type (color of the mesh) and if they featured an 'included' (green sphere) or 'excluded' (red sphere) volume.

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Mode Overview

The screenshot displays a molecular docking software interface. The main window shows a protein structure in blue ribbon representation with several grey ball-and-stick molecular models docked into its binding pocket. Two green mesh spheres are also visible, representing constraint regions. On the left, a sidebar contains a 'Docking Library (# 3)' table and a 'Generated Poses (# 0)' table. The docking library table has columns for Name, Estimated Affinity (pM, nM, μM, mM), LLE, and Tor. The bottom of the interface features a 'Target View Control' bar with a sequence viewer for protein gly216, showing residues from 1 to 30. Two buttons in the top-left corner are highlighted with red boxes: a magnifying glass icon and a green circle with a white 'S' icon.

Template or Reference Molecules (# 0)							
Docking Library (# 3)							
	Name	Estimated Affinity				LLE	Tor.
		pM	nM	μM	mM		
1	no name	0	0	0	0	0	0
2	no name	0	0	0	0	0	0
3	no name	0	0	0	0	0	0

Generated Poses (# 0)							
	Name	Estimated Affinity				LLE	Tor.
		pM	nM	μM	mM		

The number of active constraints is always displayed next to the constraint button.

You can start the docking with the 'Standard docking' button.

Table of Content

Mode Overview

The screenshot displays a molecular docking software interface. On the left, there are two tables: 'Docking Library (# 3)' and 'Generated Poses (# 30)'. The 'Generated Poses' table lists 22 poses with columns for Name, Estimated Affinity (pM, nM, μM, mM), LLE, and Tor. The 6th pose, 'no name_3_006', is highlighted. Below the tables is a 2D chemical structure of the highlighted pose, showing a benzimidazole ring system connected to a piperidine ring. The main 3D view shows the protein structure in light blue and the ligand in stick representation with green and red spheres. Two green spheres of different sizes are overlaid on the ligand, representing search volumes for specific features. The bottom of the interface shows a 'Target View Control' bar with residue numbers and names.

Docking Library (# 3)							
	Name	Estimated Affinity				LLE	Tor.
		pM	nM	μM	mM		
1	no name						
2	no name						
3	no name						

Generated Poses (# 30)							
	Name	Estimated Affinity				LLE	Tor.
		pM	nM	μM	mM		
1	no name_3_001						
2	no name_3_002						
3	no name_3_003						
4	no name_3_004						
5	no name_3_005						
6	no name_3_006						
7	no name_3_007						
8	no name_3_008						
9	no name_3_009						
10	no name_3_010						
11	no name_3_001						
12	no name_3_002						
13	no name_3_003						
14	no name_3_004						
15	no name_3_005						
16	no name_3_006						
17	no name_3_007						
18	no name_3_008						
19	no name_3_009						
20	no name_3_010						
21	no name_3_001						
22	no name_3_002						

2D
no name_3_006

Target View Control

Show Whole Protein Change Visibility of Residues

1 5 10 15 20

22FF no name_3_006

The newly generated poses display the required features: an acceptor in the dark green sphere and an aromatic heavy atom in the red sphere.

The sphere size defines the area in which the heavy atom with the required feature may be located. It may also lie on the surface of the sphere.

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Mode Overview

The screenshot displays a molecular docking software interface. The top-left panel shows constraint definitions with a table:

Act	Optional	Name	Type	Constraint	r(Å)
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	rm1	Include	acceptors	1.3
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	rm2	Include	aromatic	1.5

Below this, a text box indicates: "At least 1 optional constraints must be fulfilled." The main 3D view shows a ligand (a benzimidazole derivative) docked in a protein binding pocket, with green and red mesh spheres representing interaction regions. The bottom-left panel shows a 2D chemical structure of the ligand: C1=CC=C2C(=C1)C(=CN2)C(=O)N3CCOCC3. The bottom-right panel shows a "Target View Control" with a residue list from 1 to 30, including residues like 22FF, 4457, TYR64, TRP60, LYS60, ALA65, ASP68, ARG69, GLU74, ASP78, ASP79, ASP104, SER105, VAL113, SER114, TRP119, VAL119, GLU117, GLY119, CYS220, TRG225, GLY228, PHE227, THR228.

It is also possible to define **optional constraints** and specify how many of them must be fulfilled at a minimum. This can be especially helpful for more ambiguous SARs, as it allows key features across multiple chemotypes to be covered.

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Mode Overview

The screenshot displays the Docking software interface. On the left, the 'Define Pharmacophore' panel shows a table with columns for 'Active', 'Optional', 'Name', 'Type', 'Constraint', and 'r(A)'. Below this is a 'Generated Poses (# 30)' table with columns for 'Name', 'Estimated Affinity' (pM, nM, μM, mM), 'LLE', and 'Tor.'. The main 3D view shows a ligand (a benzimidazole derivative) docked into a protein's binding pocket. A red box highlights a specific interaction site. At the bottom left, a chemical structure viewer shows the 2D structure of the ligand. The 'Target View Control' panel at the bottom shows the protein sequence with residues 1-20 highlighted.

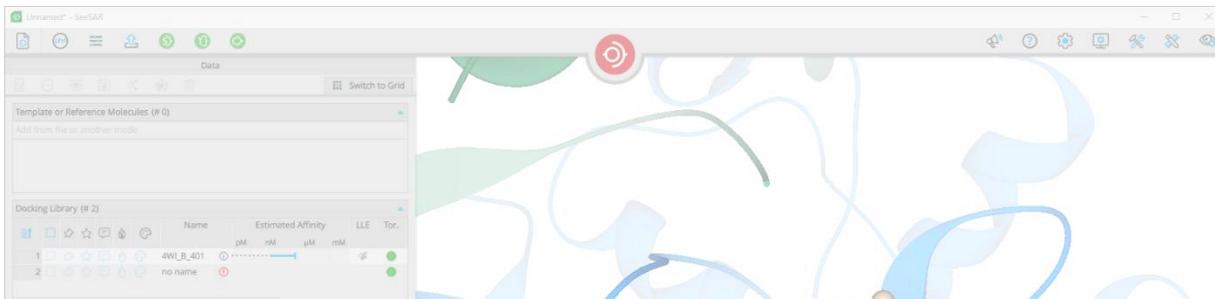
Name	Estimated Affinity	LLE	Tor.			
	pM	nM	μM	mM		
1						
2						
3						
4						
5						
6						
7						
8						
9						
10						
11						
12						
13						
14						
15						
16						
17						
18						
19						
20						
21						
22						

The constraint types 'acceptor interaction contact' and 'donor interaction contact' define the positions where the interaction partner of the ligand's hydrogen-bond donors or acceptors must be located.

Accordingly, 'acceptor interaction contact' means that a donor from the target, or one of its components, must be located within the constraint. Because these 'interaction contact' types are defined by the target, they can usually be set smaller and more precisely.

Table of Content

Mode Overview



5.2. Covalent Docking

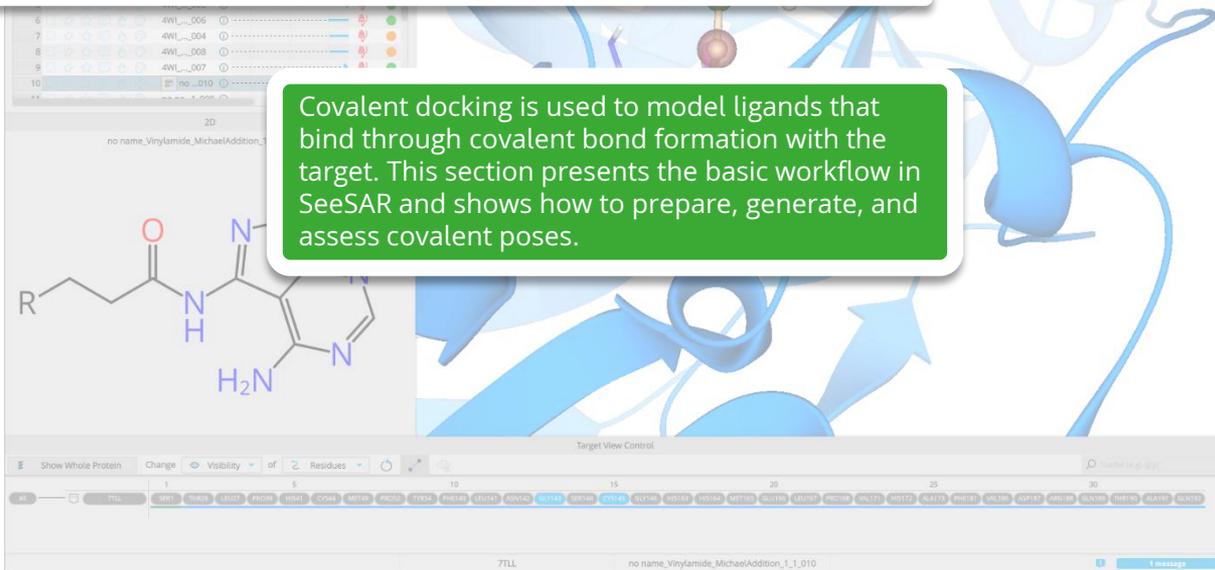


Table of Content

Mode Overview

The screenshot displays the 7TLL software interface. On the left, a panel titled "7TLL - Extract Your Ligand" contains a table of Hetero Groups:

LOI	Name	Estimated Affinity			
		pM	nM	µM	mM
1	Do not extract a ligand				
2	4WL_A_401				
3	4WL_B_401				

A red arrow points to the "Covalently bound" label next to the 4WL_B_401 entry. Below the table is a 2D chemical structure of a ligand, with a red dashed box highlighting a specific atom labeled "R". The main window shows a 3D ribbon representation of a protein structure in blue and green. At the bottom, a "Target View Control" bar shows a sequence of residues from 1 to 30, with "7TLL" and "4WL_B_401" highlighted.

You can perform covalent docking at any PDB protein structure.

PDB files that contain a covalent ligand provide this information upon loading within the info icon.

For this example, we will use the PDB 7TLL.

The linking point is represented as R in the 2D structure.

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Mode Overview

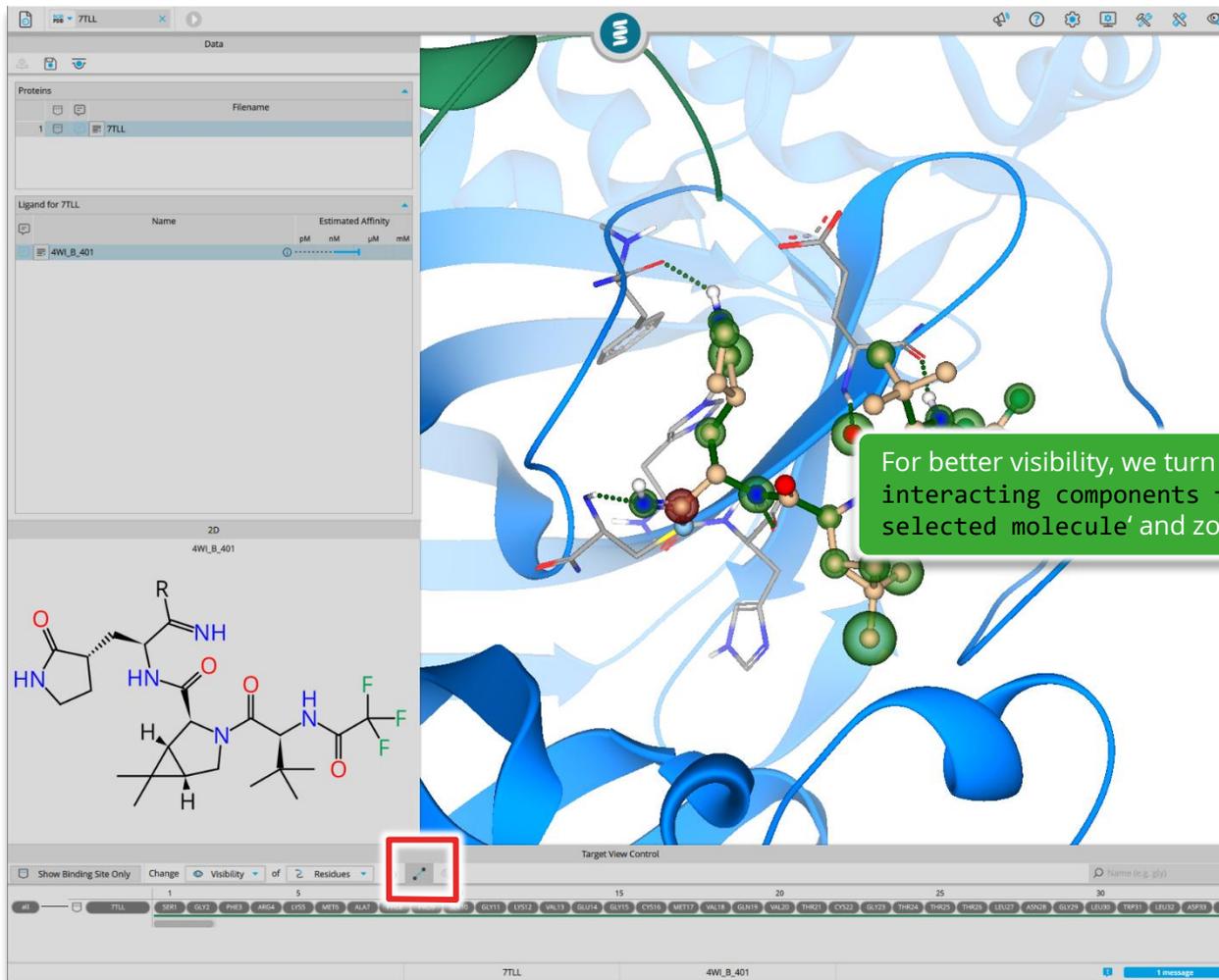


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Mode Overview

Table of Content

Mode Overview

After defining your ligand, transfer it to the **Docking Mode**.

This demo covers docking on a local machine. For remote docking, follow similar steps and additionally refer the remote docking section for details on usage.

Jump to Mode

Proteins	Filename
1	7TLL

Name	Estimated Affinity
4WL_B_401	

2D
4WL_B_401

Target View Control

Show Binding Site Only Change Visibility of Residues

1	5	10	15	20	25	30
SER1	GLY2	PRO3	ARG4	LYS5	MET6	ALA7
PRO8	SER10	GLY11	LYS12	VAL13	GLU14	GLY15
CYS16	MET17	VAL18	GLN19	VAL20	THR21	CYS22
GLY23	THR24	THR25	THR26	LEU27	ASN28	GLY29
LEU30	TRP31	LEU32	ASP33	ASP34	ASP35	ASP36

7TLL 4WL_B_401 1 message

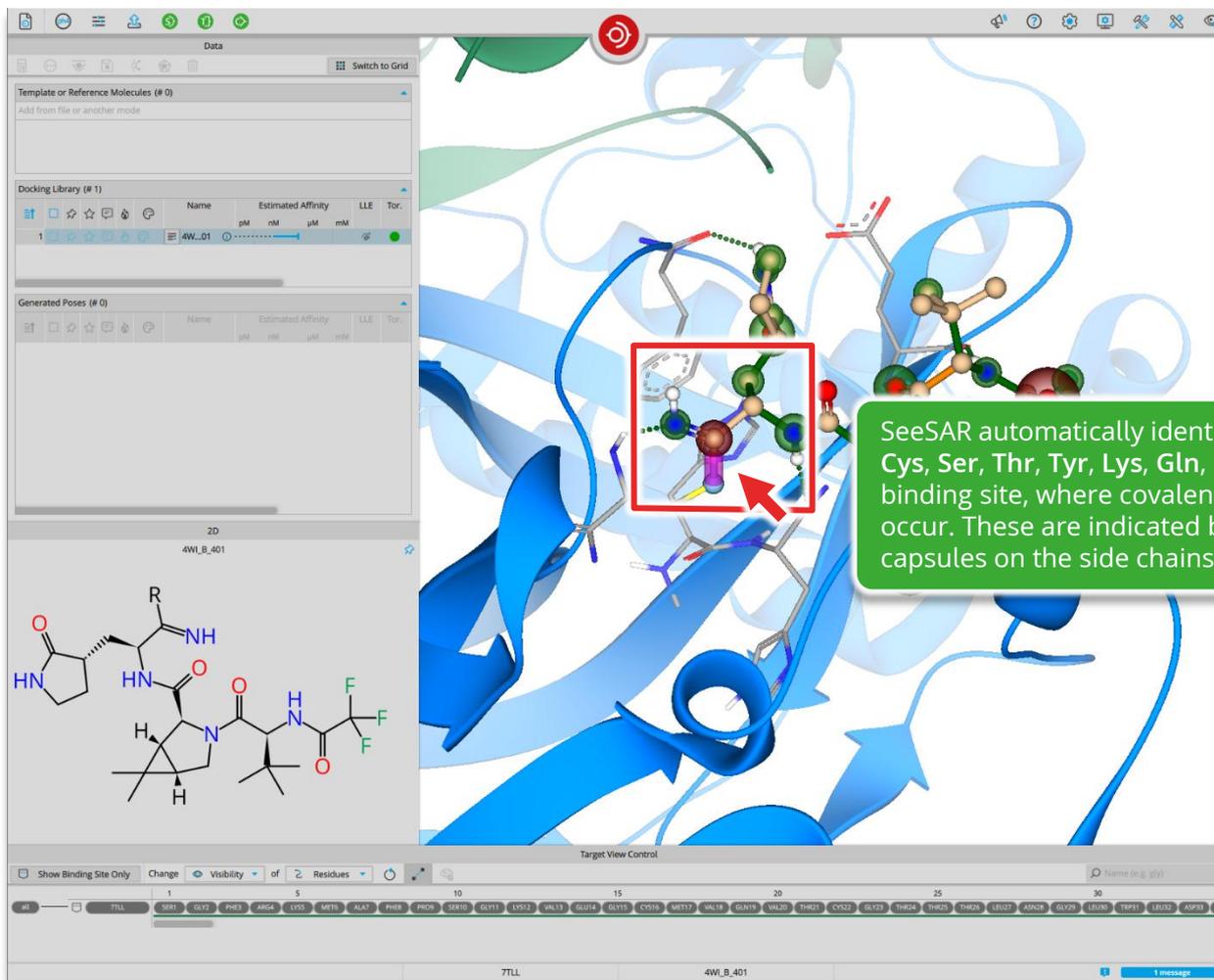


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Mode Overview

The screenshot displays a molecular docking software interface. On the left, there are panels for 'Data', 'Template or Reference Molecules (# 0)', 'Docking Library (# 1)' (containing molecule 1 with ID 4W...01), and 'Generated Poses (# 0)'. Below these is a '2D' view of the molecule 4W1_B_401, showing a complex chemical structure with various functional groups. The main window shows a 3D representation of a protein (blue ribbon) with a ligand (grey sticks) docked in its binding pocket. Green arrows point to specific residues on the protein, with a callout box stating 'Potential covalent attachment points'. Another callout box explains that to select another residue for covalent docking, one should use the 'Target View Control' to make residues visible, and a single click on the corresponding capsule is sufficient, which is visually indicated by the capsule changing to pink. At the bottom, the 'Target View Control' panel is highlighted with a red box, showing a sequence of residues from 1 to 30, with the current residue highlighted in pink.

Potential covalent attachment points

To select one another residues for covalent docking, make them visible with the Target View Control.

A single **click** on the corresponding capsule is sufficient and visually indicated by the color of the capsule changing to pink.

Target View Control

Show Whole Protein Change Visibility of Residues

1 5 10 15 20 25 30

7TL 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30

7TL 4W1_B_401 1 message

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Mode Overview

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Mode Overview

Link to FlexX Guide

Molecules without linker attachments can still be directly loaded into the docking library. Covalent docking automatically identifies warheads and modifies the ligands to attach a covalent linker.

As an example, you can copy and paste SMILES for the following compound:

NC1=C(C(NC(C=C)=O)=NN2)C2=NC=N1

The molecule contains an acrylamide warhead which will be transformed into its bound form during docking.

For details on which warheads are detected per default, refer the FlexX guide.

The screenshot displays the settings panel for a docking simulation. The panel includes the following controls:

- Maximum Number of Poses:** A slider set to 10.
- Clash Tolerance:** A slider with three positions: Standard, Medium, and High.
- Allowed Ring Conformations:** A slider with a 'W' icon below it.
- Allow Stereo Center Flipping:** A slider with four positions: Off, R/S, E/Z, and Both.
- Flexible Covalent Attachment:** A toggle switch currently turned on (green).

Red boxes highlight the menu icon (top left) and the 'Covalent docking' button (top right). A red arrow points from the menu icon to the settings panel.

The pharmacophore and docking parameters can be adjusted as usual.

For covalent docking, the parameter 'Flexible Covalent Attachment' becomes relevant. This allows you to choose whether the terminal bond of the residue involved in covalent attachment should be rotatable. By default, it is set to flexible.

Once all the parameters are set, click the third green docking button ('Covalent docking') to initiate the process.

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Mode Overview

The screenshot displays a molecular docking software interface. The main window shows a 3D representation of a protein (blue ribbon) with a ligand (grey sticks) docked in its binding pocket. The interface includes several panels:

- Data Panel (Top Left):** Contains a 'Template or Reference Molecules (# 0)' section and a 'Docking Library (# 1)' table. The docking library table has columns for Name, Estimated Affinity (pM, nM, μM, mM), LLE, and Tor. One entry is visible: '4W...01' with a green dot in the Tor column.
- Generated Poses Panel (Middle Left):** A table for 'Generated Poses (# 0)' with columns for Name, Estimated Affinity, LLE, and Tor. It is currently empty.
- 2D Panel (Bottom Left):** Shows a 2D chemical structure of the ligand, labeled '4WI_B_401'. The structure is a complex molecule with a central nitrogen atom, a carbonyl group, and a fluorinated side chain.
- Target View Control (Bottom):** A sequence viewer showing the protein sequence from residue 1 to 30. The sequence is: 1 7TLL 5 SER1 THR20 LEU27 PRO39 HIS41 CYS44 MET48 PRO52 TYR54 PHE140 LEU141 ASN142 GLY143 SER144 CYS145 GLY146 HIS153 HIS154 MET156 GLU169 LEU167 PRO169 VAL177 HIS172 MET173 PHE181 VAL188 ASP187 ARG198 GLN199 THR200 ALA192 GLN193.

Your results will be displayed in the 'Generated Poses' table.

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Mode Overview

The screenshot displays a molecular docking software interface. The main window shows a protein structure in blue ribbon representation with a ligand molecule docked in a binding pocket. The interface includes several panels:

- Data Panel:** Contains a 'Template or Reference Molecules (# 0)' section and a 'Docking Library (# 2)' table. The docking library table is as follows:

	Name	Estimated Affinity	LLE	Tor.	
		pM	nM	µM	mM
1	4Wl_B_401	→			
2	no name	→			
- Generated Poses (# 20) Panel:** A table listing 20 generated poses with columns for Name, Estimated Affinity, LLE, and Tor. The table is partially visible, showing poses 1 through 10.
- Chemical Structure Panel:** Shows a chemical structure of a ligand with a red dashed box highlighting the amide group. The structure is: R-CH2-CH2-CH2-C(=O)-NH-Indole. The amide nitrogen is labeled with H, and the indole ring has an NH group and an H2N group.
- Target View Control Panel:** Shows a sequence of residues from 1 to 30, with the current view centered on residue 7 (T7LL).

The automatic transformation of the ligand without a linker can be observed for the acrylamide group. The docking has generated poses with an attachment to this linker.

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Mode Overview



5.3 Remote Docking

For users who prefer not to run docking on their local machines, HPSee (a platform for high-performance computing, learn more [here](#)) allows you to link SeeSAR to a remote system. Using this Mode, you can initiate docking locally from SeeSAR and once completed, review and inspect the top results locally for visualization.

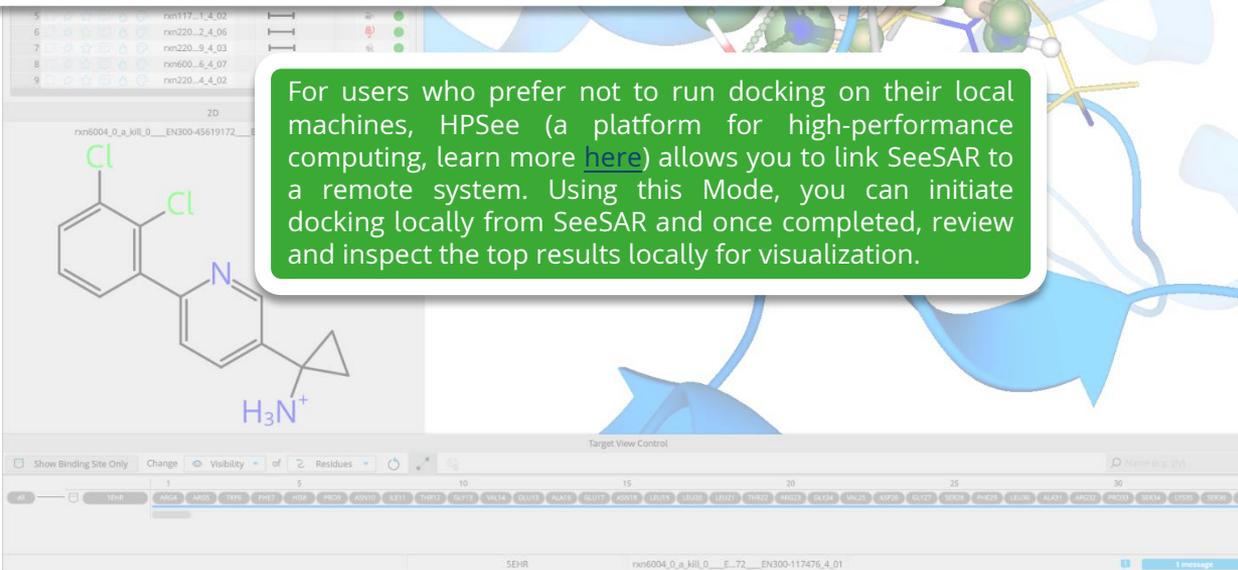
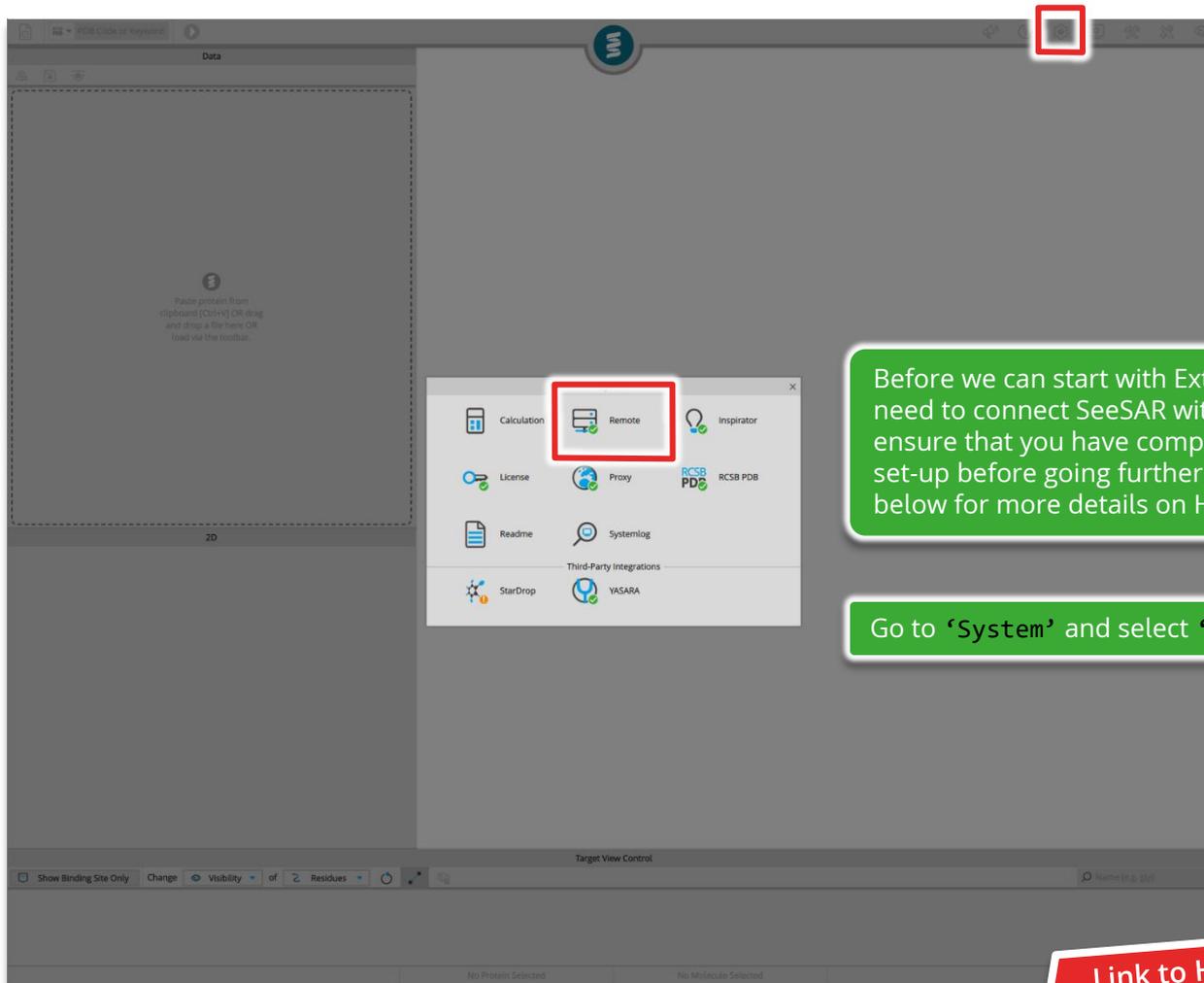


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Mode Overview



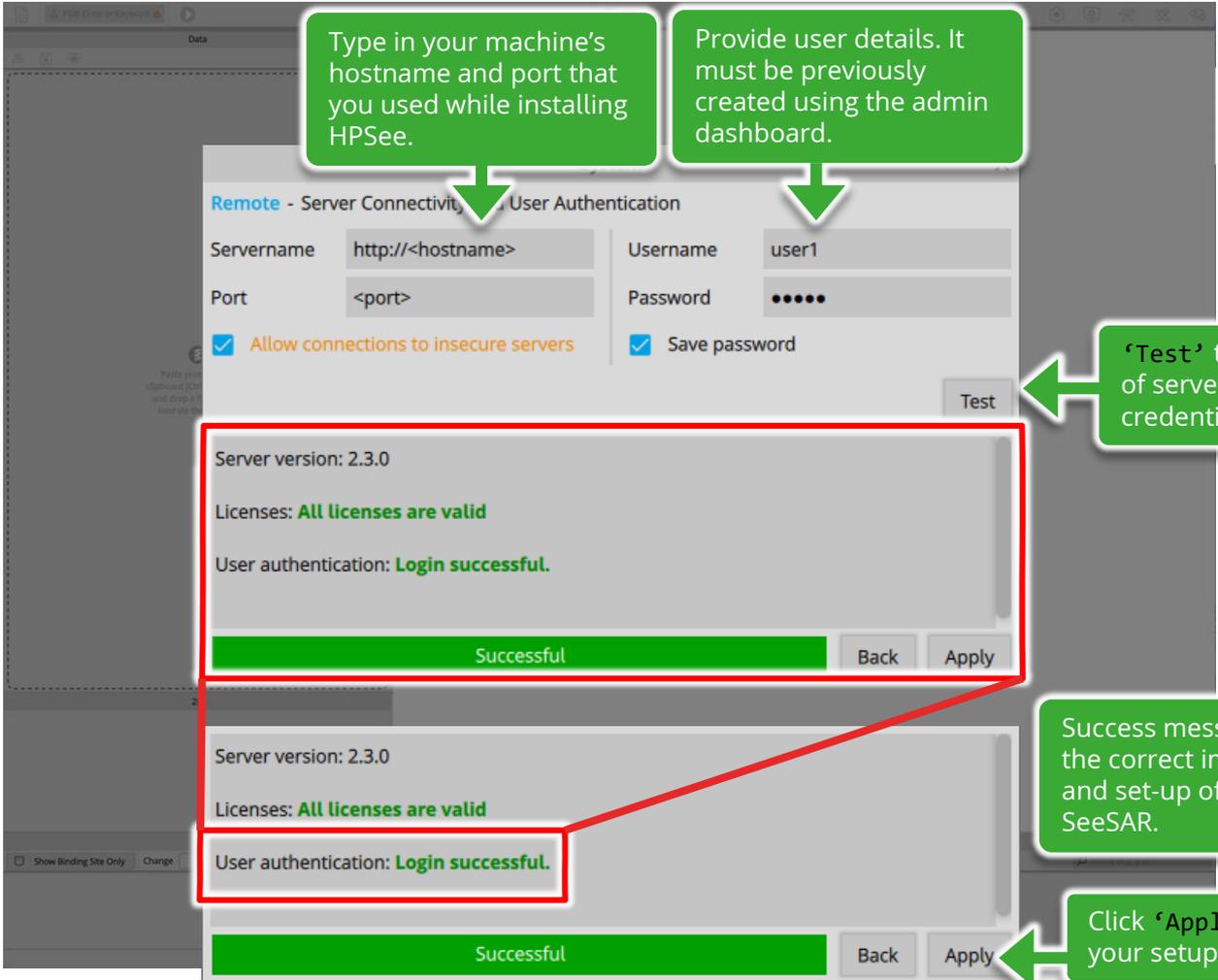
Before we can start with External Docking, we need to connect SeeSAR with HPSee. Please ensure that you have completed your HPSee set-up before going further. Refer to the guide below for more details on HPSee.

Go to 'System' and select 'Remote'.

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Mode Overview

[Link to HPSee Guide](#)



Type in your machine's hostname and port that you used while installing HPSee.

Provide user details. It must be previously created using the admin dashboard.

'Test' to check validity of server and login credentials.

Success message indicates the correct implementation and set-up of HPSee and SeeSAR.

Click 'Apply'. To confirm your setup.

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Mode Overview

The screenshot displays the SEHR software interface. On the left, a table titled "SEHR - Extract Your Ligand" lists various ligand groups. The second row, "50D_A_601", is highlighted. Below the table, the chemical structure of 50D_A_601 is shown. The main window displays a 3D ribbon representation of a protein (Chain A) in blue, with the ligand 50D_A_601 docked in the binding site. A green callout box provides instructions for the demonstration. At the bottom, a "Target View Control" bar shows the protein sequence from residue 1 to 30.

SEHR - Extract Your Ligand				
Hetero Groups				
LOI	Name	Estimated Affinity		
		pM	nM	µM
1	Do not extract a ligand			
2	50D_A_601			
3	PO4_A_602			
4	PO4_A_603			
5	PO4_A_604			
6	50D_B_601			
7	PO4_B_602			
8	PO4_B_603			
9	PO4_B_604			

2D
50D_A_601

Target View Control

Show Binding Site Only Change Visibility of Residues

1 5 10 15 20 25 30

SEHR ARG4 ARG5 TRPE PHE7 HIS8 PRO9 ASN10 LEU11 THR13 GLY13 VAL14 GLU15 ALA16 GLU17 ASN18 LEU19 LEU20 LEU21 THR22 ARG23 GLY24 VAL25 ASP26 GLY27 SER28 PHE29 LEU30 ALA31 ARG32 PRO33 SER34 LYS35 SER36

SEHR 50D_A_601

To demonstrate External Docking, we will use the PDB 5EHR.

Extract ligand 50D_A_601 from Chain A to define the binding site automatically.

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Mode Overview

The screenshot displays the SEHR software interface. On the left, there are panels for 'Proteins' (listing SEHR) and 'Ligand for SEHR' (listing SOD_A_601). Below these is a 2D chemical structure of the ligand. The main window shows a 3D molecular model of the protein (blue ribbon) with the ligand (green and orange spheres) docked. A modal menu is open, showing 'Local' and 'Remote' tabs. The 'Remote' tab is selected, and the 'Docking' option is highlighted with a red box and an arrow. Another red arrow points to the 'Remote' tab. A green callout box contains the text: 'Access Remote Docking Mode by switching into the 'Remote' Modes tab and selecting the Remote Docking Mode.'

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Mode Overview

The screenshot shows the SeeSAR software interface. The main window displays a protein structure in blue ribbon. On the left, there are several panels: 'Data', 'Template or Reference Molecules (# 0)', 'Docking Library (# 0)', and 'Generated Poses (# 0)'. The 'Docking Library (# 0)' panel is highlighted with a red box and contains two sub-sections: 'Molecules' and 'Libraries'. Below these are columns for 'Name', 'Estimated Affinity', and 'LLE'. The 'Generated Poses (# 0)' panel also has similar columns. At the bottom, there is a 'Target View Control' panel with a sequence viewer showing residues from 1 to 30, including SEHR, ARG4, ARG5, TRPE, PHE7, HIS, PRO9, ASN10, LEU11, THR13, GLY13, VAL14, GLU15, ALA16, GLU17, ASN18, LEU19, LEU20, LEU21, THR22, ARG23, GLY24, VAL25, ASP26, GLY27, SER28, PHE29, LEU30, ALA31, ARG32, PRO33, SER34, LYS35, SER36, and ASN37. The status bar at the bottom indicates 'No Molecule Selected' and '1 message'.

The window resembles the **Local Docking Mode**, but now the 'Docking Library' has two sections: 'Molecules' and 'Libraries.'

'Molecules' refers to those molecules you load locally in SeeSAR, but you intend to start docking with the remote machine.

'Libraries' refers to the molecule library already uploaded to the HPSee server.

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Mode Overview

Maximum Number of Solutions

Maximum Number of Poses

Clash Tolerance

Allowed Ring Conformations

Allow Stereo Center Flipping

Flexible Covalent Attachment

Maximum Number of Solutions

Maximum Number of Poses

Clash Tolerance

Allowed Ring Conformations

Allow Stereo Center Flipping

Flexible Covalent Attachment

Target View Control

Show Binding Site Only Change Visibility of Residues

1 5 10 15 20 25 30

SEHR ARG4 ARG5 TRPE PHE7 HIS8 PRO9 ASN10 LEU11 THR13 GLY13 VAL14 GLU15 ALA16 GLU17 ASN18 LEU19 LEU20 LEU21 THR22 ARG23 GLY24 VAL25 ASP26 GLY27 SER28 PHE29 LEU30 ALA31 ARG32 PRO33 SER34 LYS35 SER36 ASN37

SEHR No Molecule Selected 1 message

The pharmacophore and docking parameters can be modified as usual, with an additional docking parameter called 'Maximum Number of Solutions'. This defines how many top poses you wish to retrieve from the docking experiment.

Setting it to a specific number X will return the top X poses, while selecting 'Max' retrieves up to 50,000 poses, which is the maximum capacity allowed by the SeeSAR table.

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Mode Overview

Maximum Number of Solutions: [Slider]

Maximum Number of Poses: [Slider]

Clash Tolerance: [Slider]

Allowed Ring Conformations: [Slider]

Allow Stereo Center Flipping: [Slider]

Flexible Covalent Attachment: [Toggle]

Generated Poses: [List]

Docking Input Filters for Molecules

Add a Filter for

- Properties
- 3D Visibility
- Favorite
- Annotation
- Active Status
- Name
- Optimization State
- Import Source
- Estimated Affinity
- LLE
- LE
- Torsion Quality

Target View Control

Show Binding Site Only | Change | Visibility | of 2 Residues | Name (e.g. gly)

1 5 10 15 20 25 30

SEHR ARG4 ARG5 TRPE PHE7 HIS8 PRO9 ASN10 LEU11 THR12 GLY13 VAL14 GLU15 ALA16 GLU17 ASN18 LEU19 LEU20 LEU21 THR22 ARG23 GLY24 VAL25 ASP26 GLY27 SER28 PHE29 LEU30 ALA31 ARG32 PRO33 SER34 LYS35 SER36 ASN37

SEHR No Molecule Selected 1 message

In 'Docking Input Filters for Molecules', you can select parameters for filtering out molecules before the docking run. These parameters can also include columns from the docking library.

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Mode Overview

The screenshot displays the HPSee software interface. On the left, there are three panels: 'Data' (showing 'Template or Reference Molecules (# 1)' with 'SOD_A_601'), 'Docking Library (# 7)' (highlighted with a red box), and 'Generated Poses (# 0)'. The 'Docking Library' table is as follows:

	Name	Molecules	Uploaded	Description
1	Test_Comp 3D.sdf		26 5 Mar 2026	
2	Enamine_...1029.sdf	436	5 Mar 2026	
3	Library_w_...D.smi.sdf		0 5 Mar 2026	
4	all_scre...r1h1y.sdf		96 5 Mar 2026	trx

The 'Generated Poses' panel is currently empty. The main window shows a blue ribbon representation of a protein structure with a yellow stick model of a docked ligand. A green callout box on the right contains the following text:

For this experiment, we will perform docking using the library already uploaded to the HPSee server.

Instructions on how to upload a library to HPSee are provided in the HPSee Guide.

At the bottom, the 'Target View Control' panel shows a sequence of residues: SEHR, ARG4, ARG5, TRPE, PHE7, HSR, PRO9, ADN10, ILE11, THR13, GLY13, VAL14, GLU15, ALA16, GLU17, ASN18, LEU19, LEU20, LEU21, THR22, ARG23, GLY24, VAL25, ASP26, GLY27, SER28, PHE29, LEU30, ALA31, ARG32, PRO33, SER34, LYS35, SER36, ASP37.

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Mode Overview

The screenshot displays the BioSolveIT software interface. On the left, the 'Data' panel shows the protein 'SEHR' and the ligand 'SOD_A_601'. The main window shows a 3D ribbon representation of the protein with the ligand docked. A 'System' dialog box is open, showing a table of automatic calculations. The 'Calculation' section is highlighted, and the 'Generate Remote Docking Poses' and 'Switch on/off all calculations for this workflow' options are checked and green. A red box highlights these two options. The background shows a 2D chemical structure of the ligand, which is a pyrimidopyrimidinone derivative with a piperidine ring and a quaternary ammonium group.

Calculation	✓	✓	✓	✓	✗
Load Molecules from File	✓	✓	✓	✓	✗
Load Proteins	✓	✓	✓	✓	✗
Save Editor Molecules to Table	✓	✓	✓	✓	✗
Save Inspirator Molecules to Table	✓	✓	✓	✓	✗
Generate Remote Docking Poses	✓	✓	✓	✓	✗
Switch on/off all calculations for this workflow	✓	✓	✓	✓	✗

Before starting the docking process, decide what type of results you would like to retrieve from the server: FlexX (docking only) or HYDE (docking and scoring).

We recommend to use HYDE for rescoring of FlexX generated poses.

Navigate to 'System' and click on 'Calculation'. The 'Generate External Docking Poses' option can be adjusted based on your preference. If you only want docking results, uncheck the boxes.

In this demo, we will retrieve both docked and scored results, so the check marks are enabled and green. Finally, click 'Apply'.

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Mode Overview

100%

Proteins

Filename
1 SEHR

Ligand for SEHR

Name	Estimated Affinity
SOD_A_601	

Copy to Clipboard [Ctrl+C]
Calculate Estimated Affinity
Add Molecule to
Use as Reference in

- Local Docking Mode
- Remote Docking Mode
- Space Docking Mode
- Similarity Scanner

2D
SOD_A_601

CC1(C)CCN1c2nc(N)c3ccc(Cl)c(Cl)c3n2

Target View Control

Show Binding Site Only Change Visibility of Residues

1 5 10 15 20 25 30

SEHR ARG4 ARG5 TRPE PHE7 HIS8 PRO9 ASN10 LEU11 THR12 GLY13 VAL14 GLU15 ALA16 GLU17 ASN18 LEU19 LEU20 LEU21 THR22 ARG23 GLY24 VAL25 ASP26 GLY27 SER28 PHE29 LEU30 ALA31 ARG32 PRO33 SER34 GLY35 SER36 ASN37

SEHR SOD_A_601 1 message

You have the option to perform template docking by adding a template molecule.

In this case, we'll use the co-crystallized ligand as the template. To do this, return to **Proteins Mode**, right-click on the ligand, and select 'Use as Reference in' and 'Remote Docking Mode'.

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Mode Overview

After starting the docking, ensure you 'Save' the SeeSAR project file before initiating docking.

Once the run begins, you may close the SeeSAR project and later reopen to monitor the progress or download the results.

Once the template and all parameters are set, and the docking library is selected using the radio button, click the second green docking button: 'Template Docking'.

This will initiate the process, and the progress can be tracked in SeeSAR via the progress bar.

Docking in Progress (33%)

Template or Reference Molecules (# 1)
SOD_A_601

Docking Library (# 3)			
Molecules	Libraries		
Name	Molecules	Uploaded	Description
100	13 Nov 2025	for external docking mode	
11757	5 Mar 2026		
3	test_compounds.sdf	100	9 Mar 2026

Generated Poses (# 0)			
Name	Estimated Affinity	LLE	Top
pid	pid	pid	pid

Target View Control

Show Binding Site Only Change Visibility of Residues

1 5 10 15 20 25 30

SEHR ARG4 ARG5 TRPE PHE7 HOR PRO9 ASN10 ILE11 THR13 GLY13 VAL14 GLU15 ALA16 GLU17 ASN18 LEU19 LEU20 LEU21 THR22 ARG23 GLY24 VAL25 ASP26 GLY27 SER28 PHE29 LEU30 ALA31 ARG32 PRO33 SER34 LYS35 SER36 ASP37

SEHR No Molecule Selected 1 message

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Mode Overview

The screenshot shows a molecular docking software interface. On the left, there are panels for 'Template or Reference Molecules (# 1)', 'Docking Library (# 3)', and 'Generated Poses (# 0)'. The 'Docking Library' panel contains a table with the following data:

Molecules	Libraries	Name	Molecules	Uploaded	Description
1		2PLO_library.sdf	100	13 Nov 2025	for external docking mode
2		Enamine_c...1k_3D.sdf	11757	5 Mar 2026	
3		test_compounds.sdf	100	9 Mar 2026	

The main view shows a blue ribbon representation of a protein structure with a yellow and blue ligand docked in the binding site. A red box highlights the 'Download Results' button in the top toolbar, which has a sub-menu option 'Download and delete results from server'. A green callout box contains the following text:

When the run is finished, the 'Download Results' button will appear. Be aware that you can only download your results once, and after downloading, all results on the server will be deleted. Click the button to proceed.

At the bottom, there is a 'Target View Control' panel with a sequence viewer showing residues from 1 to 30. The sequence is: SEHR, ARG4, ARG5, TRPE, PHE7, HSR, PRO9, ADY10, ILE11, THR13, GLY13, VAL14, GLU15, ALA16, GLU17, ADY18, LEU19, LEU20, LEU21, THR22, ARG23, GLY24, VAL25, ASP26, GLY27, SER28, PHE29, LEU30, ALA31, ARG32, PRO33, SER34, LYS35, SER36, ASP37.

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Mode Overview

The screenshot displays a molecular docking software interface. On the left, there is a sidebar with the following sections:

- Data:** Includes a 'Switch to Grid' button and a 'Template or Reference Molecules (# 1)' section with 'SOD_A_601'.
- Docking Library (# 3):** A table listing molecules and libraries.
- Generated Poses (# 841):** A table with columns for Name, Estimated Affinity (pM, nM, μM, mM), LLE, and Tor.
- 2D:** A chemical structure of a ligand with a protonated tertiary amine group (H_3N^+).

The main window shows a 3D visualization of a protein structure (blue ribbon) with a docked ligand (grey sticks). A green callout box on the right states: "The visualization options for poses are similar to those in **Local Docking Mode**. You can color the molecules, including the template, or move the poses to **Analyzer Mode**."

At the bottom, there is a 'Target View Control' section with a sequence viewer showing residues from 1 to 30. A second green callout box on the right states: "The **Remote Docking Mode** also supports standard and covalent docking. Similar procedures can be followed for these types of docking."

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Mode Overview

	estimated Affinity	LLE	Tor	Intra-clash	Inter-clash	MPO [Radar]	MW	LogP	TPSA
1	nM	μM	mM				325.41	-0.58	69.5
2							394.47	1.70	95.7
3							353.44	1.57	74.7
4							340.40	2.61	40.6
5							322.41	2.39	49.4
6							323.43	4.08	38.3
7							327.45	2.33	66.0
8							350.46	3.17	49.4
9							323.41	1.98	65.0
10							380.51	1.00	45.1
11							394.54	1.35	45.1

- Estimated Affinity
- LLE
- LE
- Torsion Quality
- Intra Molecular Clash
- Inter Molecular Clash
- Multi-Parameter Opt.
- MW
- LogP
- TPSA

6. Analyzer Mode

The Analyzer Mode is the workspace for reviewing and narrowing down molecule sets. It is used for visual inspection after virtual screening, prioritization and filtering for the most promising molecules.

20

21

22

23

24

25

26

27

28

29

30

2D

rxn6038_0_a_kil_0_..._EN300-16215 EN300-7396612

Target View Control

Show Binding Site Only

Change Color of Residues

1 5 10 15 20 25 30

2ZF GLU1E ALA1E ASP1A CYS1E GLY2E LEU1E ARG1A PRO1E LEU1B PHE1E GLU1B LYS1B LYS1C SER1E LEU1E GLU1E ASP1A LYS1A THR1B GLU1C ARG1D GLU1D SER1P LEU1P LEU1R SER1B THR1B SER1B LEU1E VAL1E GLU1E GLY1E SER1D

2ZF rxn6038_0_a_kil_0_..._E_12_..._EN300-36481_1_010

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Mode Overview

The screenshot displays a software interface with a table of molecules on the left and a 3D protein structure on the right. The table lists 31 molecules with columns for Name, Estimated Affinity (pM, nM, μM, mM), LLE, and Tor. The 3D structure shows a protein backbone in blue with a ligand in red and yellow. A green callout box explains the Analyzer Mode.

Molecules (# 300)	Name	Estimated Affinity				LLE	Tor
		pM	nM	μM	mM		
1	rxn6..._001						
2	rxn603..._1_002						
3	rxn603..._1_003						
4	rxn603..._1_004						
5	rxn603..._1_005						
6	rxn603..._1_006						
7	rxn603..._1_007						
8	rxn603..._1_008						
9	rxn603..._1_009						
10	rxn6..._010						
11	rxn603..._1_001						
12	rxn603..._1_002						
13	rxn603..._1_003						
14	rxn603..._1_004						
15	rxn603..._1_005						
16	rxn6..._006						
17	rxn603..._1_007						
18	rxn603..._1_008						
19	rxn603..._1_009						
20	rxn603..._1_010						
21	rxn6..._001						
22	rxn603..._1_002						
23	rxn603..._1_003						
24	rxn603..._1_004						
25	rxn603..._1_005						
26	rxn603..._1_006						
27	rxn603..._1_007						
28	rxn603..._1_008						
29	rxn603..._1_009						
30	rxn603..._1_010						
31	rxn603..._1_001						

2D
rxn6034_0_a_kill_0__EN300-130956__EN300-19918_1_001

Target View Control
Show Binding Site Only Change Color of Chains

22FF rxn6034_0_a_kill_0__E_56__EN300-19918_1_001

The **Analyzer Mode** is usually used for compound management and orchestration. It offers several possibilities to filter sets and analyze generated results (e.g. from docking to select candidates for a follow up).

Table of Content
Mode Overview

The screenshot displays a docking software interface. On the left, a table lists 31 molecules with columns for Name, Estimated Affinity (pM, nM, μM, mM), LLE, and Tor. A red box highlights a funnel icon in the table, with a callout box stating: "Click to open filter options". Below the table is a 2D chemical structure of a ligand, identified as rxn6034_0_a_kill_0__EN300-130956__EN300-19918_1_001. The 3D view on the right shows a blue protein structure with a ligand (green and red spheres) docked in its binding site. A green callout box on the right states: "After loading a larger set of docking results, you can filter your results by clicking on the funnel icon." The interface also includes a 'Data' panel at the top, a 'Target View Control' at the bottom, and a search bar for chains.

Molecules (# 300)	Name	Estimated Affinity				LLE	Tor	Incl
		pM	nM	μM	mM			
1	rxn6..._001							
2	rxn603..._1_002							
3	rxn603..._1_003							
4	rxn603..._1_004							
5	rxn603..._1_005							
6	rxn603..._1_006							
7	rxn603..._1_007							
8	rxn603..._1_008							
9	rxn603..._1_009							
10	rxn6..._010							
11	rxn603..._1_001							
12	rxn603..._1_002							
13	rxn603..._1_003							
14	rxn603..._1_004							
15	rxn603..._1_005							
16	rxn6..._006							
17	rxn603..._1_007							
18	rxn603..._1_008							
19	rxn603..._1_009							
20	rxn603..._1_010							
21	rxn6..._001							
22	rxn603..._1_002							
23	rxn603..._1_003							
24	rxn603..._1_004							
25	rxn603..._1_005							
26	rxn603..._1_006							
27	rxn603..._1_007							
28	rxn603..._1_008							
29	rxn603..._1_009							
30	rxn603..._1_010							
31	rxn603..._1_001							

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Mode Overview

The screenshot displays the SeeSAR software interface. On the left, a 'Data' panel shows a list of 300 molecules with columns for Name and pKa. A 'Filter' menu is open, allowing users to select properties for filtering. The main window shows a 3D ribbon representation of a protein structure in blue, with a ligand molecule in stick representation. A yellow and black hazard symbol is overlaid on the protein. At the bottom, a 'Target View Control' panel shows a sequence of residues from 1 to 30, with a binding site highlighted. A chemical structure of a ligand is shown in the bottom left corner.

rxn6034_0_a_kill_0__EN300-130956__EN300-19918_1_009

Target View Control

1 5 10 15 20 25 30

22FF rxn6034_0_a_kill_0__E_56__EN300-19918_1_009

Within the filter menu, you can select various parameters that are calculated automatically by SeeSAR, or use SD file-specific column entries.

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Mode Overview

The screenshot displays a molecular docking software interface. On the left, a 'Data' panel lists 300 molecules. A red box highlights the 'All Filters' menu, which includes options like 'Combined Filters', 'Drug-likeness (RO5)', 'Lead-likeness', 'Fragment-likeness (RO3)', 'SMARTS Pattern', 'Properties', and '3D Visibility'. The main view shows a protein structure in blue ribbon representation with a molecule docked in the binding site. A green callout box contains the text: 'Under 'Add a Filter for', you can select preset filters or add the desired filter parameters to the current selection.' At the bottom, a 'Target View Control' panel shows a sequence of residues from 1 to 30, with a binding site highlighted.

Under 'Add a Filter for', you can select preset filters or add the desired filter parameters to the current selection.

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Mode Overview

The screenshot displays a molecular docking software interface. On the left, a 'Data' panel shows a list of 300 molecules with columns for Name and pA. A red box highlights the 'Group Molecules' checkbox, which is checked. Below the list, a 2D chemical structure is shown. The main window displays a 3D protein-ligand model. At the bottom, a 'Target View Control' panel shows a sequence of residues from 1 to 30.

Enabling 'Group Molecules' ensures that only the pose with the best score (HYDE, estimated affinity) is shown, for example from docking or 3D alignment (from the **Docking Mode(s)** and **Similarity Scanner**).

Grouping is always applied after the preset filters: first, all entries that do not match the selected parameters are removed, and then the remaining molecules are grouped.

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Mode Overview

The screenshot displays a molecular docking software interface. On the left, a 'Data' panel lists 300 molecules. A red box highlights a green 'Apply' button in the top-left corner. The central panel shows filter settings for 'Drug-likeness (RO5)', 'Intra Molecular Clash', 'Torsion Quality', and 'Inter Molecular Clash'. Below these are options for 'Pharmacophore: 0 active' and 'Group Molecules'. The main 3D view shows a blue protein structure with a yellow and black striped ligand and a green and orange ligand. A green callout box points to the 'Apply filters' button. At the bottom, a 'Target View Control' panel shows a sequence of residues from 1 to 30, with '2ZF' selected. A 2D chemical structure is shown in the bottom-left corner.

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Mode Overview

Once you are done with applying your filters, initiate the process by clicking on 'Apply filters' button.

The screenshot displays a molecular docking software interface. On the left, a table lists 18 molecules with columns for Name and pK. The 'Apply filters' button in the top-left corner is highlighted with a red box, and the flask icon representing the number of poses is also highlighted with a red box. The central panel shows filter settings for Drug-likeness (RO5), Intra Molecular Clash, Torsion Quality, and Inter Molecular Clash. The main 3D view shows a blue protein structure with a yellow and black striped ligand. A green callout box on the right explains the flask icon's meaning. The bottom panel shows the Target View Control with a residue list.

	Name	pK
1	rxn603..._1_001	
2	rxn603..._1_002	
3	rxn603..._1_001	
4	rxn603..._1_003	
5	rxn603..._1_010	
6	rxn603..._1_004	
7	rxn603..._1_003	
8	rxn603..._1_003	
9	rxn603..._1_001	
10	rxn603..._1_004	
11	rxn603..._1_007	
12	rxn603..._1_005	
13	rxn603..._1_003	
14	rxn603..._1_005	
15	rxn603..._1_008	
16	rxn603..._1_009	
17	rxn603..._1_003	
18	rxn603..._1_009	

Target View Control

1 5 10 15 20 25 30

2ZF GLU16 ALA18 ASP14 CYS1 GLY2 LEU16 ARG4 PRO5 LEU16 PHE7 GLU18 LYS10 LYS10 SER11 LEU12 GLU13 ASP14 LYS14A THR14B GLU14C ARG14D GLU14E LEU14F LEU14G LEU14H SER14I THR14K SER14L SER14M LEU14N LEU14O LEU14P LEU14Q LEU14R LEU14S LEU14T LEU14U LEU14V LEU14W LEU14X LEU14Y LEU14Z

2ZF No Molecule Selected

The number of currently applied filters will be presented next to the 'Apply filters' button. The number of poses that survived the filtering process will be presented in the flask icon.

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Mode Overview

The screenshot displays a molecular docking software interface. On the left, a table lists 18 molecules with columns for estimated Affinity (nM, μM, nM), LLE, Tor, Intra-clash, Inter-clash [Radar], MPO, MW, LogP, and TPSA. The main view shows a 3D protein target with a ligand docked. A 'Multi-Parameter Optimization' dialog box is open, featuring a radar plot and sliders for MW (200-500), LogP (5 to -5), and TPSA (30-200). Below the sliders is an 'Add Property' section with a dropdown menu. At the bottom of the dialog, there are 'Molecule 1 / 18' navigation buttons, 'Cancel', and 'Apply & Close' buttons. Red arrows point to the 'Add Property' dropdown and the 'Molecule 1 / 18' navigation buttons.

Molecules (# 18)	Checked (# 18)	estimated Affinity	LLE	Tor	Intra-clash	Inter-clash [Radar]	MPO	MW	LogP	TPSA
1		nM						294.47	1.70	95.7
2		μM						353.44	1.57	74.3
3		nM						340.40	2.61	40.6
4								322.41	2.39	49.4
5								323.43	4.08	38.3
6								327.45	2.33	66.0
7								350.46	3.17	49.4
8								380.51	1.00	45.1
9								323.43	3.83	29.5
10								322.41	2.54	49.4
11								336.43	3.13	40.6
12								362.47	3.65	49.4
13								361.44	2.99	73.2
14								364.49	3.73	49.4
15								360.45	3.10	49.4
16								370.42	3.53	58.6
17								356.44	4.01	41.6
18								410.49	1.38	103.3

In this window, you can define the desired parameter ranges and add new properties. Use the arrow keys to browse through the radar plots of the selected molecules.

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Mode Overview

The screenshot displays a software interface for molecular docking. On the left, a table lists 30 molecules with various parameters. The 'MPO radar' column is highlighted with a red box, showing traffic light indicators for each molecule. A green callout box explains that these plots are represented by a traffic light gradient: green if all parameters are within defined ranges, and red if all are outside. The 'Molecules' table header is also highlighted with a red box, and a green callout box notes that it can be scrolled using a bar at the bottom and resized by dragging its edge. A blue icon at the end of the table allows adding parameters not shown. The main view shows a 3D protein structure in blue with a ligand in stick representation. A chemical structure is shown at the bottom left, and a 'Target View Control' bar is at the bottom.

Molecules (# 30)	Checked (# 3)	Estimated Affinity	LLE	Tor.	Intra-clash	Inter-clash	MPO radar	MW	LogP	TPSA
1		25.41	-0.58	69				25.41	-0.58	69
2		194.47	1.70	95.5				194.47	1.70	95.5
3		53.44	1.57	74.3				53.44	1.57	74.3
4		40.40	2.61	40.6				40.40	2.61	40.6
5		22.41	2.39	49.4				22.41	2.39	49.4
6		23.43	4.08	38.3				23.43	4.08	38.3
7		27.45	2.33	66.0				27.45	2.33	66.0
8		50.46	3.17	49.4				50.46	3.17	49.4
9		73.41	1.98	65.0				73.41	1.98	65.0
10		80.51	1.00	45.1				80.51	1.00	45.1
11		94.54	1.35	45.1				94.54	1.35	45.1
12		23.43	3.83	29.5				23.43	3.83	29.5
13		22.41	2.54	49.4				22.41	2.54	49.4
14		36.43	3.13	40.6				36.43	3.13	40.6
15		62.47	3.65	49.4				62.47	3.65	49.4
16		61.44	2.99	73.2				61.44	2.99	73.2
17		64.49	3.73	49.4				64.49	3.73	49.4
18		60.45	3.10	49.4				60.45	3.10	49.4
19		80.49	2.90	58.6				80.49	2.90	58.6
20		80.51	1.56	45.1				80.51	1.56	45.1
21		370.42	3.53	58.6				370.42	3.53	58.6
22		356.44	4.01	41.6				356.44	4.01	41.6
23		447.35	2.65	86.3				447.35	2.65	86.3
24		337.42	3.34	52.7				337.42	3.34	52.7
25		354.43	2.21	86.3				354.43	2.21	86.3
26		382.48	2.33	95.1				382.48	2.33	95.1
27		365.47	3.46	61.4				365.47	3.46	61.4
28		353.44	1.75	74.3				353.44	1.75	74.3
29		393.48	2.51	69.7				393.48	2.51	69.7

The MPO radar plots are represented in the table by a traffic light gradient: green if all parameters are within the defined ranges, and red if all of them are outside.

The 'Molecules' table can be scrolled using the bar at the bottom. Dragging the edge can be used to resize it. If a parameter is not shown, it can be added using the blue icon at the end of the table.

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Mode Overview

The screenshot displays a molecular docking software interface. On the left, a table lists 80 molecules with various properties. A red box highlights the 'Define pharmacophore' button in the top-left corner. The main view shows a protein structure in blue with a ligand molecule in green and orange. A green callout box contains text explaining how to filter by 3D molecular features. At the bottom, a 2D chemical structure is shown, and a 'Target View Control' bar is visible.

Molecules (# 300)	(Checked (# 18))	estimated Affinity	LLE	Tor.	Intra-clash	Inter-clash	MPO [Radar]	MW	LogP	TPSA
		nM	μM	mM						
50								322.41	2.39	49.4
51								323.43	4.08	38.3
52								323.43	4.08	38.3
53								323.43	4.08	38.3
54								323.43	4.08	38.3
55								323.43	4.08	38.3
56								323.43	4.08	38.3
57								323.43	4.08	38.3
58								323.43	4.08	38.3
59								323.43	4.08	38.3
60								323.43	4.08	38.3
61								327.45	2.33	66.0
62								327.45	2.33	66.0
63								327.45	2.33	66.0
64								327.45	2.33	66.0
65								327.45	2.33	66.0
66								327.45	2.33	66.0
67								327.45	2.33	66.0
68								327.45	2.33	66.0
69								327.45	2.33	66.0
70								327.45	2.33	66.0
71								350.46	3.17	49.4
72								350.46	3.17	49.4
73								350.46	3.17	49.4
74								350.46	3.17	49.4
75								350.46	3.17	49.4
76								350.46	3.17	49.4
77								350.46	3.17	49.4
78								350.46	3.17	49.4
79								350.46	3.17	49.4
80								350.46	3.17	49.4

2D
rxn6038_0_a_kil_0____EN300-16215 EN300-7396612____EN300-36481_1_010

Target View Control

Show Binding Site Only Change Color of Residues

1 5 10 15 20 25 30
2ZF GLU16 ALA18 ASP14 CYS1 GLY2 LEU18 ARG4 PRO5 LEU16 PHE7 GLU18 LYS10 LYS10 SER11 LEU12 GLU13 ASP14 LYS14A THR14B GLU14C ARG14D GLU14E LEU14F LEU14G GLU14H SER14I THR14K SER14L SER14M VAL17 GLU18 GLY19 SER20

2ZF rxn6038_0_a_kil_0____E_12____EN300-36481_1_010

It is also possible to filter by 3D molecular features (pharmacophore constraints). To do this, you first need to define the 3D features using 'Define Pharmacophore'.

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Mode Overview

The screenshot displays a molecular docking software interface. A protein structure is shown in light blue ribbon representation. A ligand molecule is docked in the binding site, shown in stick representation with green and orange atoms. A dialog box titled "Define Pharmacophore" is open, with a red box highlighting it. The dialog contains the text "New spheres will be created in center of selected objects." and a "Define New Constraint" button. Below the dialog is a table of constraints. At the bottom left, a 2D chemical structure of the ligand is shown. At the bottom right, a "Target View Control" bar shows the protein sequence from residue 1 to 30.

Residue	Atom	Distance	Angle	Planarity
58		323.43	4.08	38.3
59		323.43	4.08	38.3
60		323.43	4.08	38.3
61		327.45	2.33	66.0
62		327.45	2.33	66.0
63		327.45	2.33	66.0
64		327.45	2.33	66.0
65		327.45	2.33	66.0
66		327.45	2.33	66.0
67		327.45	2.33	66.0
68		327.45	2.33	66.0
69		327.45	2.33	66.0
70		327.45	2.33	66.0
71		350.46	3.17	49.4
72		350.46	3.17	49.4
73		350.46	3.17	49.4
74		350.46	3.17	49.4
75		350.46	3.17	49.4
76		350.46	3.17	49.4
77		350.46	3.17	49.4
78		350.46	3.17	49.4
79		350.46	3.17	49.4
80		350.46	3.17	49.4

Add a new feature with 'Define New Constraint'.

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Mode Overview

The screenshot displays a molecular docking software interface. On the left, a 'Define Pharmacophore' panel includes a 'Mole' section with a 'Set Sphere to Center' button highlighted by a red box. Below this is a table of pharmacophore features. The main 3D view shows a protein structure in blue with a ligand in green and orange. A red box highlights a purple sphere on the ligand, with red arrows pointing to it. A green callout box explains that this sphere can be positioned by left-clicking or by selecting heavy atoms and using the 'Set sphere to center of selected objects' command. At the bottom, a 'Target View Control' panel shows a sequence of residues from 1 to 20.

Residue	Feature	Color	Distance	Score	Score
53					
54					
55					
56	I	Red	323.43	4.08	38.3
57	I	Red	323.43	4.08	38.3
58	I	Red	323.43	4.08	38.3
59	I	Red	323.43	4.08	38.3
60	I	Red	323.43	4.08	38.3
61					
62	>	Green	327.45	2.33	66.0
63	>	Green	327.45	2.33	66.0
64	>	Green	327.45	2.33	66.0
65	>	Green	327.45	2.33	66.0
66	>	Green	327.45	2.33	66.0
67	>	Green	327.45	2.33	66.0
68	>	Green	327.45	2.33	66.0
69	>	Green	327.45	2.33	66.0
70	>	Green	327.45	2.33	66.0
71	I	Red	350.46	3.17	49.4
72	I	Red	350.46	3.17	49.4
73	I	Red	350.46	3.17	49.4
74	I	Red	350.46	3.17	49.4
75	I	Red	350.46	3.17	49.4
76	I	Red	350.46	3.17	49.4
77	I	Red	350.46	3.17	49.4
78	I	Red	350.46	3.17	49.4
79	I	Red	350.46	3.17	49.4
80	I	Red	350.46	3.17	49.4

Chemical structure: O=C(NCC1=CC=CC=C1)C2=CC=CC=C2

The generated sphere can be positioned at the desired location in 3D by dragging them with a left-click.

Alternatively, you can select one or more heavy atoms (selected atoms are highlighted in purple) and position the sphere using 'Set sphere to center of selected objects'.

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Mode Overview

Molecules (# 15)	Checked (# 1)	Estimated Affinity	LLE	Tor.	Intra-clash	Inter-clash	MPO [Radar]	MW	LogP	TPSA				
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	II	327.45	2.33	66.0	●	●	●	327.45	2.33	66.0	●	●	●	●
2	II	380.51	1.00	45.1	●	●	●	380.51	1.00	45.1	●	●	●	●
3	II	322.41	2.54	49.4	●	●	●	322.41	2.54	49.4	●	●	●	●
4	II	322.41	2.54	49.4	●	●	●	322.41	2.54	49.4	●	●	●	●
5	II	362.47	3.65	49.4	●	●	●	362.47	3.65	49.4	●	●	●	●
6	II	360.45	3.10	49.4	●	●	●	360.45	3.10	49.4	●	●	●	●
7	II	380.49	2.90	58.6	●	●	●	380.49	2.90	58.6	●	●	●	●
8	II	354.43	2.21	86.3	●	●	●	354.43	2.21	86.3	●	●	●	●
9	II	354.43	2.21	86.3	●	●	●	354.43	2.21	86.3	●	●	●	●
10	II	365.47	3.46	61.4	●	●	●	365.47	3.46	61.4	●	●	●	●
11	II	365.47	3.46	61.4	●	●	●	365.47	3.46	61.4	●	●	●	●
12	II	365.47	3.46	61.4	●	●	●	365.47	3.46	61.4	●	●	●	●
13	II	365.47	3.46	61.4	●	●	●	365.47	3.46	61.4	●	●	●	●
14	II	365.47	3.46	61.4	●	●	●	365.47	3.46	61.4	●	●	●	●
15	II	365.47	3.46	61.4	●	●	●	365.47	3.46	61.4	●	●	●	●

Chemical structure: c1ccc(cc1)CN(C)C(=O)Cc2ccccc2

Target View Control: Show Binding Site Only | Change | Color | Residues | Name (e.g. gly)

Residues: 1 5 10 15 20 25 30

Residues: 22FF | GLU12 | ALA18 | ASP14 | CYS1 | GLY2 | LEU18 | ARG4 | PRO5 | LEU16 | PHE7 | GLU18 | LYS10 | LYS10 | SER11 | LEU12 | GLU13 | ASP14 | LYS14A | THR14B | GLU14C | ARG14D | GLU14E | LEU14F | LEU14G | GLU14H | SER14I | THR14J | SER14K | SER14L | VAL17 | GLU18 | GLY19 | SER20 | ASP22

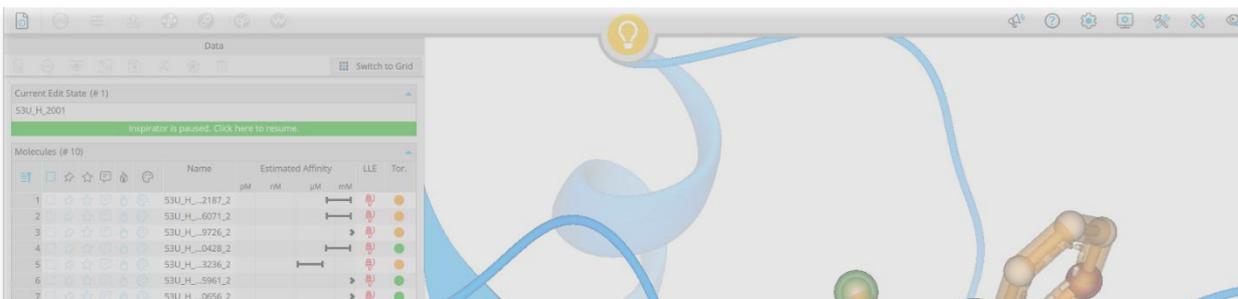
The number of currently active pharmacophore constraints will be displayed next to the icon.

Additional details of pharmacophore constraints are explained in the dedicated section.

Jump to Section

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Mode Overview



7. Inspirator

Inspirator Mode helps you explore ways to improve your compound. Grow into unoccupied binding sites, test small modifications, or even replace entire scaffolds.

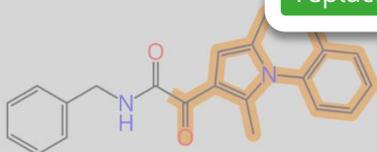


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Mode Overview



The screenshot displays the ZZZF software interface. At the top left, a dropdown menu shows 'ZZZF' (1) and a play button (2). A red box highlights the play button with the number '3.' next to it. The main window is titled 'ZZZF - Extract Your 1. and' and contains a table of Hetero Groups:

	Name	Estimated Affinity
		pM nM μ M mM
1	Do not extract a ligand	
2	53U_H_2001	

Below the table, a 2D chemical structure of the ligand 53U_H_2001 is shown. The main 3D view shows a protein structure in blue ribbon representation with a ligand in stick representation. A green callout box contains the text: 'For this guide we will use PDB 2ZFF as example. Load it in the **Proteins Mode** and select a ligand to work with.'

At the bottom, the 'Target View Control' panel shows a sequence of residues from 1 to 30, with 'ZZFF' and '53U_H_2001' selected.

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Mode Overview

The screenshot displays the software interface for molecular docking. On the left, a 'Data' panel shows a table of proteins and ligands. The 'Ligand for Z2FF' table lists the molecule '53U_H_2001'. A red box highlights the 'Use as Reference in' menu option, which is set to 'Inspirator'. Below the table, the 2D chemical structure of the ligand is shown. On the right, a 3D visualization of the protein-ligand complex is displayed. A green callout box contains the text: 'Transfer your ligand to the **Inspirator Mode** with a right-click on the molecule in the table.'

Proteins	Filename
1	Z2FF

Ligand for Z2FF	
Name	Estimated Affinity
	pM nM μ M mM
53U_H_2001	

2D
53U_H_2001

C1CCN(C1)C(=O)N(Cc2ccccc2)C(=O)N(Cc3ccccc3)C(=O)N

Target View Control

Show Binding Site Only Change Visibility of Residues

1	5	10	15	20	25	30
GLU1C	ALA1B	ASP1A	CYS1	GLY2	LEU3	ARG4
PRO5	LEU6	PHE7	GLU8	LYS9	LYS10	SER11
LEU12	GLU13	ASP14	LYS16A	THR16B	GLU16C	ARG16D
GLU16E	LEU16F	LEU16G	GLU16H	SER16I	THR16J	LEU16K
LEU16L	VAL17	GLU18	GLY19	SER20	ASP	

Z2FF 53U_H_2001 1 message

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Mode Overview

Current Edit State (# 1)
53U_H_2001

Molecules (# 1)

Name	Estimated Affinity	LLE	Tor.
1 53U_H_2001	pM mM μM mM		

2D
53U_H_2001

Target View Control

Show Binding Site Only Change Visibility of Residues

1	5	10	15	20	25	30																												
22FF	GLUC	ALAN	ASPA	CYS1	GLY2	LEU3	ARG4	PRO5	LEU6	PHI7	GLU8	LYS9	LYS10	SER11	LEU12	GLU13	ASP14	LYS14A	THR14B	GLU14C	ARG14D	GLU14E	LEU14F	LEU14G	GLU14H	SER14I	THR14J	LEU14K	LEU14L	VAL17	GLU18	GLY19	SER20	ASP

The **Inspira Mode** features several tools and applications to generate ideas how to improve your compound or to find novel scaffolds.

Linking & Merging:
Connects two fragments

Analoging:
Creates a series of analogs

ReCore:
Replaces scaffolds

FastGrow:
Grows into binding pockets

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Mode Overview

The screenshot shows the SeeSAR software interface. On the left, there is a 'Data' panel with 'Current Edit State (# 1)' and 'Molecules (# 1)' sections. The main window displays a 3D molecular model of a protein-ligand complex. A 'System' menu is open in the center, with 'Inspirator' highlighted by a red box. Below the menu, a 2D chemical structure of the ligand is shown. At the bottom, there is a 'Target View Control' panel with a sequence viewer showing residues from 1 to 30.

ReCore: This tool screens millions of molecular fragments to identify 3D scaffold replacements. To use it, download and add a ReCore index (fragment library) to SeeSAR.

ReCore indices can be accessed and downloaded directly from SeeSAR or from our website:

Download more files

Got to 'System' and select 'Inspirator'.

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Mode Overview

Here you can download and add ReCore files to SeeSAR. Once you are done adding your indices, confirm everything with 'Apply'. Then you can close the window.

System

one indices and fragment growing files for inspirator mode.

ReCore Indices	Fragment Growing Files
<input type="radio"/> Inspirator.PDB2022-06_pkg	<input type="radio"/> FastGrowDB_51k_2024-05
<input type="radio"/> maglrings3D_2022-05	<input type="radio"/> FastGrowDB_61k_2024-05
<input type="radio"/> recore	<input type="radio"/> FastGrowDB_61k_2024-05
<input type="radio"/> ErtlLinkers	<input type="radio"/> FastGrowDB_24k_2023-03
<input type="radio"/> Inspirator.PDB2022-06_pkg	<input type="radio"/> hinge_binders_44k

A valid ReCore index is selected.

Target View Control

Show Binding Site Only Change Visibility of Residues

1 5 10 15 20 25 30

GLUC1C ALA18 ASP14A CYS1 CYS2 LEU18 ARG4 PRO5 LEU16 PHE7 GLU8 LYS9 LYS10 SER11 LEU12 GLU13 ASP14 LYS14A THR14B GLU14C ARG14D GLU14E LEU14F LEU14G LEU14H SER14B THR14A SER14K SER14L MET14 VAL17 GLU18 GLY19 SER22 ASP

22FF No Molecule Selected

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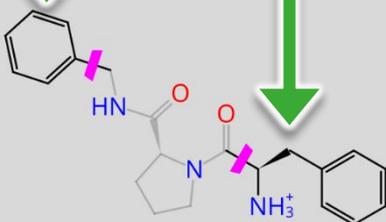
Mode Overview

Click on a bond to set a constraint (exchange vector) on your molecule—in either 2D or 3D view.

Clicking the same bond again toggles the vector direction, defining which part of the molecule to keep and which to replace.

A third click removes the vector entirely.

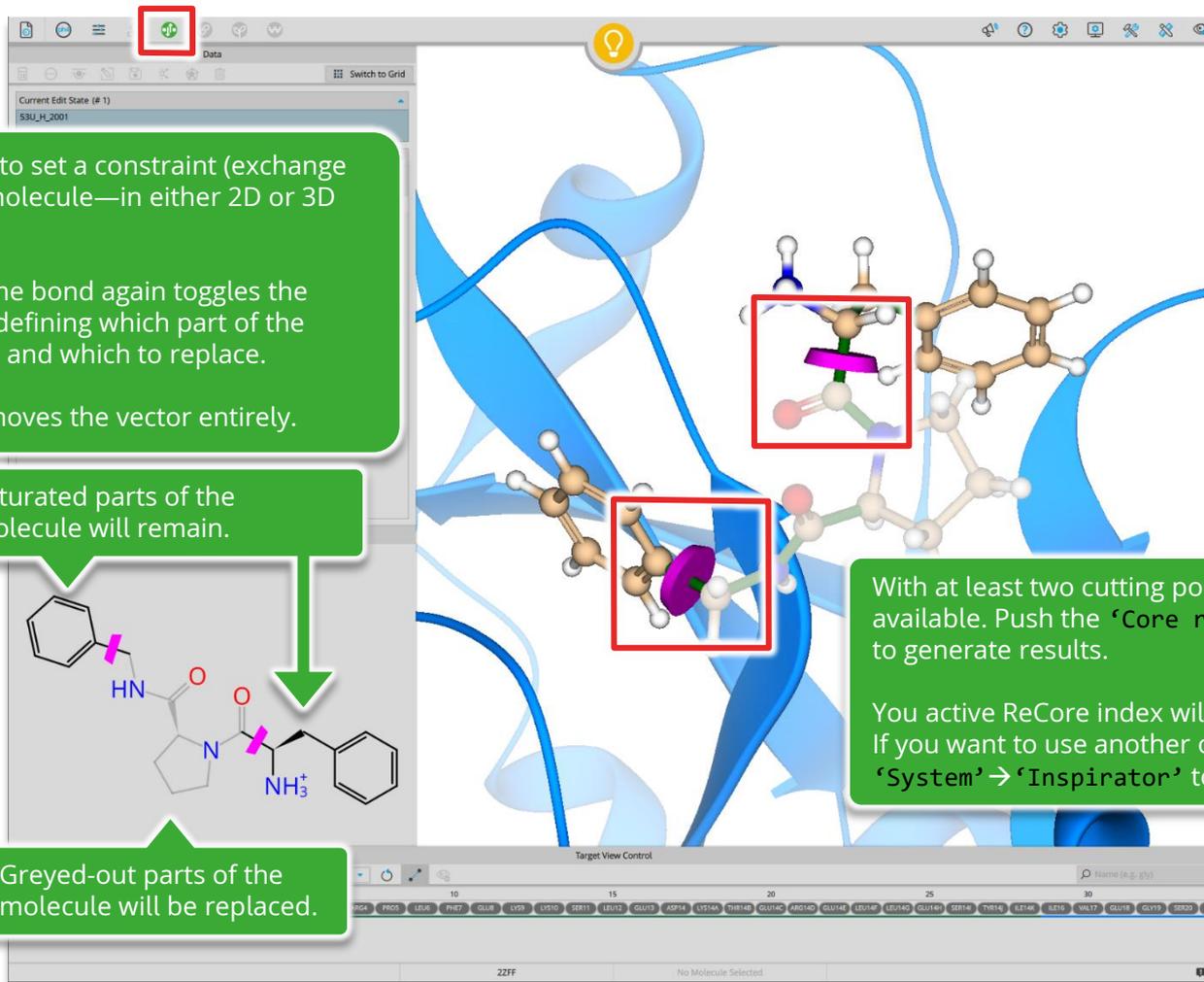
Saturated parts of the molecule will remain.



Greyed-out parts of the molecule will be replaced.

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Mode Overview



With at least two cutting points ReCore becomes available. Push the 'Core replacement' button to generate results.

You active ReCore index will be used for this. If you want to use another one, go back to 'System' → 'Inspirator' to change the index.

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Mode Overview

Once the computation is complete, the results will appear in the Molecules' table.

The region replaced by ReCore will be highlighted within each resulting molecule.

Molecules (# 10)	Name	Estimated Affinity				LLE	Tor.
		pM	nM	μ M	mM		
1	S3U___1						
2	S3U_H_X___1						
3	S3U___1						
4	S3U___1						
5	S3U___1						
6	S3U_H_D___1						
7	S3U_H_B___1						
8	S3U_H_C___1						
9	S3U_H_E___1						
10	S3U_H_E___1						

Target View Control

1 5 10 15 20 25 30

22FF GLU1C ALA1B ASP1A CYS1 GLY2 LEU3 ARG4 PRO5 LEU6 PHE7 GLU8 LYS9 LYS10 SER11 LEU12 GLU13 ASP14 LYS16A THR16B GLU16C ARG16D GLU16E LEU16F LEU16G LEU16H SER16I THR16K SER16L SER16M VAL17 GLU18 GLY19 SER20

22FF S3U_H_2001_6115_PEF_1_a_605_RB___1

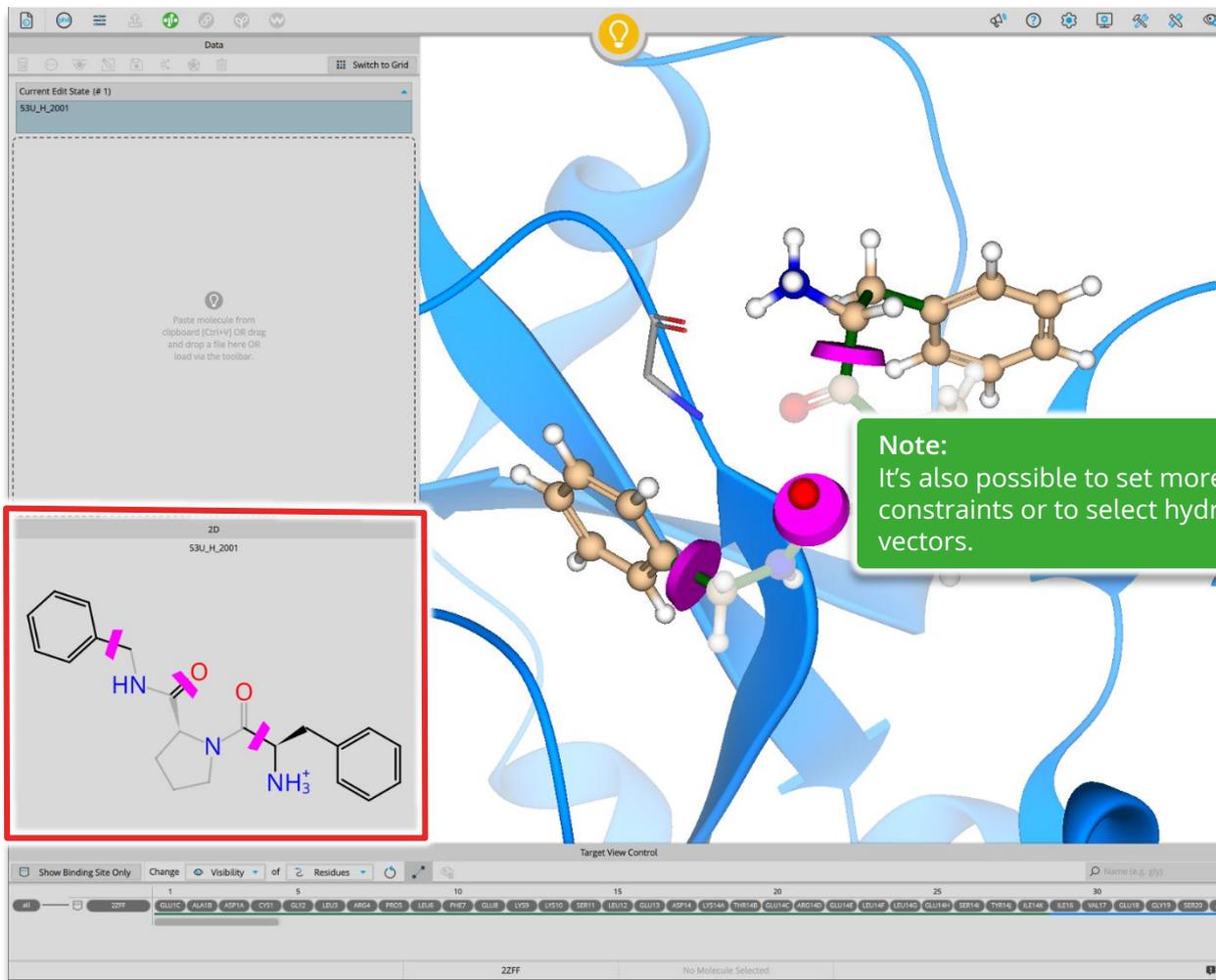
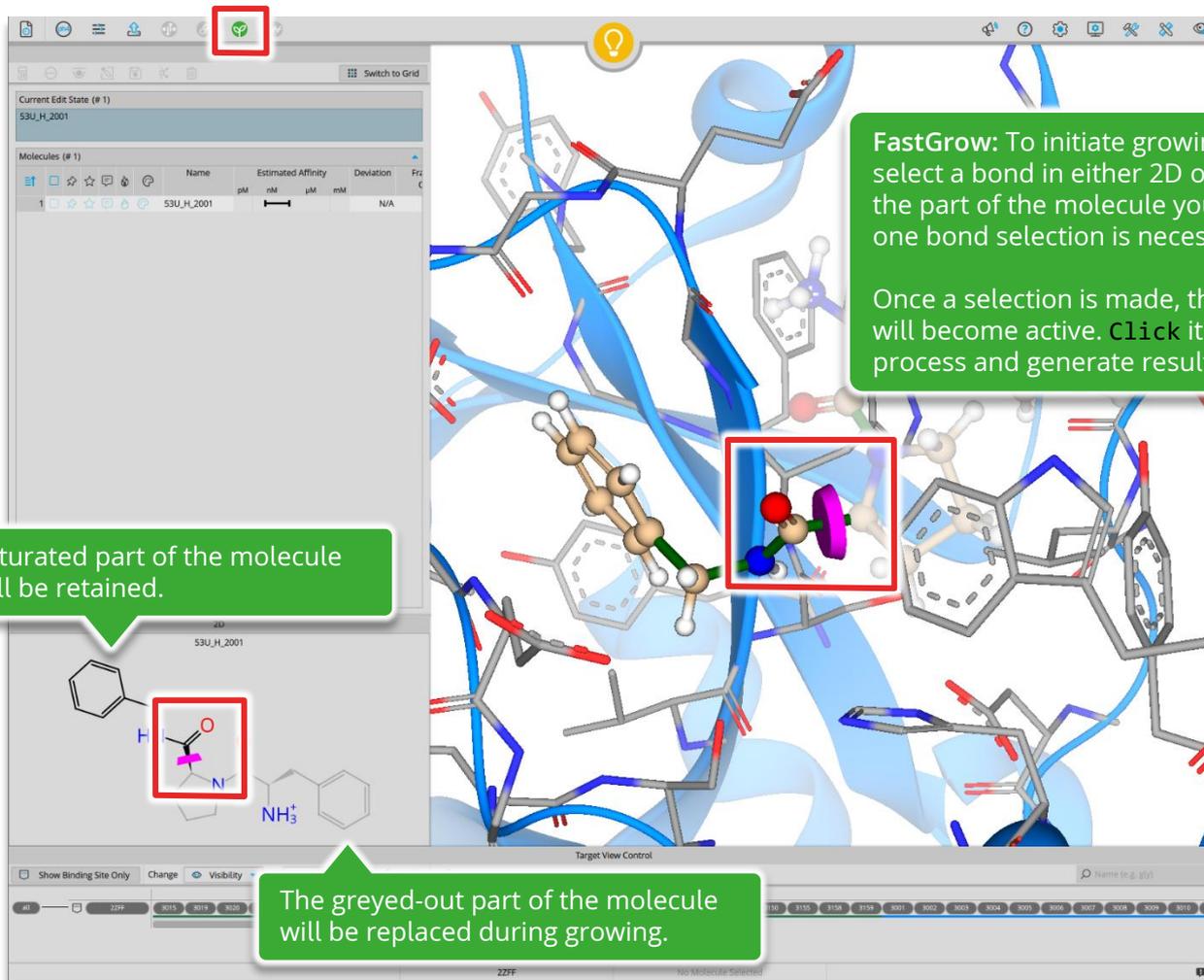


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Mode Overview



The screenshot displays a molecular docking software interface. The central part shows a protein structure in blue ribbon representation with a ligand molecule docked in a binding pocket. The ligand is shown in a stick representation with green and orange atoms. A green callout box explains that the results will be listed in the 'Molecules' table and that the grown part will be highlighted, with the name of the fragment used appended to the molecule's name.

Below the protein view, there is a 'Molecules (# 10)' table with the following columns: Name, Estimated Affinity (pM, nM, μM, mM), LLE, and Tor. The table contains 10 rows of molecule data, with the last row (10) highlighted in blue. A red box highlights the entire table.

Below the table, there is a '2D' view showing the chemical structure of the molecule 53U_H_2001_CSS800000286055_2. The structure is a complex organic molecule with a benzene ring, a carbonyl group, and a nitrogen atom. A green callout box notes that you can also select any bond to grow from, even a single hydrogen.

At the bottom, there is a 'Target View Control' section with a sequence of residues: 1 5 10 15 20 25 30. The residues are: 22FF, GLU1C, ALA1B, ASP1A, CYS1, GLY2, LEU3, ARG4, PRO5, LEU6, PHE7, GLU8, LYS9, LYS10, SER11, LEU12, GLU13, ASP14, LYS16A, THR16B, GLU16C, ARG16D, GLU16E, LEU16F, LEU16G, GLU16H, SER16I, THR16J, LEU16K, LEU16L, VAL17, GLU18, GLY19, SER20, ARG21.

The results will be listed in the 'Molecules' table.

The grown part will be **highlighted**, and the name of the fragment used is appended to the molecule's name.

Note:
You can also select any bond to grow from, even a single hydrogen.

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Mode Overview

The screenshot displays the SeeSAR software interface. On the left, a 'Data' panel shows the 'Current Edit State (# 1)' as 'S3U_H_2001'. Below this is a 'Molecules (# 10)' table with columns for Name, Estimated Affinity (pM, nM, μM, mM), LLE, and Tor. The table lists 10 molecules, with the 10th molecule, S3U_H_55_2, highlighted. Below the table is a '2D' view showing the chemical structure of S3U_H_2001_CSS800000286055_2, which is a complex organic molecule with a benzamide-like core and a fused ring system.

The main window shows a 3D ribbon representation of a protein (blue) with a ligand (orange and green spheres) bound to its binding site. A yellow question mark icon is visible in the top right corner of the main window.

At the bottom, a 'Target View Control' panel shows a sequence of residues from 1 to 30, with a search bar for 'Name (e.g. gly)'. The residues listed are: 1: 2ZFF, 2: GLYC, 3: ALA18, 4: ASP14, 5: CYS1, 6: GLY2, 7: LEU3, 8: ARG4, 9: PRO5, 10: LEU6, 11: PHE7, 12: GLU8, 13: LYS9, 14: LYS10, 15: SER11, 16: LEU12, 17: GLU13, 18: ASP14, 19: LYS14A, 20: THR14B, 21: GLU14C, 22: ARG14D, 23: GLU14E, 24: LEU14F, 25: LEU14G, 26: LEU14H, 27: SER14I, 28: THR14J, 29: LEU14K, 30: LEU14L, 31: VAL17, 32: GLU19, 33: GLY19, 34: SER20, 35: ARG.

SeeSAR comes with a growing library featuring +12,000 fragments.

More and larger libraries be downloaded for free from our website:

[Download more libraries](#)

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Mode Overview

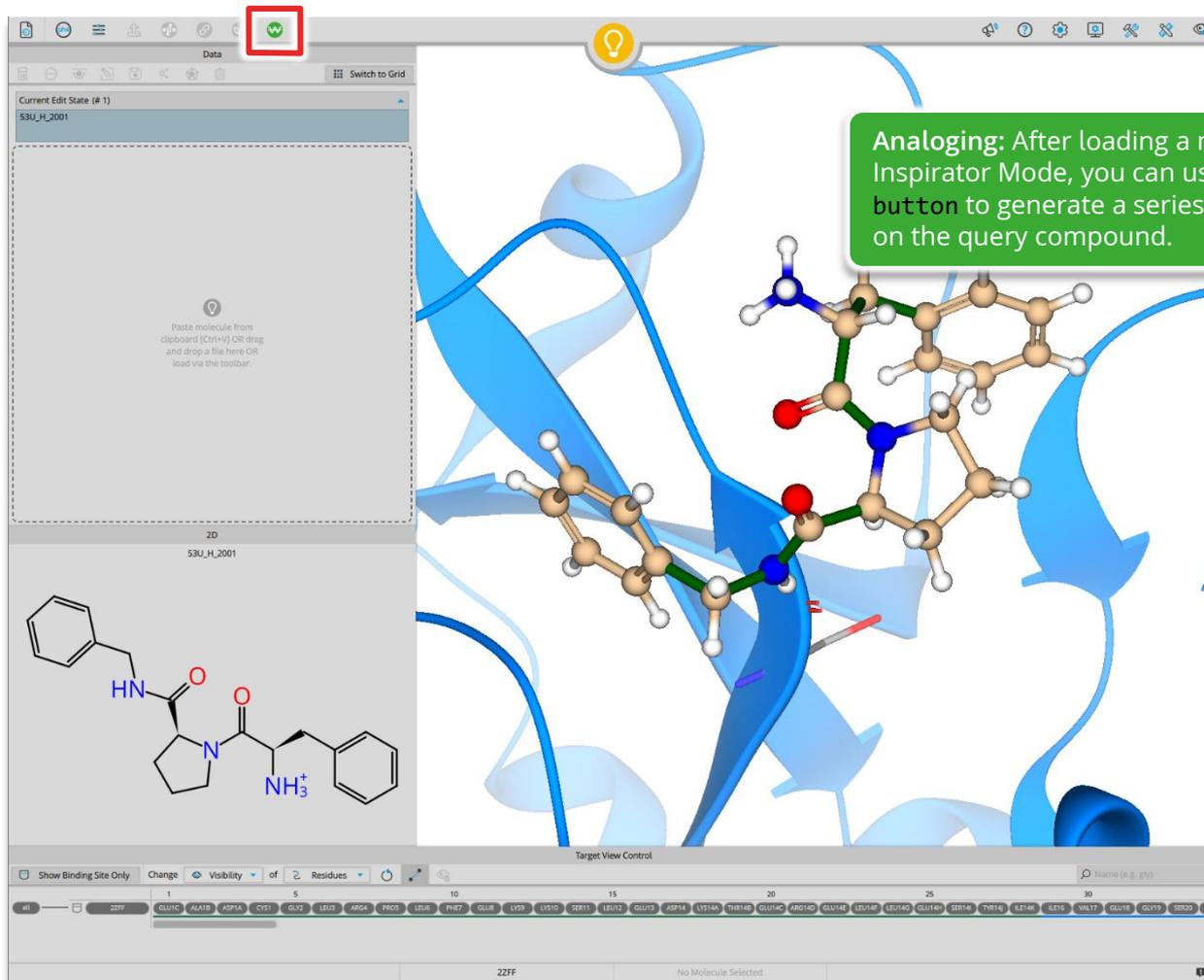


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Mode Overview

The screenshot displays a molecular docking software interface. On the left, a 'Molecules' table lists 10 molecules with their names and estimated affinity values. The table is as follows:

	Name	Estimated Affinity	LLE	Tor.
		pM	µM	mM
1	S3U_H_1_3	---	---	---
2	S3U_H_1_20_2_3	---	---	---
3	S3U_H_1_20_3_3	---	---	---
4	S3U_H_1_20_4_3	---	---	---
5	S3U_H_1_20_5_3	---	---	---
6	S3U_H_1_20_6_3	---	---	---
7	S3U_H_1_20_7_3	---	---	---
8	S3U_H_1_20_8_3	---	---	---
9	S3U_H_1_20_9_3	---	---	---
10	S3U_H_1_20_10_3	---	---	---

Below the table, a chemical structure editor shows a molecule with a highlighted H_2N group. The structure is a complex molecule with a benzene ring, a secondary amine, a pyrrolidine ring, and a primary amine.

At the bottom, a 'Target View Control' panel shows a sequence of residues: 1 5 10 15 20 25 30. The residues are: 22FF, GLU1C, ALA1E, ASP1A, CYS1, GLY2, LEU3, ARG4, PRO5, LEU6, PHE7, GLU8, LYS9, LYS10, SER11, LEU12, GLU13, ASP14, LYS16A, THR16B, GLU16C, ARG16D, GLU16E, LEU16F, LEU16G, GLU16H, SER16I, THR16J, LEU16K, LEU16L, VAL17, GLU18, GLY19, SER20, ASP21.

The results will appear in the 'Molecules' table.

The transformed region will be highlighted, and the applied medicinal chemistry transformation will be appended to the molecule's name.

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Mode Overview

The screenshot displays the Inspira software interface. On the left, the 'Data' panel shows a list of molecules: S3U_H_2001, S3U_H_01_3, and S3U_H_2001_2. The 'Add Molecules to' button is highlighted with a red box, and the 'Inspira' mode is selected in the 'Molecules' list, also highlighted with a red box. Below the 'Data' panel, a 2D chemical structure of a molecule is shown, featuring a carboxylate group, a protonated amine group (NH_3^+), and a benzene ring. The main window shows a blue ribbon representation of a protein structure with a ball-and-stick model of a molecule docked in the binding site. At the bottom, the 'Target View Control' bar shows the sequence of residues: 1 (GLUC), 5 (ALAT), 10 (ASPA), 15 (CYS), 20 (GLY), 25 (LEU), 30 (ARG), 35 (PRO), 40 (LEU), 45 (PHE), 50 (GLU), 55 (LYS), 60 (LYS), 65 (SER), 70 (LEU), 75 (GLU), 80 (ASP), 85 (LYS), 90 (THR), 95 (GLU), 100 (ARG), 105 (GLU), 110 (LEU), 115 (LEU), 120 (GLU), 125 (SER), 130 (THR), 135 (LEU), 140 (SER), 145 (VAL), 150 (GLU), 155 (GLY), 160 (SER), 165 (ASP).

Linking & Merging: To connect two different fragments or molecules, load both into **Inspira Mode** at the same time.

To do so check both molecules in any Mode and select 'Add Molecules to' → 'Inspira'.

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Mode Overview

The screenshot displays the Inspira software interface. On the left, a 'Data' panel contains a 'Docking Library (# 2)' table with columns for Name, Estimated Affinity (pM, nM, uM, mM), LLE, and Tor. Two molecules, 53U_H_2001_1 and 53U_H_2001_2, are listed. Below this is a 'Generated Poses (# 32) Checked (# 2)' table with columns for Name, Estimated Affinity, LLE, and Tor. Two poses are checked, indicated by blue boxes. At the bottom left, a 2D chemical structure of a ligand is shown. The main window displays a 3D molecular model of a protein (blue ribbon) with a ligand (grey sticks) docked in its binding site. A green callout box on the right contains the following text:

The simultaneous loading of two molecules into **Inspirator Mode** works in any mode where multiple ligands can be selected (e.g., **Docking Mode**, **Molecule Editor Mode**, **Similarity Scanner Mode**, **Analyzer Mode**, even **Inspirator Mode** itself, ...).

Check the molecules that are to be merged and transfer them via: 'Add Molecules to' → 'Inspira'

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Mode Overview

Define vectors to connect the two molecules. During this process, undesired parts can be replaced, resulting in a fragment merge.

Once at least two vectors are defined, the 'Linking & Merging' button will become active. Click it to generate the results.

Current Edit State (# 2)			
S3U_H_2001_1, S3U_H_2001_2			
Molecules (# 2)			
Name	Estimated Affinity	LLE	Tor.
1	pM nM μ M mM	→	→
S3U_H_2001_1		→	→
2	pM nM μ M mM	→	→
S3U_H_2001_2		→	→

2D

Target View Control

Show Binding Site Only Change Visibility of Residues

1 5 10 15 20 25 30

GLU1C ALA1B ASP1A CYS1 CYS2 LEU3 ARG4 PRO5 LEU6 PHE7 GLU8 LEU9 LEU10 SER11 LEU12 GLU13 ASP14 LEU16 THR18 LEU19C ARG14D GLU14E LEU14F LEU14G LEU14H SER14E THR16E LEU16E LEU17 VAL17E GLU18E GLU19E SER20E ASP

2ZF No Molecule Selected

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Mode Overview

Data

Current Edit State (# 2)
 S3U_H_2001_1, S3U_H_2001_2

Inspirator is paused. [Click here to resume.](#)

Molecules (# 12)

Name	Estimated Affinity				LLE	Tor.
	pM	nM	µM	mM		
1 S3U_H_2001_1						
2 S3U_H_2001_2						
3 S3U_..._4						
4 S3U_H_2_..._4						
5 S3U_H_..._4						
6 S3U_H_..._4						
7 S3U_H_..._4						
8 S3U_..._4						
9 S3U_H_..._4						
10 S3U_H_..._4						
11 S3U_H_..._4						
12 S3U_H_..._4						

2D
 S3U_H_2001_1_S3U_H_2001_2_6wnw_L16M_1_D_402_..._4

Target View Control

Show Binding Site Only Change Visibility of Residues

1 5 10 15 20 25 30

GLU1C ALA1B ASP1A CYS1 GLY2 LEU3 ARG4 PRO5 LEU6 PHE7 GLU8 LYS9 LYS10 SER11 LEU12 GLU13 ASP14 LYS16A THR16B GLU16C ARG16D GLU16E LEU16F LEU16G LEU16H SER16I THR16J SER16K SER16L VAL17I GLU17J GLY17K SER20A

22FF S3U_H_2001_1_S3U_H_200...wn_L16M_1_D_402_..._4

Note:
 Linking & Merging uses the currently active ReCore index. You can change the fragment set in 'System' → 'Inspirator'.

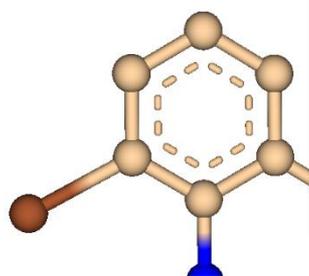
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Mode Overview

The screenshot shows the BioSolveIT software interface. The 'Data' panel on the left contains a table of molecules and a 2D chemical structure view of a reference molecule.

	Name	Tor.	Intra-clash	MW	LogP	TPSA
1	refer_e_mol	●	●	383.11	4.15	34.9
2	mol1	●	●	242.28	1.80	47.2
3	mol2	●	●	377.66	3.76	32.3

The 2D view shows a complex molecule with a benzene ring, a bromine atom (Br), and a cyclobutane ring with two fluorine atoms (F). The reference molecule is labeled 'reference_mol'.



The **Similarity Scanner** can be used for ligand-based drug discovery (LBDD). You can add molecules as SMILES by copy-and-paste those with 'Ctrl+V' or load those via the toolbar.

For this example, we will work with a set of compounds:

```

O=C(c1ccc2N([C@H](CC3)C3(F)F)C(C(F)(F)F)=Nc1c2Br reference_mol
O=C(c(ccc(C1)c1)c1N1)N([C@H](C2)C[C@]2(CBr)F)C1=S mol1
O=C(/C=C(/C(F)(F)F)\c(cc1)ccc1Cl)O[C@@H](CC1)C1(F)F mol2
C[C@H]([C@@](C1CC1)(C(F)(F)F)Oc(c1ccc2)c2Cl)C1=O mol3
C[C@H]([C@@](C1CC1)(C(F)(F)F)Oc(c1ccc2)c2Cl)C1=O mol4
O=C(c(cc(cc1)F)c1N1)N(C2CC2)C1=S mol5
O=C(c1ccc2N(C[C@H](CC3)C3(F)F)C(C(F)(F)F)=Nc1c2Br mol6
O=C([C@H]1C1)c(cc(cc2)F)c2O[C@@]1(C1CC1)C(F)(F)F mol7

```

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Mode Overview

The screenshot displays a molecular docking software interface. On the left, a sidebar contains a 'Molecules' table with the following data:

	Name	Tor.	Intra-clash	MW	LogP	TPSA
1	refer_e_mol			383.11	4.15	34.9
2	mol1					47.2
3	mol2					32.3

Below the table, a context menu is open, showing options such as 'Use as Reference in', 'Local Docking Mode', 'Remote Docking Mode', and 'Similarity Scanner'. The 'Use as Reference in' option is highlighted with a red box, and a sub-menu is visible with 'Similarity Scanner' also highlighted. A green callout box on the right contains the text: 'Select the reference_mol ligand with right-click to 'Use as Reference' → 'In Similarity Scanner'.'

The main window shows a 3D ball-and-stick model of a ligand (reference_mol) docked into a protein binding site. The protein is shown as a grey mesh, and the ligand is shown as a ball-and-stick model with orange, blue, green, and red atoms. Below the 3D model, a 2D chemical structure of the reference molecule is displayed, featuring a benzimidazole core with a bromine atom, a cyclobutane ring, and a trifluoromethyl group.

At the bottom of the interface, there is a 'Target View Control' section with options for 'Show Binding Site Only', 'Change', 'Visibility', 'of', 'Residues', and a search field for 'Name (e.g. gly)'.

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Mode Overview

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Mode Overview

	Name	Tor	Intra-clash	MW	LogP	TPSA
1	refer_e_mol	●	●	383.11	4.15	34.9
2	mol1	●	●	242.28	1.80	47.2
3	mol2	●	●	377.66	3.76	32.3

2D
reference_mol

Target View Control
Show Binding Site Only Change Visibility of Residues Name (e.g. gly)

reference_mol

You can see the active template in the respective table. This is also where you can remove molecules if they are no longer needed.

You can start the molecule alignment with the 'Run Similarity Scanner' button.

It is also possible to apply pharmacophore constraints to keep key motifs in the generated results in desired locations.

The screenshot displays a molecular docking software interface. On the left, a 'Generated Poses' table lists 49 poses, with the first row highlighted in blue and a red arrow pointing to the 'Similarity Rating' column. The table includes columns for Name, Similarity Rating, Tor, Intra-class, and MW. Below the table, a 2D chemical structure of a molecule is shown, labeled 'mol6_1_1 (Template: reference_mol)'. On the right, a 3D ball-and-stick model of the molecule is displayed, showing its interaction with a target protein. A green callout box contains text explaining that aligned results are listed in the 'Generated Poses' table and can be ranked by clicking on the respective column.

Generated Poses (# 49)		Name	Similarity Rating	Tor	Intra-class	MW
1	mol6_1_1	★★★★★	★★★★★	●	●	236.27
2	mol6_1_2	★★★★★	★★★★★	●	●	236.27
3	mol6_1_3	★★★★★	★★★★★	●	●	236.27
4	mol6_1_4	★★★★★	★★★★★	●	●	236.27
5	mol6_1_5	★★★★★	★★★★★	●	●	236.27
6	mol2_1_01	★★★★★	★★★★★	●	●	377.66
7	mol2_1_02	★★★★★	★★★★★	●	●	377.66
8	mol2_1_03	★★★★★	★★★★★	●	●	377.66
9	mol2_1_04	★★★★★	★★★★★	●	●	377.66
10	mol2_1_05	★★★★★	★★★★★	●	●	377.66

mol6_1_1 (Template: reference_mol)

Target View Control

mol6_1_1

1 message

Aligned results will be listed in the 'Generated Poses' table. They can be ranked based on their Similarity Rating by clicking on the respective column.

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Mode Overview

Active & Inactive Molecules (# 14 / 1000)

	Name	Tor.	Intra-clash [Radars]	MPO	MW	LogP
1	ref_mol				383.11	4.15
2	mol1_1_1				397.14	4.22
3	mol2_1_1				304.69	4.26
4	mol3_1_1				308.66	3.72
5	mol4_1_1				377.66	3.76
6	mol5_1_1				362.27	4.33
7	mol6_1_1				387.55	4.48

Activity Spots (# 17) Checked (# 3)
Activity Spots | Inactivity Spots

9. Activity Spotter

The Activity Spotter identifies the key molecular features responsible for biological activity based on aligned molecules and the assignment of compounds as active or inactive.

Important note:
Molecular pre-alignment is required to achieve consistent results with the Activity Spotter (e.g., via Similarity Scanner, Docking Poses, or binding site superposition).

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Mode Overview

The **Activity Spotter** requires a pre-aligned ligand set. For this exercise, we will use the following compounds, starting in the **Similarity Scanner**. Copy and paste the ligands using 'Ctrl+V':

```

0=C(c1ccc2N([C@H](CC3)C3(F)F)C(C(F)(F)F)=Nc1c2Br reference_mol
0=C(c1ccc2N(C[C@H](CC3)C3(F)F)C(C(F)(F)F)=Nc1c2Br mol1
C[C@H]([C@@](C1CC1)(C(F)(F)F)Oc(c1ccc2)c2C1)C1=O mol2
0=C([C@H]1C1)c(cc(cc2)F)c2O[C@@]1(C1CC1)C(F)(F)F mol3
0=C(c(ccc(C1)c1)c1N1)N([C@H](C2)C[C@]2(CBr)F)C1=S mol4
CC(C1)(C2)CC12N(c(cc(C(F)(F)F)cc1)c1N=C1C(F)(F)F)C1=O mol5
0=C([C@@H]([C@@](C1CC1)(C(F)(F)F)Oc1c2)C1)c1cc(Br)c2F mol6
0=C1c(cccc2)c2O[C@@](C2CC2)(C(F)(F)F)C1(F)F mol7
COC([C@](C1CC1)(C(F)(F)F)Nc(cc1)cc(F)c1F)=O mol8
0=C(c(cc(cc1)F)c1N1)N(C2CC2)C1=S mol9
0=C(Cc1c(C(F)(F)F)[nH]c2c1cccc2)O[C@@H](CC1)C1(F)F mol10
0=C1NC(c(cc2)cc(F)c2F)=NC(C(F)(F)F)=C1 mol11
[O-][N+](c(cccc1C2=CNC(C3CC3)=NC2=O)c1F)=O mol12
0=C(/C=C(/C(F)(F)F)\c(cc1)ccc1C1)O[C@@H](CC1)C1(F)F mol13

```

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Mode Overview

The screenshot displays the software interface with the following components:

- Data Panel:** Shows a list of molecules. The 'reference_mol' entry is selected, and a context menu is open over it. The menu options include 'Use as Reference in', 'Local Docking Mode', 'Remote Docking Mode', and 'Similarity Scanner'. The 'Similarity Scanner' option is highlighted with a red box.
- Molecules Table:**

	Name	Tor.	Intra-clash	MW	LogP	TPSA
1	refer_e_mol			383.11	4.15	34.9
2	mol1					47.2
3	mol2					32.3
- Generated Poses Panel:** Shows 'Generated Poses (# 0)' with options like 'Open Radar Plot Settings...', 'Calculate Torsion Quality', 'Calculate Molecular Clashes', 'Calculate Optimum Properties', and 'Add Molecule to'.
- 2D View:** Displays the chemical structure of the 'reference_mol' molecule, which is a complex heterocyclic compound with fluorine (F) and bromine (Br) substituents.
- 3D View:** Shows a ball-and-stick model of the 'reference_mol' molecule docked into a target binding site.
- Target View Control:** Located at the bottom, it includes options for 'Show Binding Site Only', 'Change', 'Visibility', 'of', 'Residues', and a search field for 'Name (e.g. gly)'.

Callout Box: Select the reference_mol ligand with a right click to 'Use as Reference' → 'In Similarity Scanner'.

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Mode Overview

The screenshot displays a software interface for molecular docking. On the left, a 'Data' panel contains a 'Template Molecules (# 1)' section with a red border around 'reference_mol'. Below it is a 'Molecules (# 9)' table:

	Name	Tor.	Intra-clash	MW	LogP	TPSA
1	refer_e_mol	●	●	383.11	4.15	34.9
2	mol1	●	●	242.28	1.80	47.2
3	mol2	●	●	377.66	3.76	32.3

Below the table is a 'Generated Poses (# 0)' section. At the bottom left, a 2D chemical structure of 'reference_mol' is shown, featuring a benzimidazole core with a bromine atom, a cyclobutane ring, and two trifluoromethyl groups. On the right, a 3D ball-and-stick model shows the molecule docked into a target site, with yellow dashed lines indicating interactions. A green callout box points to the 'reference_mol' entry in the table.

You can see the active template in the respective table. This is also where you can remove molecules if they are no longer needed.

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Mode Overview

	Intra-dash	MW	LogP	TPSA
1	reference_mot	383.11	4.15	34.9
2	mol1	377.66	3.76	32.3
3	mol2	340.67	4.63	26.3

Generated Poses (# 0)

Name	Similarity Rating	Tor.	Intra-dash	Mov
------	-------------------	------	------------	-----

Target View Control

Show Binding Site Only Change Visibility of Residues

No Molecule Selected

Go to 'Similarity Scanner Parameters' and set the 'Maximum Number of Poses' to '1'.

Here, we do this to keep the exercise as straightforward as possible. In the later slides, we will show how to work with larger sets of poses of the same molecule.

Important note:
In some cases, lowering the 'Minimum Similarity Rating' can help when no poses can be generated for a ligand.

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Mode Overview

Active	Optional	Name	Type	Constraint	r[A]
<input checked="" type="checkbox"/>	<input type="checkbox"/>	pharm1	include	donors	1.0
<input checked="" type="checkbox"/>	<input type="checkbox"/>	pharm2	include	any N	1.0
<input checked="" type="checkbox"/>	<input type="checkbox"/>	pharm3	include	halogens	1.1

At least 1 optional constraint must be fulfilled.

Define New Constraint

	reference_mot		383.11	4.15	34.9
1					
2		mol1	377.66	3.76	32.3
3		mol2	340.67	4.63	26.3

Generated Poses (# 0)

Name	Similarity Rating	Tot. Intra-clash	Mov
------	-------------------	------------------	-----

Target View Control

Show Binding Site Only Change Visibility of Residues

No Molecule Selected

Again, it is also possible to apply pharmacophore constraints to keep key motifs in the generated results in desired locations.

Please visit the pharmacophore section for further details and instructions.

Jump to Section

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Mode Overview

Data

Template Molecules (# 1)

- reference_mol

Molecules (# 8)

	Name	Tor.	Intra-clash	MW	LogP	TPSA
1	reference_mol	●	●	383.11	4.15	34.9
2	mol1	●	●	377.66	3.76	32.3
3	mol2	●	●	340.67	4.63	26.3

Generated Poses (# 0)

	Name	Similarity Rating	Tor.	Intra-clash	MW
--	------	-------------------	------	-------------	----

2D

Target View Control

Show Binding Site Only Change Visibility of Residues

No Molecule Selected

You can start the molecule alignment with the 'Run Similarity Scanner' button.

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Mode Overview

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Mode Overview

Check reference_mol and the generated poses and transfer them to the Activity Spotter Mode via 'Add Molecules to' → 'Activity Spotter'.

Molecules (# 8) Checked (# 1)			
Name	TPSA		
reference_mol	1.15	34.9	
mol1	377.66	3.76	32.3
mol2	340.67	4.63	26.3

Generated Poses (# 7) Checked (# 7)					
Name	Similarity Rating	Tor.	Intra-clash	MW	
mol5_3_1	★★★★★	●	●	236.27	
mol1_3_1	★★★★★	●	●	377.66	
mol3_3_1	★★★★★	●	●	304.69	
mol4_3_1	★★★★★	●	●	304.69	
mol2_3_1	★★★★★	●	●	340.67	
mol6_3_1	★★★★★	●	●	397.14	
mol7_3_1	★★★★★	●	●	308.66	

The screenshot shows a software interface with a 3D molecular model in the center. On the left, there are three panels: 'Template Molecules (# 1)' containing 'reference_mol'; 'Molecules (# 8) Checked (# 1)' with a table of molecule properties; and 'Generated Poses (# 7) Checked (# 7)' with a table of pose properties. A dialog box titled 'Action impacting multiple tables' is overlaid on the model, with the 'Continue' button highlighted by a red box. A green callout box on the right contains the following text:

You will be informed that you want to move molecules from different tables. Since this is our intention, press 'Continue'.

Name	Tor.	Intra-clash	MW	LogP	TPSA
reference_mol	●	●	383.11	4.15	34.9
mol1	●	●	377.66	3.76	32.3
mol2	●	●	340.67	4.63	26.3

Name	Similarity Rating	Tor.	Intra-clash	MW
mol5_3_1	★★★★☆	●	●	236.27
mol1_3_1	★★★★★	●	●	377.66
mol3_3_1	★★★★★	●	●	304.69
mol4_3_1	★★★★★	●	●	304.69
mol2_3_1	★★★★★	●	●	340.67
mol6_3_1	★★★★★	●	●	397.14
mol7_3_1	★★★★★	●	●	308.66

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Mode Overview

	Name	Tor.	Intra-clash	MPO [Radar]	MW	LogP	T
1	ref_mol	●	●	●	383.11	4.15	
2	mol5_3_1	●	●	●	236.27	2.14	
3	mol1_3_1	●	●	●	377.66	3.76	
4	mol3_3_1	●	●	●	304.69	4.26	
5	mol4_3_1	●	●	●	304.69	4.26	
6	mol2_3_1	●	●	●	340.67	4.63	
7	mol6_3_1	●	●	●	397.14	4.22	

reference_mol

Target View Control

reference_mol

Now in the Activity Spotter, you will find your aligned molecules in the 'Active & Inactive Molecules' table. Up to 1,000 molecules can be used in the Activity Spotter to perform an SAR analysis.

Your input molecules can also come from different sources, e.g., docking, binding site alignment, external sd files.

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Mode Overview

The screenshot displays a software interface for molecular docking. On the left, a 'Data' table lists several molecules. A red box highlights the 'Active Status' column, and a red arrow points to the flame icon for the molecule 'reference_mol'. Below the table is a 3D ball-and-stick model of a molecule, and at the bottom left is a 2D chemical structure of a complex molecule with fluorine (F) and bromine (Br) atoms.

Active	Tor.	Intra-clash [Radar]	MPO	MW	LogP
ref_mol	●	●	●	383.11	4.15
mol1_1	●	●	●	397.14	4.22
mol2_1	●	●	●	304.69	4.26
mol3_1	●	●	●	308.66	3.72
mol4_1_1	●	●	●	377.66	3.76
mol5_1_1	●	●	●	362.27	4.33
mol6_1_1	●	●	●	387.55	4.48

Activity Spots (# 0)

Click the play button on the toolbar to compute activity and inactivity spots.

2D
reference_mol

Target View Control
Show Binding Site Only Change Visibility of Residues

To determine interactions driving the biological activity, you need to assign an activity status to each compound of your set.

In the 'Active & Inactive Molecules' table, click on the icon in the 'Active Status' column to change it to 'active' (flame icon). A second click can be used to change it to 'inactive' (ice icon).

Change the status of `reference_mol` to 'active' (represented by a flame icon).

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Mode Overview

The screenshot shows a software interface for molecular docking. On the left, a table lists 'Active & Inactive Molecules (# 5 / 1000)'. The table has columns for Name, Tor, Intra-clash [Radar], MPO, MW, and LogP. The first five molecules (mol1_1_1 to mol5_1_1) have their status icons highlighted with a red box and a red arrow. Below the table is a 2D chemical structure of a reference molecule. On the right, a 3D ball-and-stick model shows a protein structure with a ligand bound to it. A green callout box contains the following text:

After changing the status of one molecule, 'Shift+click' a second molecule applies the change to all molecules between the two.

Change the status of the first five molecules to 'active'.

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Mode Overview

The screenshot displays a software interface for molecular simulation. On the left, a 'Data' panel shows a table of 'Active & Inactive Molecules (# 6 / 1000)'. A red box highlights the status column for molecule 6, with a red arrow pointing to a snowflake icon. Below the table is an 'Activity Spots' section with a play button and instructions. The main window shows a 3D ball-and-stick model of a protein-ligand complex. A green callout box explains that two clicks on the status of a molecule change its status to 'inactive' (represented by a snowflake icon) and instructs to set the status of molecule 6 to 'inactive'. At the bottom left, a 2D chemical structure of molecule 6 is shown, labeled 'mol5_1_1 (Template: reference_mol)'. The bottom of the interface includes a 'Target View Control' bar with options like 'Show Binding Site Only', 'Change', 'Visibility', 'of', 'Residues', and a search field for 'Name (e.g. gly)'.

	Name	Tor.	Intra-clash [Radar]	MPO	MW	LogP
1	refer_e_mol			383.11	4.15	
2	mol1_1_1			397.14	4.22	
3	mol2_1_1			304.69	4.26	
4	mol3_1_1			308.66	3.72	
5	mol4_1_1			377.66	3.76	
6	mol5_1_1			362.27	4.33	
7	mol6_1_1			387.55	4.48	

Activity Spots (# 0)

Click the play button on the toolbar to compute activity and inactivity spots.

2D

mol5_1_1 (Template: reference_mol)

Target View Control

Show Binding Site Only Change Visibility of Residues Name (e.g. gly)

mol5_1_1

Two clicks on the status of a molecule change its status to 'inactive' (represented by a snowflake icon).

Set the status of molecule 6 to 'inactive'.

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Mode Overview

The screenshot displays a software interface for molecular docking. On the left, a table lists molecules with their properties. A red box highlights the 'Active & Inactive' column, and a red arrow points to the play button icon in the first row of this column. Below the table, a 2D chemical structure of 'mol13_1' is shown. On the right, a 3D ball-and-stick model of the same molecule is displayed. A green callout box contains instructions on how to toggle the status of molecules.

Active & Inactive	Name	Tor.	Intra-clash	MPO [Radar]	MW	LogP
<input type="checkbox"/>	mol7_1_1	●●	●●	●●	292.20	3.61
<input type="checkbox"/>	mol8_1_1	●●	●●	●●	309.23	3.26
<input type="checkbox"/>	mol9_1_1	●●	●●	●●	236.27	2.14
<input type="checkbox"/>	mol10_1_1	●●	●●	●●	333.25	4.07
<input type="checkbox"/>	mol11_1_1	●●	●●	●●	276.16	2.73
<input type="checkbox"/>	mol12_1_1	●●	●●	●●	275.24	2.01
<input type="checkbox"/>	mol13_1_1	●●	●●	●●	340.67	4.63

mol13_1_1 (Template: reference_mol)

Target View Control

mol13_1_1

Again, [Shift+click] can be used to change the status of all molecule between the first and the second.

Do this to change the status of the remaining molecules to 'inactive'.

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Mode Overview

Name	Tor	Intra-clash [Radar]	MPO	MW	LogP	T
ref_mol				383.11	4.15	
mol1_1				397.14	4.22	
mol2_1				304.69	4.26	
mol3_1				308.66	3.72	
mol4_1				377.66	3.76	
mol5_1				362.27	4.33	
mol6_1				387.55	4.48	

Activity Spots (# 0)

Click the play button on the toolbar to compute activity and inactivity spots.

2D
reference_mol

Target View Control

Show Binding Site Only Change Visibility of Residues Name (e.g. gly)

reference_mol

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Mode Overview

The screenshot displays a molecular modeling software interface. On the left, there are two data tables. The top table, titled 'Active & Inactive Molecules (# 14 / 1000)', lists molecules with columns for Name, Tor, Intra-clash, MPO, MW, and LogP. The bottom table, titled 'Activity Spots (# 17)', is highlighted with a red box and shows columns for Rank, Type, and two percentage columns. The main window shows a 3D molecular model with several yellow and orange spheres representing activity spots. A green callout box explains the 'Spot' table and the 'Spot' table. At the bottom left, there is a 2D chemical structure of a complex molecule with fluorine (F) and bromine (Br) atoms.

Active & Inactive Molecules (# 14 / 1000)						
	Name	Tor	Intra-clash	MPO	MW	LogP
1	ref_mol				383.11	4.15
2	mol1_1_1				397.14	4.22
3	mol2_1_1				304.69	4.26
4	mol3_1_1				308.66	3.72
5	mol4_1_1				377.66	3.76
6	mol5_1_1				362.27	4.33
7	mol6_1_1				387.55	4.48

Activity Spots (# 17)				
Activity Spots	Inactivity Spots	Rank	Type	
1		1	nonpolar exposed atom	60 11
2		2	nonpolar exposed atom	40 0
3		3	nonpolar exposed atom	40 0
4		4	nonpolar exposed atom	40 0
5		5	nonpolar exposed atom	40 0
6		6	acceptor atom interaction	80 33
7		7	acceptor atom	100 44
8		8	acceptor atom interaction	100 44

The 'Spot' table will be populated with entries of 'Activity Spots' and 'Inactivity Spots'. You can switch between both tabs to explore each category.

Each Spot displays how many of the active and inactive molecules are covered by it.

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Mode Overview

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Mode Overview

Table of Active & Inactive Molecules (# 14 / 1000)

	Name	Tor.	Intra-clash	MPO [Radar]	MW	LogP
8	mol7_1_1	●●●●●	●●●●●	292.20	3.61	
9	mol6_1_1	●●●●●	●●●●●	387.55	4.48	
10	mol5_1_1	●●●●●	●●●●●	362.27	4.33	
11	mol3_1_1	●●●●●	●●●●●	308.66	3.72	
12	mol11_1_1	●●●●●	●●●●●	276.16	2.73	
13	mol12_1_1	●●●●●	●●●●●	275.24	2.01	
14	ref._mol	●●●●●	●●●●●	383.11	4.15	

Activity Spots (# 17)

Activity Spots	Inactivity Spots	Rank	Type	Δ [%]	Σ [%]
1	●	1	acceptor atom	60	0
2	●	2	donor atom	60	0
3	●	3	donor atom interaction	60	0
4	●	4	acceptor atom interaction	40	0
5	●	5	acceptor atom interaction	40	0
6	●	6	nonpolar exposed atom	80	38
7	●	7	nonpolar exposed atom	40	13
8	●	8	nonpolar exposed atom	40	13
9	●	9	nonpolar exposed atom	40	25
10	●	10	aromatic ring	100	75
11	●	11	nonpolar exposed atom	80	75
12	●	12	acceptor atom	60	63
13	●	13	acceptor atom interaction	60	63
14	●	14	acceptor atom interaction	60	63
15	●	15	nonpolar exposed atom	60	88

Visualization Options:

- Hyde Coloring
- H-bonds
- Torsion Coloring
- Molecular Clashes
- Unoccupied Space
- Unresolved Segments
- Possible Atom Interactions**
- Target Clipping

Callout Text: You can also display geometrically potential H-bond interactions of your active molecule under 'Visualization' → 'Possible Atom Interactions'.

2D reference_mol:

BrC1=CC=C2C(=O)N(C(F)(F)F)C(F)(F)F2

The screenshot displays a software interface for molecular docking. On the left, a table titled 'Active & Inactive Molecules (# 14 / 1000)' lists various molecules with their properties. Below it, a table titled 'Activity Spots (# 17)' lists specific interaction points. A red box highlights the first entry in this table: '1 | nonpolar exposed atom | 60 | 11'. To the right, a 3D molecular model shows a protein structure with several yellow and orange spheres representing activity spots. A red arrow points to one of these spheres. At the bottom left, a 2D chemical structure of a reference molecule is shown, featuring a benzimidazole core with a cyclobutane ring, fluorine atoms, and a bromine atom.

Name	Tor.	Intra-clash [Radar]	MPO	MW	LogP
ref_mol			383.11	4.15	
mol1_1_1			397.14	4.22	
mol2_1_1			304.69	4.26	
mol3_1_1			308.66	3.72	
mol4_1_1			377.66	3.76	
mol5_1_1			362.27	4.33	
mol6_1_1			387.55	4.48	

Activity Spots	Inactivity Spots
1 nonpolar exposed atom	60 11
3 nonpolar exposed atom	40 0
4 nonpolar exposed atom	40 0
5 nonpolar exposed atom	40 0
6 acceptor atom interaction	80 33
7 acceptor atom	100 44
8 acceptor atom interaction	100 44

reference_mol

reference_mol

Clicking on a Spot in the table or 3D will also highlight the Spot in the other section.

Note: Sphere can belong to ligands OR predicted interaction points at the target.

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Mode Overview

The screenshot displays a software interface for molecular docking. On the left, there are two tables:

Active & Inactive Molecules (# 14 / 1000)

	Name	Tor.	Intra-clash [Radar]	MPO	MW	LogP
1	ref_mol				383.11	4.15
2	mol1_1_1				397.14	4.22
3	mol2_1_1				304.69	4.26
4	mol3_1_1				308.66	3.72
5	mol4_1_1				377.66	3.76
6	mol5_1_1				362.27	4.33
7	mol6_1_1				387.55	4.48

Inactivity Spots (# 42)

Activity Spots	Inactivity Spots	Type	Δ [%]	∞ [%]
1	1	acceptor atom	0	11
2	2	acceptor atom	0	11
3	3	acceptor atom	0	11
4	4	acceptor atom	0	11
5	5	acceptor atom	0	11
6	6	acceptor atom	0	11
7	7	acceptor atom	0	11

Below the tables is a 'Molecule Coverage' section with a slider set to 22%. It shows 9 inactive molecules and 5 active molecules. A red box highlights this section.

The main window shows a 3D molecular model of a ligand (orange and blue spheres) docked into a protein's binding site (blue spheres). A green callout box explains the 'Inactivity Spots' feature.

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Mode Overview

After switching to the 'Activity Spots' tab, you can select 'Inactivity Spots'. These help exclude inactive molecules and shift the molecule coverage toward a lower number of inactive compounds.

Select the top two Inactivity Spots. The coverage of inactive molecules will decrease.

The screenshot displays a software interface for molecular docking analysis. On the left, there are two tables:

Active & Inactive Molecules (# 14 / 1000)

Name	Tor.	Intra-clash [Radar]	MPO	MW	LogP
refer_e_mol			383.11	4.15	
mol1_1_1			397.14	4.22	
mol2_1_1			304.69	4.26	
mol3_1_1			308.66	3.72	
mol4_1_1			377.66	3.76	
mol5_1_1			362.27	4.33	
mol6_1_1			387.55	4.48	

Activity Spots (# 17)

Rank	Type	Δ [%]	Σ [%]
1	1 nonpolar exposed atom	60	11
2	2 nonpolar exposed		
3	3 nonpolar exposed		
4	4 nonpolar exposed		
5	5 nonpolar exposed		
6	6 acceptor atom interact		33
7	7 acceptor atom		44
8	8 acceptor atom interaction	100	44

Below the tables, there is a 'Molecule Coverage' section showing 'Activity Spots (# 3)' and 'Inactivity Spots (# 2)' with a progress bar at 22%. A 'Show Contributing' button is highlighted with a red box.

The main 3D view shows a protein structure with a ligand (green sticks) and several activity spots (yellow spheres). A red box highlights a specific spot on the ligand. A green callout box explains that right-clicking on a spot and selecting 'Show Contributing' → 'Actives/Inactives' will visualize all molecules covered by that spot and pin them to the table.

At the bottom, there is a 'Target View Control' panel with options for 'Show Binding Site Only', 'Change', 'Visibility', 'of', 'Residues', and a search field for 'Name (e.g. gly)'.

You can visualize all molecule covered by a Spot by right-clicking on it, then 'Show Contributing' → 'Actives/Inactives'. The molecules involved in this spot will also become pinned in the 'Active & Inactive Molecules' table.

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Mode Overview

The screenshot shows a software interface with a data table and a 3D molecular model. The data table is as follows:

	Intra-clash	MPO	MW	LogP
			383.11	4.15
			14	4.22
			69	4.26
4			66	3.72
5			377.66	3.76
6			362.27	4.33
7			387.55	4.48

The 'Activity Spots' table is also visible:

Rank	Type	Δ [%]	Σ [%]
1	nonpolar exposed atom	60	11
2	nonpolar exposed atom	40	0
3	nonpolar exposed atom	40	0
4	nonpolar exposed atom	40	0
5	nonpolar exposed atom	40	0
6	acceptor atom interaction	80	33
7	acceptor atom	100	44
8	acceptor atom interaction	100	44

The 3D model shows a molecule with several activity spots represented as yellow and orange spheres. A red arrow points to the 'Add Spots' button in the 'Calculate Molecule Coverage of Checked Spots' menu. A green callout box provides instructions on how to use the 'Add Spots' feature.

For a mass conversion of Spots, select a combination of Activity Spots and Inactivity Spots. Go to 'Checked molecule assignments' → 'Calculate Molecule Coverage of Checked Spots' → 'Add Spots'. You can also use this feature to remove checked Spots from the combination selection.

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Mode Overview

The screenshot displays a software interface with a table of molecules and activity spots on the left, and a 3D molecular model on the right. A callout box points to a 'Convert to Sphere Constraint' button in the activity spots table.

	Name	Tor.	Intra-clash [Radar]	MPO	MW	LogP
1	refer_e_mol				383.11	4.15
2	mol1_1_1				397.14	4.22
3	mol2_1_1				304.69	4.26
4	mol3_1_1				308.66	3.72
5	mol4_1_1				377.66	3.76
6	mol5_1_1				362.27	4.33
7	mol6_1_1				387.55	4.48

Rank	Type	Δ [%]	⊞ [%]
1	nonpolar	60	11
2	nonpolar exp	40	0
3	nonpolar e	0	0
4	nonpolar e	0	0
5	nonpolar e	0	0
6	acceptor a	100	33
7	acceptor atom	100	44
8	acceptor atom interaction	100	44

Molecule Coverage: Activity Spots (# 3) Inactivity Spots (# 2)
22% 80%

Inactives (#9) Actives (#5)

Target View Control
Show Binding Site Only Change Visibility of Residues

No Molecule Selected

In order to convert a Spot into a pharmacophore constraint (e.g., for Similarity Scanner or docking), right-click on a Spot and select 'Convert to Sphere constraint'.

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Mode Overview

The screenshot displays a software interface for defining a pharmacophore. A dialog box titled "Define Pharmacophore" is open, showing the "Include" dropdown set to "hydrophobic" and the "Radius" set to "1.0 Å". Below the dialog, a table lists "Activity Spots" with columns for Rank, Inactivity Spots, Type, and two percentage columns. The table contains 8 rows of data. A green callout box on the right contains text explaining the dialog's function. In the bottom left, there are green callout boxes for "Table of Content" and "Mode Overview".

Define Pharmacophore

Include: hydrophobic
Radius: 1.0 Å
My Own SMARTS

Cancel Apply

Rank	Inactivity Spots	Type	Δ [%]	Σ [%]
1	60	nonpolar exposed atom	11	
2	40	nonpolar exposed atom	0	
3	40	nonpolar exposed atom	0	
4	40	nonpolar exposed atom	0	
5	40	nonpolar exposed atom	0	
6	80	acceptor atom interaction	33	
7	100	acceptor atom	44	
8	100	acceptor atom interaction	44	

Molecule Coverage: Activity Spots (# 3) Inactivity Spots (# 2)
22% 80%

Inactives (#9) Actives (#5)

2D

Target View Control

Show Binding Site Only Change Visibility of Residues

No Molecule Selected

Table of Content

Mode Overview

The pharmacophore menu will open up. You can increase or decrease the size of the constraint or the type is required. Once you are done, confirm your setup with 'Apply'.

The screenshot displays a software interface with the following components:

- Data Table:** A table titled "Active & Inactive Molecules (# 14 / 1000)".
- Activity Spots Table:** A table titled "Activity Spots (# 17) Checked (# 3)".
- Molecule Coverage:** A progress bar showing 22% activity spots and 80% inactivity spots.
- 2D Structure:** A chemical structure of a reference molecule with fluorine (F) and bromine (Br) atoms highlighted.
- 3D Model:** A 3D ball-and-stick model of a molecule with several activity spots represented as semi-transparent spheres.

Name	Tor.	Intra-clash [Radar]	MPO	MW	LogP
ref_mol				383.11	4.15
mol1_1				397.14	4.22
mol2_1				304.69	4.26
mol3_1				308.66	3.72
mol4_1				377.66	3.76
mol5_1				362.27	4.33
mol6_1				387.55	4.48

Rank	Type	Δ [%]	Σ [%]
1	nonpolar exposed atom	60	11
2	nonpolar exposed atom	40	0
3	nonpolar exposed atom	40	0
4	nonpolar exposed atom	40	0
5	nonpolar exposed atom	40	0
6	acceptor atom interaction	80	33
7	acceptor atom	100	44
8	acceptor atom interaction	100	44

Activity Spots will be handled as 'include' constraints per default, and Inactivity Spots as 'exclude'.

Your pharmacophore constraints will now be active in all other modes and can be adjusted there if needed (e.g., deactivated, re-sized, etc.). You can use them for virtual screening campaigns in the **(Remote) Docking Mode/Chemical Space Docking® Mode**, or for ligand-based screenings in the **Similarity Scanner**.

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Mode Overview

The screenshot shows a software interface with a table of molecules and a 3D molecular model. A green callout box provides instructions on how to group molecules in Analyzer Mode.

Table of Molecules:

	Name	Tor.	Intra-clash	MW	LogP	TPSA
1	mol1	●	●	397.14	4.22	34.9
2	mol2	●	●	304.69	4.26	26.3
3	mol3	●	●	308.66	3.72	26.3
4	mol4	●	●	377.66	3.76	32.3
5	mol5	●	●	362.27	4.33	34.9
6	mol6	●	●	387.55	4.48	26.3
7	mol7	●	●	292.20	3.61	26.3
8	mol8	●	●	309.23	3.26	38.3
9	mol9	●	●	276.27	2.14	32.3

	Name	Similarity Rating	Tor.	Intra-clash	MW
1	1_2_01	★★★★★	●	●	397.14
2	1_2_02	★★★★★	●	●	397.14
3	1_2_03	★★★★★	●	●	397.14
4	1_2_04	★★★★★	●	●	397.14
5	1_2_05	★★★★★	●	●	397.14
6	1_2_06	★★★★★	●	●	397.14
7	mol1_2_07	★★★★★	●	●	397.14
8	mol1_2_08	★★★★★	●	●	397.14
9	mol1_2_09	★★★★★	●	●	397.14
10	mol1_2_10	★★★★★	●	●	397.14
11	mol2_2_01	★★★★★	●	●	304.69
12	mol2_2_02	★★★★★	●	●	304.69

Callout Box Text:

In cases where more than one pose of a ligand is available (e.g., more than one pose was generated during the **Similarity Scanner/Docking Mode** run was generated), a grouping in the **Analyzer Mode** can be performed.

For this, select all your molecules by right-click → 'Check all'.

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Mode Overview

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Mode Overview

Transfer the compound to the Analyzer Mode: 'Add Molecules to' → 'Analyzer'.

Molecules (# 13)		Name	TPSA
1	mol1	1.22 34.9
2	mol2	●●●●●●	304.69 4.26 26.3
3	mol3	●●●●●●	308.66 3.72 26.3
4	mol4	●●●●●●	377.66 3.76 32.3
5	mol5	●●●●●●	362.27 4.33 34.9
6	mol6	●●●●●●	387.55 4.48 26.3
7	mol7	●●●●●●	292.20 3.61 26.3
8	mol8	●●●●●●	309.23 3.26 38.3
9	mol9	●●●●●●	236.27 2.14 32.3

Generated Poses (# 102)		Checked (# 102)	Name	Similarity Rating	Tor.	Intra-clash	MW
1	mol1_2_01	★★★★★	●●	397.14			
2	mol1_2_02	★★★★★	●●	397.14			
3	mol1_2_03	★★★★★	●●	397.14			
4	mol1_2_04	★★★★★	●●	397.14			
5	mol1_2_05	★★★★★	●●	397.14			
6	mol1_2_06	★★★★★	●●	397.14			
7	mol1_2_07	★★★★★	●●	397.14			
8	mol1_2_08	★★★★★	●●	397.14			
9	mol1_2_09	★★★★★	●●	397.14			
10	mol1_2_10	★★★★★	●●	397.14			
11	mol2_2_01	★★★★★	●●	304.69			
12	mol2_2_02	★★★★★	●●	304.69			

The screenshot displays a software interface for molecular docking. On the left, a table lists 102 molecules with columns for Name, Estimated Affinity (pM, nM, μM, mM), LLE, and Target. A red box highlights a funnel icon in the table, with a tooltip that says "Click to open filter options". Below the table is a 2D chemical structure of molecule mol13_2_4, which is a complex organic molecule with a benzene ring, a chlorine atom, and a cyclobutane ring. On the right, a 3D ball-and-stick model shows the molecule (mol13_2_4) docked into a protein target. A green callout box points to the funnel icon in the top toolbar, stating: "Once in the Analyzer Mode, click on the funnel icon." At the bottom, there is a "Target View Control" panel with options for "Show Binding Site Only", "Change", "Visibility", "of", "Residues", and a search field for "Name (e.g. gly)".

	Name	Estimated Affinity				LLE	Tar.	In cl.
		pM	nM	μM	mM			
72	mol10_2_10							●
73	mol4_2_07							●
74	mol4_2_08							●
75	mol9_2_2							●
76	mol6_2_08							●
77	mol6_2_09							●
78	mol7_2_08							●
79	mol11_2_1							●
80	mol11_2_2							●
81	mol9_2_3							●
82	mol7_2_09							●
83	mol7_2_10							●
84	mol6_2_10							●
85	mol11_2_3							●
86	mol12_2_1							●
87	mol12_2_2							●
88	mol12_2_3							●
89	mol12_2_4							●
90	mol11_2_4							●
91	mol4_2_09							●
92	mol9_2_4							●
93	mol12_2_5							●
94	mol4_2_10							●
95	mol12_2_6							●
96	mol9_2_5							●
97	mol13_2_1							●
98	mol12_2_7							●
99	mol12_2_8							●
100	mol13_2_2							●
101	mol13_2_3							●
102	mol13_2_4							●

Table of Content

Mode Overview

The screenshot displays a software interface for molecular docking. On the left, a table lists 102 molecules with columns for Name and pK. The 'Group Molecules' option is highlighted with a red box and a red arrow. The main area shows a 3D ball-and-stick model of a molecule. A green callout box contains the text: "Activate the 'Group Molecules' option." Below the 3D model is a 2D chemical structure of the selected molecule, mol13_2_4.

Name	pK
mol10_2_10	
mol4_2_07	
mol4_2_08	
mol9_2_2	
mol6_2_08	
mol6_2_09	
mol7_2_08	
mol11_2_1	
mol11_2_2	
mol9_2_3	
mol7_2_09	
mol7_2_10	
mol6_2_10	
mol11_2_3	
mol12_2_1	
mol12_2_2	
mol12_2_3	
mol12_2_4	
mol11_2_4	
mol4_2_09	
mol9_2_4	
mol12_2_5	
mol4_2_10	
mol12_2_6	
mol9_2_5	
mol13_2_1	
mol12_2_7	
mol12_2_8	
mol13_2_2	
mol13_2_3	
mol13_2_4	

mol13_2_4 (Template: reference_mol)

CC1(F)C(F)C1OC(=O)C=C(C(F)(F)F)C1=CC=C(Cl)C=C1

Table of Content

Mode Overview

The screenshot displays a molecular docking software interface. On the left, a table lists 102 molecules with columns for Name and pH. A red box highlights a green checkmark icon in the top toolbar, with a red arrow pointing to it. Below the table, a 2D chemical structure of molecule 'mol13_2_4' is shown, featuring a benzene ring with a chlorine atom, a trifluoromethyl group, and a cyclobutane ring with two fluorine atoms. On the right, a 3D ball-and-stick model of the same molecule is shown in a stick representation. A green callout box with the text 'Apply the filter.' points to the 3D model. The interface also includes a 'Pharmacophore: 0 active' section and a 'Group Molecules' section with a checked checkbox and a note: 'For identical molecules, show only best estimated affinity.' At the bottom, there is a 'Target View Control' section with options for 'Show Binding Site Only', 'Change', 'Visibility', 'of', 'Residues', and a search field for 'Name (e.g. gly)'. The status bar at the very bottom indicates 'No Protein Selected' and 'mol13_2_4'.

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Mode Overview

The screenshot displays a software interface for molecular docking. On the left, a table lists 13 molecules, with the first 13 rows highlighted by a red box. The table has columns for 'Molecules (# 13)', 'Name', and 'pH'. The molecules listed are mol1_2_01 through mol13_2_1. Below the table, a 2D chemical structure of mol13_2_1 is shown, featuring a benzene ring with a chlorine atom, a vinyl group, and a cyclobutane ring with two fluorine atoms. On the right, a 3D ball-and-stick model of the same molecule is displayed. A green callout box points to the 3D model with the text: "Only the top-ranking pose of each molecule will be displayed. You can now transfer them into the Activity Spotter to perform an SAR analysis." The interface also includes a 'Data' panel at the top with various filters and a 'Target View Control' panel at the bottom.

Molecules (# 13)	Name	pH
1	mol1_2_01	
2	mol2_2_01	
3	mol3_2_01	
4	mol4_2_01	
5	mol5_2_01	
6	mol6_2_01	
7	mol7_2_01	
8	mol8_2_1	
9	mol9_2_1	
10	mol10_2_01	
11	mol11_2_1	
12	mol12_2_1	
13	mol13_2_1	

Only the top-ranking pose of each molecule will be displayed. You can now transfer them into the Activity Spotter to perform an SAR analysis.

Table of Content

Mode Overview

Template or Reference Molecules (# 0)		Molecules (# 6)				
Name	Estimated Affinity	LE	Tor.	Intra-clash	Inter-clash	MW
	pM	nM	µM	mM		
1 rxn5_AS_2						348.43
2 rxn501__A1_1						310.38
3 rxn501__AS_5						348.43
4 rxn501__A1_1						332.36
5 rxn501__A1_2						347.42
6 rxn501__A1_5						396.47

10. Chemical Space Docking®

Chemical Space Docking (C-S-D) is a structure-based method that screens billion- or even trillion-sized Chemical Spaces for the most promising drug candidates.

Important note:
In order to perform C-S-D, you need a running instance of HPSee.

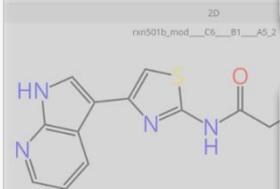
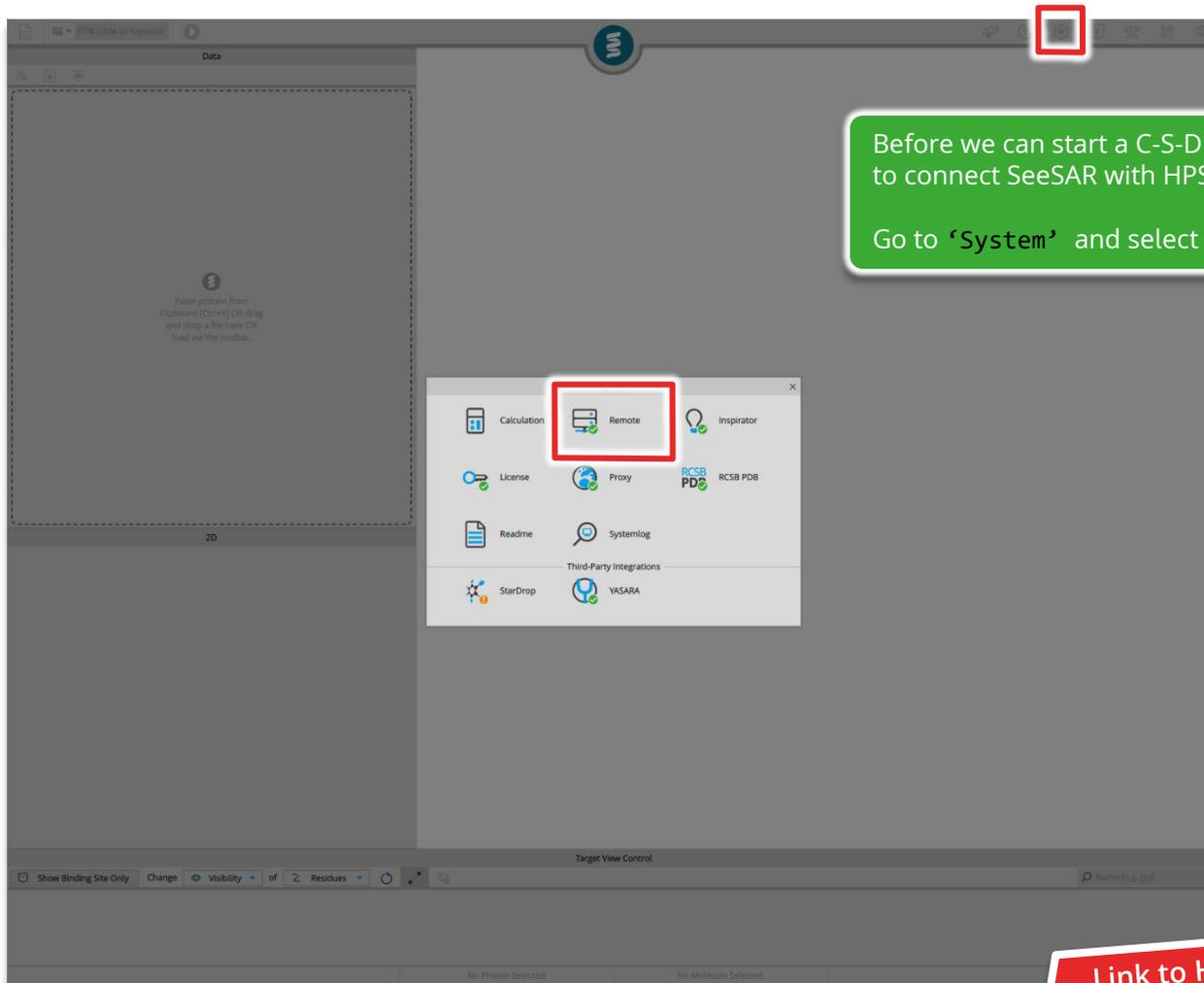


Table of Content

Mode Overview



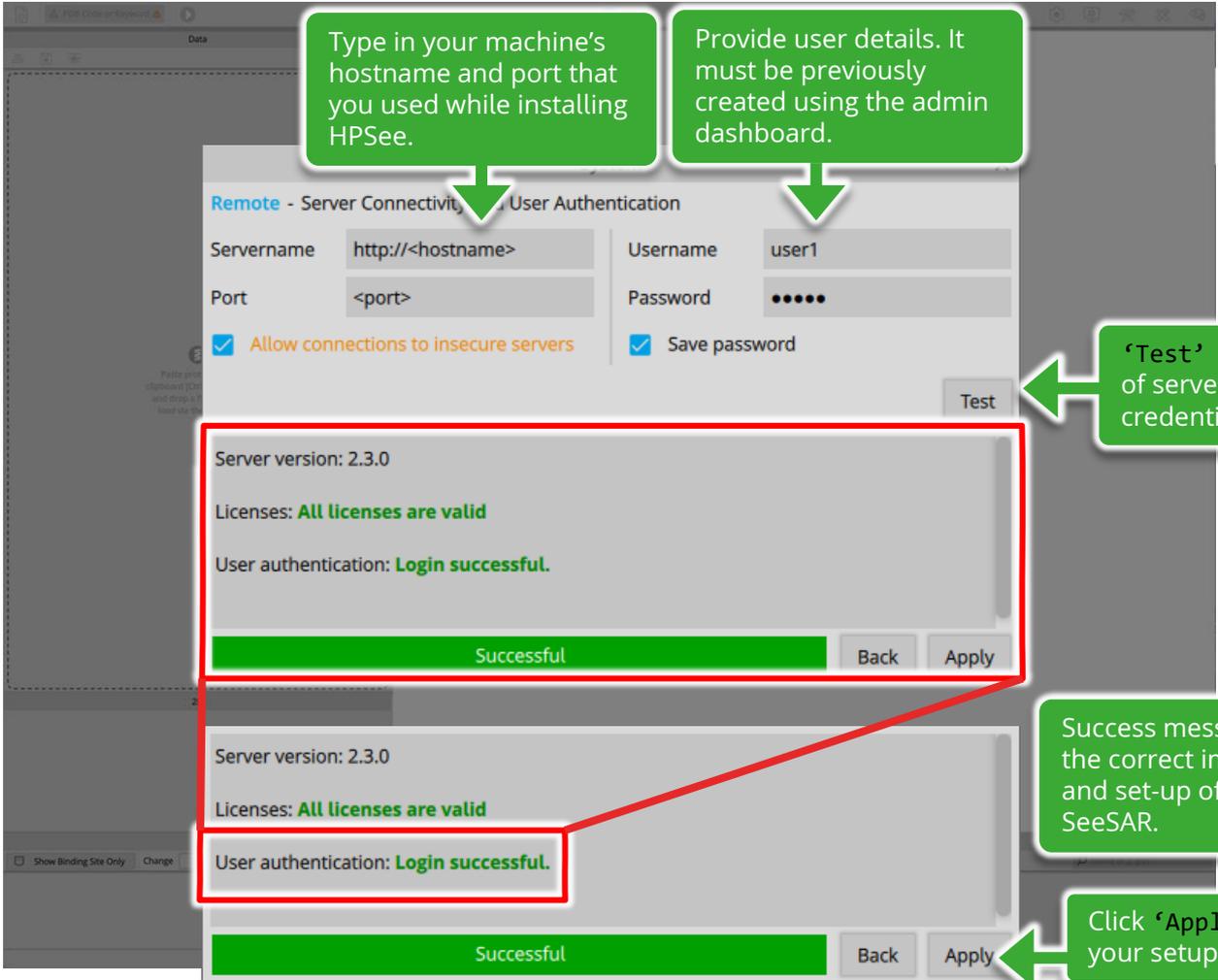
Before we can start a C-S-D workflow, we need to connect SeeSAR with HPSee.

Go to 'System' and select 'Remote'.

Table of Content

Mode Overview

[Link to HPSee Guide](#)



Type in your machine's hostname and port that you used while installing HPSee.

Provide user details. It must be previously created using the admin dashboard.

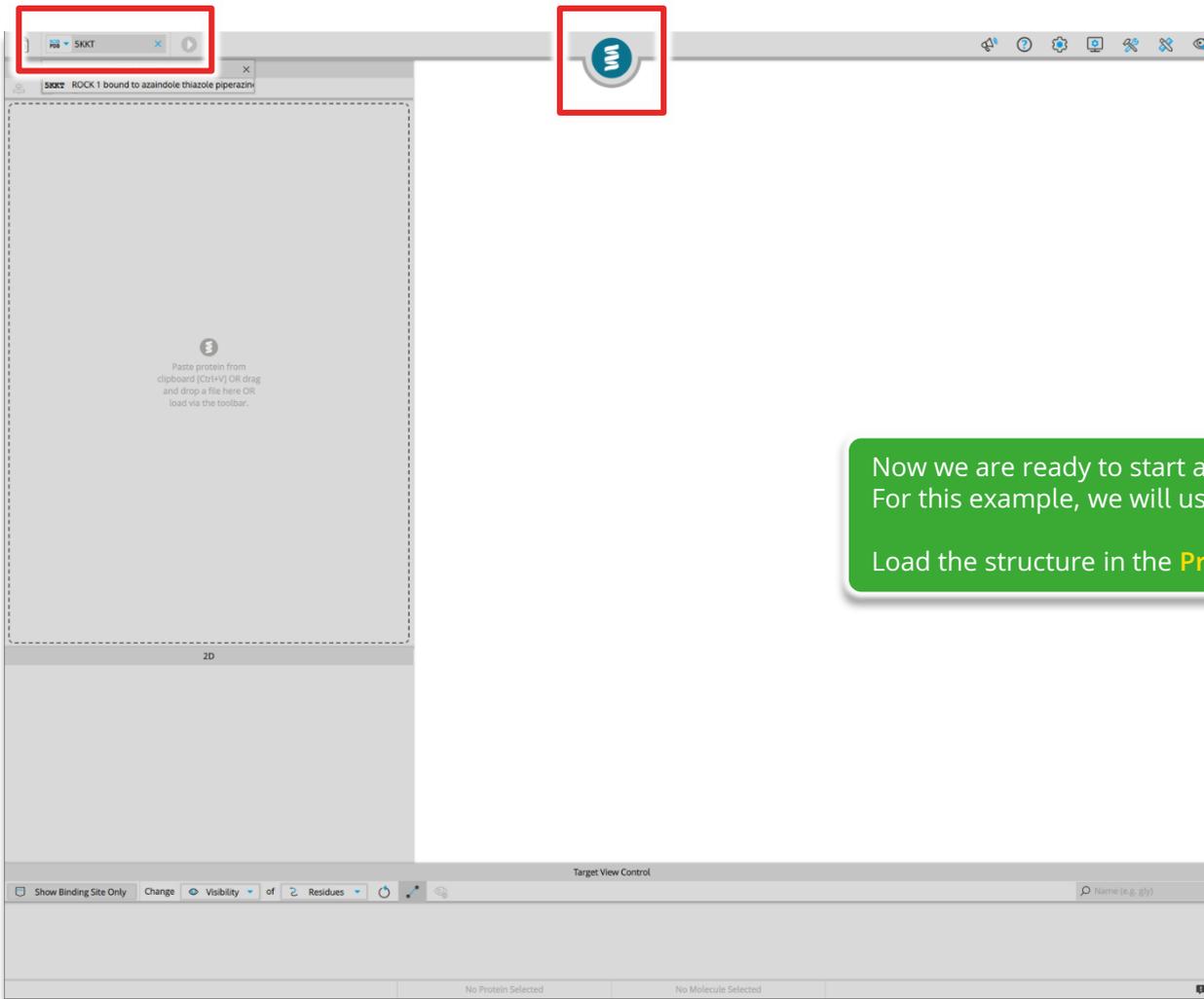
'Test' to check validity of server and login credentials.

Success message indicates the correct implementation and set-up of HPSee and SeeSAR.

Click 'Apply'. To confirm your setup.

Table of Content

Mode Overview



Now we are ready to start a C-S-D run.
For this example, we will use 5KKT as PDB.
Load the structure in the **Proteins Mode**.

Table of Content

Mode Overview

SKKT - Extract Your Ligand

Hetero Groups

ID	Name	PKM	COM	PKM	COM
1	Do not extract a ligand				
2	6U2_A_501				
3	6U2_A_501				

2D
6U2_A_501

C1CN(CCN1)CCOC(=O)Cc2ccc(cc2)NC(=O)c3nc4c(ncn4)c5cccnc35

Target View Control

Show Binding Site Only Change Visibility of Residues

1 5 10 15 20 25 30

all SKKT SERE PHET GLUR THR8 ARG10 PHET11 GLU12 LYS13 MET14 ASP15 ASN16 LEU17 LEU18 ARG19 ASP20 PRO21 LYS22 SER23 GLU24 VAL25 ASN26 SER27 ASP28 CYS29 LEU30 LEU31 ASP32 GLY33 LEU34 ASP35 ALA36 LEU37 VAL38 TYR39

SKKT 6U2_A_501

Select the first ligand and confirm your binding site.

Table of Content

Mode Overview

The screenshot displays the Docking software interface. On the left, a sidebar contains a 'Proteins' table with one entry 'SKKT' and a 'Ligand for SKKT' table with one entry '6U2_A_501'. Below these is a 2D chemical structure of the ligand. The main window shows a 3D molecular model of the protein SKKT (green ribbon) with the ligand 6U2_A_501 (stick representation) docked in its binding site. A semi-transparent grey overlay is positioned in the upper center, containing two buttons: 'Docking' and 'Space Docking®'. The 'Space Docking®' button is highlighted with a red box, and a green arrow points from a green callout box to it. The callout box contains the text 'Switch to Space Docking® Mode.' in yellow and green. Another red box highlights the 'MM' icon in the top toolbar, with a red arrow pointing to the 'Remote' button in the top right. At the bottom, a 'Target View Control' bar shows a sequence of residues from 1 to 30, with 'SKKT' and '6U2_A_501' labels below it.

Table of Content

Mode Overview

Name	Fragments
ROCK1-test-space	30
Freedom Space	382747
eXplore	551401
mini REAL Space - Evaluation	15690

Target View Control

Show Binding Site Only Change Visibility of Residues

1 5 10 15 20 25 30 Name (e.g. gly)

all SKKT SERE PHET GLUR THRS ARG10 PHET11 GLU12 LYS13 MET14 ASP15 ASN16 LEU17 LEU18 ARG19 ASP20 PRO21 LYS22 SER23 GLU24 VAL25 ASN26 SER27 ASP28 CYS29 LEU30 LEU31 ASP32 GLY33 LEU34 ASP35 ALA36 LEU37 VAL38 TYR39

SKKT ROCK1-test-space No Molecule Selected 1 message

Chemical Spaces that were previously uploaded using the Dashboard can be seen here.

We will use a small custom Space for this tutorial, called 'ROCK1-test-space'.

You download the ROCK1-test Space file [here](#). It's a small Chemical Space than can conveniently be used to test if your setup works as intended.

Select the Chemical Space you want to work with and click on the green button  on the top to start the C-S-D run with the current protein and binding site.

Table of Content

Mode Overview

In order to upload a Chemical Space, please go to your HPSee dashboard and enter the 'Spaces' section.

Here you can upload your Chemical Space. Please take note that the Chemical Space needs to be fully processed before it can be used for a C-S-D run.

Admin Dashboard

- Home
- Licenses
- Users
- Libraries
- Spaces
- Workflows

Chemical Spaces ?

	Status	Filename	Description	# Fragments	Created At	Created By
		ROCK1_1k_2025-07	ROCK-1_Test-Space	30	11/13/2025 12:49:59 PM	
		FreedomSpace_296bn_2026-03	release testing 2026-03-04	382747	3/4/2026 9:03:25 AM	
		eXplore_5tr_2025-07		551401	3/4/2026 9:42:32 AM	
		miniREALSpace_100k_2025-12		15690	3/6/2026 2:49:23 PM	

Rows per page: 10 ▾ 1-4 of 4 |< < > >|



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Mode Overview

The screenshot displays the SeeSAR software interface. At the top, a 'Data' panel is highlighted with a red box, containing the text 'Template or Reference Molecules (4/0)' and 'Add from file or another mode'. A green arrow points from this panel to a green callout box. The main window shows a protein structure with a green ribbon and a blue ribbon, with two yellow and black striped rods representing anchor fragments. A bullhorn icon is visible in the top right corner of the main window. At the bottom, a 'Target View Control' panel shows a sequence of residues: SER1, PHE2, GLU3, THR3, ARG10, PHE11, GLU12, LYS13, MET14, ASP15, ASN16, LEU17, LEU18, ARG18, ASP20, PRO21, LYS22, SER23, GLU24, VAL25, ASN26, SER27, ASP28, CYS29, LEU30, LEU31, ASP32, GLY33, LEU34, ASP35, ALA36, LEU37, VAL38, TYR39.

- You now have a choice to either perform 'Template C-S-D' or a 'Standard C-S-D':
- ◆ 'Template C-S-D' will place the anchor fragment in reference to the 'Template Molecule'.
 - ◆ 'Standard C-S-D' explores the binding site freely to find the best possible pose to bind the anchor fragments.

The bullhorn icon informs you if a new version of SeeSAR is available.

If you choose to perform a 'Standard C-S-D', skip the next slide and continue the demo. If you choose to perform a 'Template C-S-D', the next slide shows how to add one.

Table of Content

Mode Overview

'Template Docking'

The screenshot displays the Docking Explorer interface. On the left, the 'Ligand for SKKT' panel shows the molecule '6U2_A_501' with a context menu open, highlighting 'Use as Reference in' and 'Space Docking Mode'. The main 3D view shows the protein SKKT (green ribbon) and the ligand 6U2_A_501 (stick representation). A red box highlights the 'MM' button in the top right corner of the 3D view area. The bottom panel shows the 'Target View Control' with a sequence viewer for SKKT and 6U2_A_501.

The extracted ligand from PDB can be used as a 'Template Molecule' in this demo.

Go to **Proteins Mode** and right-click on the ligand and choose the options 'Use as Reference in' → 'Space Docking Mode'.

You could also load an SDF directly in **Space Docking® Mode**.

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Mode Overview

'Template Docking'

The screenshot displays a molecular docking software interface. On the left, a table titled 'Template or Reference Molecules (# 1)' contains one entry: '6U2_A_501'. The main 3D view shows a protein structure in green ribbon representation with a yellow template molecule docked in the binding site. A 'Target View Control' bar at the bottom shows a sequence of residues: SERE, PHE7, GLUR, THR8, ARG10, PHE11, GLU12, LYS13, MET14, ASP15, ASN16, LEU17, LEU18, ARG19, ASP20, PRO21, LYS22, SER23, GLU24, VAL25, ASN26, SER27, ASP28, CYS29, LEU30, LEU31, ASP32, GLY33, LEU34, ASP35, ALA36, LEU37, VAL38, TYR39.

You should see your Template Molecule in this box, if you decide to perform a 'Template C-S-D'. Up to five template molecules are supported during a C-S-D run.

The Template Molecule is displayed in 3D after its import to the Space Docking Mode. You can remove visibility or change color using  from the table.

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Mode Overview

'Template Docking'

The screenshot displays a molecular docking software interface. On the left, a panel titled 'Template or Reference Molecules (# 1)' contains a list with one entry: '6U2_A_501'. A red-bordered button with a trash icon is highlighted in this panel. A green callout box with a white arrow points to this button, containing the text: 'You can remove the Template Molecule here.' The main 3D view shows a protein structure in green ribbon representation with a yellow and blue template molecule docked. At the bottom, a 'Target View Control' panel shows a sequence of residues from 1 to 30, including SER1, PHE7, GLU8, THR8, ARG10, PHE11, GLU12, LYS13, MET14, ASP15, ASN16, LEU17, LEU18, ARG18, ASP20, PRO21, LYS22, SER23, GLU24, VAL25, ASN26, SER27, ASP28, CYS29, LEU30, LEU31, ASP32, GLY33, LEU34, ASP35, ALA36, LEU37, VAL38, and TYR39. The status bar at the bottom indicates 'No Molecule Selected'.

If you want to continue with the Template Molecule, keep it in the table and continue with the next slides of 'Standard Docking'.

Table of Content

Mode Overview

Docking Input Filters for Molecules

MW
≥ 300

Rotatable Bonds
≤ 10

Add a Filter for
- Select a Property -

Before starting the C-S-D run, you can apply additional filters that will be applied on the generated molecules. The filters are applied to **full molecules** (assembled molecules and molecules without extension vectors) before remote compute is allocated.

Target View Control

Show Binding Site Only Change Visibility of Residues

1 5 10 15 20 25 30 Name (e.g. gly)

all SKT SERE PHET GLUR THRE ARG10 PHET11 GLU12 LYS13 MET14 ASP15 ASN16 LEU17 LEU18 ARG19 ASP20 PRO21 LYS22 SER23 GLU24 VAL25 ASN26 SER27 ASP28 CYS29 LEU30 LEU31 ASP32 GLY33 LEU34 ASP35 ALA36 LEU37 VAL38 TYR39

SKT ROCK1-test-space No Molecule Selected 1 message

Table of Content

Mode Overview

The screenshot displays a molecular docking software interface. At the top left, a red box highlights a green button with a power icon and the text "Start a new Space Docking". Below this is a panel titled "Template or Reference Molecules (# 1)" containing a single entry "6U2_A_501". The main window shows a 3D ribbon representation of a protein structure in green, with a yellow and blue ligand molecule docked in the binding site. A green callout box on the right contains the text: "To start the first step of the C-S-D workflow, use the green button." At the bottom, there is a "Target View Control" panel with a sequence viewer showing residues from 1 to 30, including SER1, PHE7, GLU8, THR8, ARG10, PHE11, GLU12, LYS13, MET14, ASP15, ASN16, LEU17, LEU18, ARG18, ASP20, PRO21, LYS22, SER23, GLU24, VAL25, ASN26, SER27, ASP28, CYS29, LEU30, LEU31, ASP32, GLY33, LEU34, ASP35, ALA36, LEU37, VAL38, and TYR39. The bottom status bar shows "SKKT", "ROCK1-test-space", "No Molecule Selected", and "1 message".

Table of Content

Mode Overview

The image shows a screenshot of a molecular docking software interface. A protein structure is displayed in a ribbon representation, colored in shades of green and blue. A yellow and blue chemical structure is docked into the protein's binding site. A dialog box titled "Define Pharmacophore" is open, with a red box around it and a green arrow pointing to it. The dialog box contains the text "New spheres will be created in center of selected objects." and "At least 3 general constraints must be fulfilled." with a "Define New Constraint" button. A green callout box with an arrow pointing to the dialog box contains the text: "Set your docking parameters here." Another green callout box with an arrow pointing to the protein structure contains the text: "Guide your Anchoring stage of docking with desired pharmacophore constraints. Hint: Check out 'linker constraints'! This is a pharmacophore definition for the extension vector of your building blocks/synthons." A third green callout box with an arrow pointing to the protein structure contains the text: "The initialization steps of the Template Docking and Standard Docking are the same." At the bottom of the interface, there is a "Target View Control" panel with a sequence viewer showing residues from 1 to 30. The sequence is: 1 SKT, 5 SER, 6 PHE, 7 GLU, 8 THR, 9 ARG, 10 PHE, 11 GLU, 12 LYS, 13 MET, 14 ASP, 15 ASN, 16 LEU, 17 LEU, 18 ARG, 19 ASP, 20 PRO, 21 LYS, 22 SER, 23 GLU, 24 VAL, 25 ASN, 26 SER, 27 ASP, 28 CYS, 29 LEU, 30 LEU. The interface also shows a "Show Binding Site Only" checkbox and a "Residues" dropdown menu.

Guide your Anchoring stage of docking with desired pharmacophore constraints.

Hint: Check out 'linker constraints'!
This is a pharmacophore definition for the extension vector of your building blocks/synthons.

The initialization steps of the Template Docking and Standard Docking are the same.

Table of Content

Mode Overview

The screenshot displays a molecular docking software interface. The central 3D view shows a protein structure in green ribbon representation with a yellow and blue ligand molecule docked in its binding site. A red box highlights the 'Docking Parameters' panel on the left, which includes settings for 'Maximum Number of Poses' (set to 5), 'Clash Tolerance' (set to Standard), and 'Allowed Ring Conformations'. The 'Docking input Filters for Fragments' panel is also visible, showing 'Max. # Consec. Rot. Bonds' set to 5. The bottom of the interface features a 'Target View Control' panel with a sequence viewer showing residues from 1 to 30, including SER1, PHE2, GLU3, THR3, ARG10, PHE11, GLU12, LYS13, MET14, ASP15, ASN16, LEU17, LEU18, ARG19, ASP20, PRO21, LYS22, SER23, GLU24, VAL25, ASN26, SER27, ASP28, CYS29, LEU30, LEU31, ASP32, GLY33, LEU34, ASP35, ALA36, LEU37, VAL38, and TYR39. The bottom status bar shows 'No Molecule Selected' and a '1 message' button.

In the Docking Parameters, you can adjust the settings for the generated poses or add more filter parameters for the to-be-docked anchor blocks.

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Mode Overview

Start Anchoring step of C-S-D.

S button lets you perform a standard docking of anchors in CSD.

T button can be used for template-based docking in anchoring step of C-S-D.

This guide will follow a standard C-S-D.

Table of Content

Mode Overview

Target View Control

1 5 10 15 20 25 30

all SKT SER PHET GLU THR ARG10 PHET11 GLU12 LYS13 MET14 ASP15 ASN16 LEU17 LEU18 ARG19 ASP20 PRO21 LYS22 SER23 GLU24 VAL25 ASN26 SER27 ASP28 CYS29 LEU30 LEU31 ASP32 GLY33 LEU34 ASP35 ALA36 LEU37 VAL38 TYR39

SKT ROCK1-test-space No Molecule Selected 1 message

Terminate a running workflow.

Progress bar at top can be used to monitor.

Docking In Progress (16%)

After the run is complete, click on 'View Results' to access Anchoring results.

View Results

Please ensure you 'Save' the SeeSAR project file after initiating C-S-D.

Once the run begins, you may close the SeeSAR project and later reopen to monitor the progress or download the results to proceed to next steps.

Important note

Table of Content

Mode Overview

The screenshot shows the SeeSAR software interface. At the top, a progress bar indicates 'Docking Pending (0%)' and 'Docking In Progress (16%)'. A 'View Results' button is visible below the progress bar. The main area displays a 3D molecular model of a protein (green) and a ligand (yellow and blue). At the bottom, the 'Target View Control' panel shows a sequence of residues: SER1, PHE2, GLU3, THR3, ARG10, PHE11, GLU12, LYS13, MET14, ASP15, ASN16, LEU17, LEU18, ARG18, ASP20, PRO21, LYS22, SER23, GLU24, VAL25, ASN26, SER27, ASP28, CYS29, LEU30, LEU31, ASP32, GLY33, LEU34, ASP35, ALA36, LEU37, VAL38, TYR39. The interface also shows a 'Show Binding Site Only' button and a 'Change Visibility of Residues' dropdown menu.

The screenshot displays a software interface for molecular docking. At the top left, a table lists fragments with columns for Name, Estimated Affinity (pM, nM), LE, Tor., Intra-clash, Inter-clash, and MW. A red box highlights a button in the top toolbar. A green callout box explains that torsion and clash filters are applied automatically and results are sorted by LE. A green callout box points to a '+' button in the table, stating it is used to select fragments for the Extension step. A large 3D visualization shows a protein structure in light blue with a green ligand bound to it. A yellow and black striped rod is also visible. A green callout box explains that the anchor fragment is visualized in 3D and can be compared to a template molecule. A red callout box labeled 'Important note' states that 111 poses were generated and that a light-blue dummy atom is the extension vector. At the bottom, a chemical structure of a pyridole derivative is shown with an 'R' group. A 'Target View Control' bar at the bottom shows a sequence of residues: SKKT, SERE, PHET, GLUR, THRS, ARG10, PHET1, GLU13, LYS13, MET14, ASP15, ADN16, LEU17, LEU18, ARG18, ASP20, PRO21, LYS22, SER23, GLU24, VAL25, ASN26, SER27, ASP28, CYS29, LEU30, LEU31, ASP32, GLY33, LEU34, ASP35, ALA36, LEU37, VAL38, TYR39.

Torsion and clash filters are applied automatically. The results are sorted based on LE.

Click '+' to select fragments for the Extension step.

Visualize your anchor fragment to the right in 3D. Optionally compare it with respect to your Template Molecule.

For this run, 111 poses were generated. Visually assess them for their binding modes. Keep in mind that the **light-blue dummy atom** is the **extension vector** for this synthon: All built-up molecules will grow from it. If it points towards an undesired area (e.g., solvent-exposed lumen or a binding site you do not want to fill), do not pick this pose for the next step.

Important note

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Mode Overview

The screenshot displays a molecular docking software interface. On the left, there are two tables of fragments. The top table, 'Fragments on Server: (# 111)', lists 18 fragments with columns for Name, Estimated Affinity (pM, nM, μM, mM), LE, Tor., Intra-clash, Inter-clash, and MW. A red box highlights a filter icon in the top right of this table. The bottom table, 'Fragments: (# 6 / 500)', lists 6 fragments with similar columns. Below the tables is a 2D chemical structure of a fragment labeled '#E322758_3', which is a thiophene ring with an 'R' group and an 'NH' group. The main window shows a protein structure in green ribbon representation with a linker atom highlighted in blue and yellow. A green callout box with an arrow points to the linker atom, stating 'Visualization shows feasible extension directions from the linker atom of the fragments in the next step.' Another green callout box with an arrow points to the filter icon, stating 'Change filters as desired.' The bottom of the interface shows a 'Target View Control' bar with a sequence of residues: SKKT, SERE, PHEI, GLUR, THRS, ARGIO, PHEII, GLUII, LVYIS, METI4, ASPIS, ADNI6, LEUI7, LEUI8, ARGIS, ASPD2, PROSI, LVYS2, SERI3, GLIUI4, VALI5, ADNI6, SERI7, ASPF8, CYI29, LEUI0, LEUI1, ASPD2, GLIUI3, LEUI4, ASPD3, ALADI, LEUI7, VALI8, TYI.

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Mode Overview

After selection of the desired fragments, start the extension step by clicking this button.

The screenshot displays a molecular docking software interface. The main window shows a protein structure in green ribbon representation with a small molecule docked in the binding site. A table of fragments is visible, and a chemical structure is shown below it.

Table 1: Fragments on Server (# 111)

Name	Estimated Affinity	LE	Tor.	Intra-clash	Inter-clash	MW
	pM	nM	µM	mM		
14 + #E322762_5						1
13 + #E322760_3						6
14 + #E322774_5						1
16 + #E322752_2						1
17 + #E322774_3						15
18 + #E322758_3						5

Table 2: Fragments (# 6 / 500)

Name	Estimated Affinity	LE	Tor.	Intra-clash	Inter-clash	MW
	pM	nM	µM	mM		
1 #E322766_2						67.07
2 #E322768_2						93.11
3 #E322771_4						117.13
4 #E322772_3						117.13
5 #E322751_2						149.17
6 #E322751_1						149.17

Chemical Structure: A 2D chemical structure of a fragment, labeled #E322758_3, is shown below the table. It consists of a five-membered ring with a sulfur atom (S) and a nitrogen atom (NH), with two R groups attached to the ring.

Selected fragments are moved to this table. You can also remove no longer desired fragments to exclude them from the next steps.

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Mode Overview

The screenshot displays a molecular docking software interface. At the top, a red box highlights the 'Extension 2' button. The main window shows a protein structure in green and yellow, with a small molecule docked in the binding site. On the left, there are two tables of fragments. The top table, 'Fragments on Server (# 103)', lists fragments with their names, estimated affinity, and various flags. The bottom table, 'Fragments: (# 10 / 500)', lists fragments with their names, estimated affinity, and various flags. Below the tables, a chemical structure of a fragment is shown, labeled '#E1466199_2'. The structure is a benzene ring with an R group, a pyridine ring, and an amino group. At the bottom, there is a 'Target View Control' section with a sequence viewer showing residues 1 to 30.

Fragments on Server: (# 103)		Results on Server (# 8)	
Name	Estimated Affinity	LE	Tor.
	pM nM μM mM		
23	#E1466195_2	11	11
24	#E1466195_2	11	11
25	#E1466196_1	11	11
26	#E1466181_3	11	11
27	#E1466202_1	11	11
28	#E14_99_2	11	11

Fragments: (# 10 / 500)	
Name	Estimated Affinity
	pM nM μM mM
1	#E1466199_1
2	#E1466180_1
3	#E1466200_1
4	#E1466180_2
5	#E1466216_1
6	#E1466198_1
7	#E1466197_1
8	#E393193_2
9	#E1466195_2
10	#E1466199_2

Chemical structure of #E1466199_2:

RNc1ccc(cc1)-c2ccncc2N

The procedure for the next step remains the same. You will receive full/complete molecules and fragments, that can be further extended.

Select the fragments you want to grow and continue with the extension.

Your results may differ!

The molecules produced depend on the fragments you chose to extend.

Once you are finished selecting your compound, proceed with 'Extension 2'.

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Mode Overview

The screenshot displays the SeeSAR software interface. On the left, there are two tables of molecules. The top table, 'Molecules on Server: (# 147)', lists various molecules with columns for Name, Estimated Affinity (pM, nM, μM, mM), LE, Tor., Intra-clash, Inter-clash, and MW. The bottom table, 'Molecules: (# 6)', shows a filtered list of molecules. Below these tables is a 2D chemical structure of a molecule, identified as rxn501b_mod__C6__B1__A5_3. The main window shows a 3D ribbon representation of a protein (green) with a ligand (orange and blue spheres) bound to it. The bottom of the interface features a 'Target View Control' with a sequence viewer showing residues from SKKT to VAL38.

Molecules on Server: (# 147)						
Name	Estimated Affinity	LE	Tor.	Intra-clash	Inter-clash	MW
	pM nM μM mM					
1	rxn501__A5_2					34
2	rxn5__A5_3					34
3	rxn501__A5_2					34
4	rxn501__A5_1					34
5	rxn501__A5_5					34
6	rxn501__A5_5					34
7	rxn501__A1_2					11

Molecules: (# 6)						
Name	Estimated Affinity	LE	Tor.	Intra-clash	Inter-clash	MW
	pM nM μM mM					
1	rxn501__A5_2					348.43
2	rxn501__A1_1					310.38
3	rxn501__A5_5					348.43
4	rxn501__A1_1					332.36
5	rxn501__A1_2					347.42
6	rxn501__A1_5					396.47

2D
rxn501b_mod__C6__B1__A5_3

Target View Control

Show Binding Site Only Change Visibility of Residues

1 5 10 15 20 25 30 Name (e.g. gly)

SKKT SERE PHEI GLUR THR8 ARG10 PHE13 GLU13 LYS13 MET14 ASP15 ASN16 LEU17 LEU18 ARG18 ASP20 PRO21 LYS22 SER23 GLU24 VAL25 ASN26 SER27 ASP28 CYS29 LEU30 LEU31 ASP32 GLY33 LEU34 ASP35 ALA36 LEU37 VAL38 TYR39

SKKT ROCK-test-space rxn501b_mod__C6__B1__A5_3 5 messages

You have reached the last stage of the C-S-D workflow. Select your final molecules.

At this stage, you can save your SeeSAR project and return to it whenever you wish.

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Mode Overview

The screenshot displays a molecular docking software interface. The main view shows a protein structure in green ribbon representation with a ligand molecule docked in a binding site. The ligand is shown as a ball-and-stick model with green, blue, and red atoms. A yellow and black striped vertical bar is visible on the right side of the protein.

On the left side, there is a panel titled "Molecules: (# 6)" containing a table of results:

Name	Estimated Affinity	LE	Tor.	Intra-clash	Inter-clash	MW
	μM	mM	μM			
1 rxn501___A5_2	348.43					348.43
2 rxn501___A1_1	310.38					310.38
3 rxn501___A5_5	348.43					348.43
4 rxn501___A1_1	332.36					332.36
5 rxn501___A1_2	347.42					347.42
6 rxn501___A1_5	396.47					396.47

Below the table, a chemical structure is shown with the label "rxn501b_mod___C6___B1___A5_3". The structure is a complex organic molecule with a benzimidazole ring system, a thiazole ring, and a propyl chain attached to a nitrogen atom.

At the bottom, there is a "Target View Control" panel showing a sequence of residues: SKKT, SERE, PHET, GLUR, THRS, ARGIO, PHETI, GLU12, LYS13, MET14, ASP15, ADN16, LEU17, LEU18, ARG19, ASP20, PRO21, LYS22, SER23, GLU24, VAL25, ASN26, SER27, ASP28, CYS29, LEU30, LEU31, ASP32, GLY33, LEU34, ASP35, ALA36, LEU37, VAL38, TYR39.

Annotations on the screenshot include:

- A red box around the "Result" dropdown menu in the top toolbar.
- A red box around a menu with options: "Anchoring", "Extension 1", "Extension 2", and "Result" (checked).
- A green callout box with the text: "This page shows all the full molecules. You can go to any of the steps and re-run the calculations."

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Mode Overview

Alternatively, you have the option to end the workflow.

The 'Terminate' button will only show the full molecules that are selected below, into a Results page. All remaining intermediate fragments/molecules will be deleted. You can no longer navigate to any of the previous steps after you 'Terminate'.

Note: The 'Terminate' button also releases the allocated storage on the HPSee cluster.

Molecules on Server: (# 147)	
Name	Estimated Affinity
	pM nM μM mM
1	rxn501___A5_2
2	rxn5___A5_3
3	rxn501___A5_2
4	rxn501___A5_1
5	rxn501___A5_5
6	rxn501___A5_5
7	rxn501___A1_2

Molecules: (# 6)	
Name	Estimated Affinity
	pM nM μM mM
1	rxn501___A5_2
2	rxn501___A1_1
3	rxn501___A5_5
4	rxn501___A1_1
5	rxn501___A1_2
6	rxn501___A1_5

2D

rxn501b_mod___C6___B1___A5_3

C1=CC=C(C=C1)CCCNC(=O)c2nc3c(s2)nc4c3cnc4

Target View Control

Show Binding Site Only Change Visibility of Residues

1 5 10 15 20 25 30

SKKT SERE PHE7 GLU8 THR8 ARG10 PHE11 GLU12 LYS13 MET14 ASP15 ASN16 LEU17 LEU18 ARG18 ASP20 PRO21 LYS22 SER23 GLU24 VAL25 ASN26 SER27 ASP28 CYS29 LEU30 LEU31 ASP32 GLY33 LEU34 ASP35 ALA36 LEU37 VAL38 TYR39

SKKT ROCK1-test-space rxn501b_mod___C6___B1___A5_3 5 messages

The screenshot displays a molecular docking software interface. On the left, a table lists six molecules with their names, estimated affinities, and molecular weights. Below the table is a 2D chemical structure of the selected molecule, rxn501b_mod__C6__B1__A5_2. The main window shows a 3D ribbon representation of a protein structure in green, with a yellow and black striped hazard symbol indicating a warning. A green callout box on the right contains the text: "This is the final page with all selected full molecules so far. Congratulations! You finished your first C-S-D run!". At the bottom, a target view control shows a sequence of residues from 1 to 30, with the selected molecule's name and a message count (5 messages) displayed.

Molecules: (# 6)	Name	Estimated Affinity				LE	Tor.	Intra-clash	Inter-clash	MW
		pM	nM	µM	mM					
1	rxn5__A5_2	→								348.43
2	rxn501__A1_1									310.38
3	rxn501__A5_5									348.43
4	rxn501__A1_1									332.36
5	rxn501__A1_2									347.42
6	rxn501__A1_5									396.47

2D
rxn501b_mod__C6__B1__A5_2

Target View Control

Show Binding Site Only Change Visibility of Residues

1 5 10 15 20 25 30 Name (e.g. gly)

SKKT SERE PHET GLUR THR8 ARG10 PHET11 GLU13 LYS13 MET14 ASP15 ASN16 LEU17 LEU18 ARG18 ASP20 PRO21 LYS22 SER23 GLU24 VAL25 ASN26 SER27 ASP28 CYS29 LEU30 LEU31 ASP32 GLY33 LEU34 ASP35 ALA36 LEU37 VAL38 TYR39

SKKT ROCK1-test-space rxn501b_mod__C6__B1__A5_2 5 messages

This is the final page with all selected full molecules so far.

Congratulations! You finished your first C-S-D run!

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Mode Overview



11. Protein Editor Mode

The YASARA module is a third-party integration that enables you to perform structure refinement of your target of interest or complex.

Important note:
To run the energy minimization a valid YASARA license for SeeSAR is required.

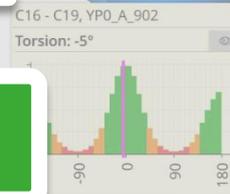


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Mode Overview

ZZZF - Extract Your Ligand

Hetero Groups	LOI	Name	Estimated Affinity			
			pM	nM	µM	mM
<input type="checkbox"/>		Do not extract a ligand				
<input checked="" type="checkbox"/>		53U_H_2001				

2D
53U_H_2001

C1CCN(C1)C(=O)N(Cc2ccccc2)C(=O)N(Cc3ccccc3)C

Target View Control

Show Binding Site Only Change Visibility of Residues

1 5 10 15 20 25 30

GLU16 ALA18 ASP14 CYS1 CYS2 GLU3 LEU3 ARG4 PRO5 LEU6 PHE7 GLU8 LYS9 LYS10 SER11 LEU12 GLU13 ASP14 LYS14A THR14B GLU14C ARG14D GLU14E LEU14F LEU14G LEU14H LEU14I SER14E THR14E SER14K SER14L VAL17 GLU18 GLY19 SER20 ASP

ZZZF 53U_H_2001

Load PDB 2ZFF and select 53U_H_2001 as the ligand.

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Mode Overview

The screenshot displays a software interface for protein-ligand interaction analysis. On the left, a 'Data' panel shows a table of proteins and ligands. A red arrow points to a context menu for the protein 'ZZFF', with the option 'Add to Protein Editor' highlighted in a red box. The main window shows a 3D ribbon representation of a protein structure in blue, with a red ligand molecule bound to it. A green callout box with white text reads: 'Right-click on your target and transfer it to the Protein Mode.' The bottom of the interface features a 'Target View Control' panel with a sequence viewer showing amino acid residues from 1 to 30, including GLU1C, ALA1B, ASP1A, CYS1, GLY2, LEU3, ARG4, PRO5, LEU6, PHE7, GLU8, LYS9, LYS10, SER11, LEU12, GLU13, ASP14, LYS16A, THR16B, GLU16C, ARG16D, GLU16E, LEU16F, LEU16G, LEU16H, LEU16I, SER16J, THR16K, SER16L, SER16M, VAL17, GLU18, GLY19, SER20, and ASP21.

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Mode Overview

The screenshot displays the ChimeraX software interface. On the left, two panels are highlighted with red boxes: the 'Current Edit State' panel, which shows 'Z2FF_1' as the active state, and the 'Proteins (# 1)' panel, which lists a protein with filename 'Z2FF' and description 'Exploring Thrombin S1-pocket'. The central area features a 3D ribbon representation of a protein structure in blue, with a red stick model of a ligand bound to it. At the bottom, the 'Target View Control' panel shows a sequence viewer for the protein, with residues 1 through 30 visible. The interface includes various toolbars and a search bar at the top.

In 'Current Edit State' you will find the active protein you are currently working with. This is also where you can resume your editing process.

All proteins currently featured in the **Proteins Mode** can be found in the 'Proteins' window.

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Mode Overview

The screenshot shows a protein structure visualization software interface. The main window displays a 3D ribbon representation of a protein structure in blue, with a segment highlighted in green. The interface includes a top toolbar with various icons, a left sidebar with panels for 'Data', 'Current Edit State', 'Unresolved Segments', and 'Proteins (# 1)'. The 'Unresolved Segments' panel is highlighted with a red box and contains the following table:

N-Term	Unresolved	C-Term
1 THR_H_147	--- WTIANVVK	① --- GLY_H_150

The 'Proteins (# 1)' panel shows a table with columns for 'Filename' and 'Description':

Filename	Description
1 Z2FF	Exploring Thrombin S1-pocket

At the bottom, there is a 'Target View Control' panel with a 'Show Binding Site Only' checkbox, a 'Change' button, and a 'Residues' dropdown menu. A sequence viewer at the bottom shows the protein sequence: 1 5 10 15 20 25 30. The sequence is: 1 GLUIC ALAIE ASPIA CYST GLVZ LEIIE ARG4 PROS LEI4E PHE7 GLIIE LYSO LYSIO SERII LEIIE GLIIE ASP14 LYS14A THR14E GLIIE4C ARG14D GLIIE4E LEIIE4P LEIIE4Q GLIIE4R SER14E THR14E LEIIE4E LEIIE4E VAL17E GLIIE4E GLIIE4E SER22E ASP

If part of a protein is unresolved, the missing segment can be displayed as a suggested sequence, provided this information is available in the file format.

The segment can then be remodeled by energy minimization.

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[Mode Overview](#)

The screenshot displays the Proteins Plus Server web interface. At the top, a search bar is highlighted with a red box and contains the text "Search for similar binding sites in the PDB". The main area shows a 3D ribbon representation of a protein structure in blue, with a grey stick model of a ligand bound to it. On the left, a sidebar contains several panels: "Current Edit State" showing "Z2FF_1", "Unresolved Segments" with a table, "Proteins (# 1)" with a table, and a "2D" panel. At the bottom, a "Target View Control" panel shows a sequence viewer with residue numbers from 1 to 30 and amino acid abbreviations like GLU1C, ALA1B, ASP1A, etc.

N-Term	Unresolved	C-Term
1 THR_H_147	--- WTANVGK	① --- GLY_H_150

Filename	Description
Z2FF	Exploring Thrombin S1-pocket

Residue	Amino Acid
1	GLU1C
2	ALA1B
3	ASP1A
4	CYS1
5	GLY2
6	LEU3
7	ARG4
8	PRO5
9	LEU6
10	PHE7
11	GLU8
12	LYS9
13	LYS10
14	SER11
15	LEU12
16	GLU13
17	ASP14
18	LYS14A
19	THR14B
20	GLU14C
21	ARG14D
22	GLU14E
23	LEU14F
24	LEU14G
25	GLU14H
26	SER14I
27	THR14J
28	LEU14K
29	LEU14L
30	VAL17
31	GLU18
32	GLY19
33	SER20
34	ASP21

Unedited PDB structures can be used as templates to search for similar binding sites via the SIENA – Proteins Plus Server.

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Mode Overview

The screenshot displays the Proteins Plus Server interface. On the left, there is a sidebar with sections for 'Data', 'Current Edit State' (showing 'Z2FF_1'), 'Unresolved Segments' (listing '1 THR_H_147' and 'GLY_H_150'), and 'Proteins (# 1)' (listing 'Z2FF Exploring Thrombin S1-pocket'). The main area shows a 3D ribbon representation of a protein structure in blue and grey. A dialog box titled 'SIENA - Proteins Plus Server' is overlaid on the structure. The dialog contains a green circular logo, the Proteins Plus logo, and a privacy warning: 'You are going to use the remote Proteins Plus server. Be sure that your search does not violate the privacy policy of your company. For more details see [Privacy Policy Uni-Freiburg](#).' Below the warning are three buttons: 'Privacy warning...' (highlighted in orange), 'Advanced Settings...' (highlighted with a red box), and 'Search' (highlighted with a red box). At the bottom of the interface, there is a 'Target View Control' section with a sequence viewer showing residues from 1 to 35, including 'GLUC', 'ALAN', 'ASPAR', 'CYS', 'GLUT', 'LEUC', 'ARGI', 'PROL', 'LEUC', 'PHE', 'GLUC', 'LEUC', 'LEUC', 'GLUC', 'SERI', 'LEUC', 'GLUC', 'ASPAR', 'LEUC', 'THR', 'GLUC', 'ASPAR', 'GLUC', 'LEUC', 'LEUC', 'GLUC', 'SERI', 'THR', 'SERI', 'SERI', 'VAL', 'GLUC', 'GLUC', 'SERI', 'ASP'. The status bar at the bottom indicates 'No Protein Selected' and '1 message'.

You can initiate the search with the 'Search' button. Similarity of retrieved structures is based on binding site topology (not sequence).
Per default, 10 structures will be retrieved. If more are required, visit 'Advanced Settings...'.

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Mode Overview

The screenshot displays the Proteins Plus Server interface. On the left, there are panels for 'Data' (Current Edit State: Z2FF_1, Unresolved Segments: 1 THR_H_147 --- WTAVNGK --- GLY_H_150) and 'Proteins (# 1)' (Filename: Z2FF, Description: Exploring Thrombin S1-pocket). The main area shows a 3D protein structure in blue ribbon representation. A dialog box titled 'SIENA - Proteins Plus Server' is open, featuring a green circular icon with a white 'C' and a 'PROTEINS PLUS' logo. It includes a slider for 'Maximum Number of Solutions' set to 10, and buttons for 'Cancel', 'Advanced Settings...', and 'Search'. At the bottom, there is a 'Target View Control' bar with a sequence of residues: 1 Z2FF_1, 5 GLUC, ALAN, ASPA, CYST, GLYS, LEUC, ARG, PRO, LEUC, PHE, GLU, LYS, LYS, SER1, LEUC, GLUC, ASP4, LYS1A, THR1B, GLUC1C, ARG1D, GLUC1E, LEUC1F, LEUC1G, GLUC1H, SER1I, THR1L, SER1K, SER1L, VAL1T, GLUC1J, GLYS1K, SER2D, ASP2E.

Here, you can increase the number of structures to-be-retrieved up to 500.

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Mode Overview

Protein editing is paused. Click here to resume.

Unresolved Segments

N-Term	Unresolved	C-Term
THR_H_147	--- WTRMVGK	GLY_H_150

Proteins (# 11)

Filename	Description
1 Z2FF	Exploring Thrombin S1-pocket
2 1AGH	THE X-RAY CRYSTAL STRUCTURE OF PPACK-MEIZOTHR...
3 1AGH	THE X-RAY CRYSTAL STRUCTURE OF PPACK-MEIZOTHR...
4 1AZC	STRUCTURE OF THROMBIN INHIBITED BY AERUGINOS...
5 1A3B	COMPLEX OF HUMAN ALPHA-THROMBIN WITH THE BL...
6 1A3E	COMPLEX OF HUMAN ALPHA-THROMBIN WITH THE BL...
7 1A46	THROMBIN COMPLEXED WITH HIRUGEN AND A BETA...
8 1A4W	CRYSTAL STRUCTURES OF THROMBIN WITH THIAZOLE...
9 1A5G	HUMAN THROMBIN COMPLEXED WITH NOVEL SYNTHL...
10 1A61	THROMBIN COMPLEXED WITH NOVEL SYNTHETIC PEPT...
11 1ABI	STRUCTURE OF HUMAN ALPHA-THROMBIN

2D

Target View Control

Show Binding Site Only Change Visibility of Residues

1 5 10 15 20 25 30

all 1ABI SERIE GLYID GLIIC ALAID ASPIA CYSC GLVC LEIIS ARQ4 PRQD LEIIS PHE7 GLI8 LYS3 LYSID SER11 LEU12 GLI13 ASP14 LYS16A THR16B GLI16C ARG16D GLI16E LEU16F LEU16G GLI16H SER16 THR16I LEI16J ASP16K GLY16L ARG16M

1ABI

1 message

Once you have your structure retrieved or edited, you can export them back to the **Proteins Mode** for follow-up investigations with a **right-click** on the structure of interest and 'Add to Protein Mode'.

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Mode Overview

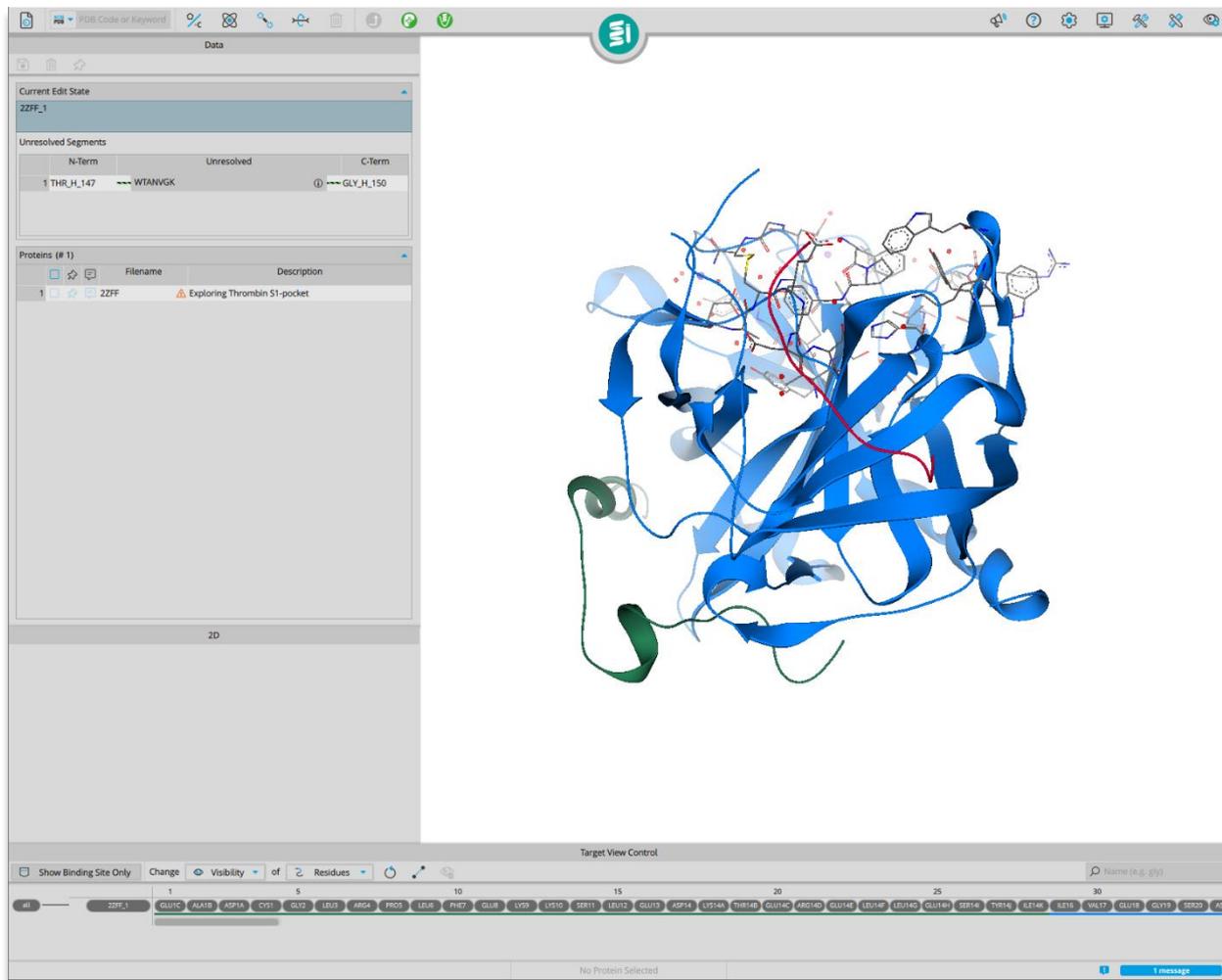


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Mode Overview

Data

Current Edit State
ZZFF_1

Unresolved Segments	N-Term	Unresolved	C-Term
1	THR_H_147	--- WTIANVKG	GLV_H_150

Proteins (# 1)

Filename	Description
ZZFF	Exploring Thrombin S1-pocket

2D

CC1=CC=C2C(=C1)C(=CN2)C[C@@H](C(=O)R)N(R)

Target View Control

Show Binding Site Only Change Visibility of Residues

1 5 10 15 20 25 30

all --- ZZFF_1 GLYC ALA18 ASP14 CYS1 GLY2 LEU3 ARG4 PRO5 LEU6 PHE7 GLU8 LYS9 LYS10 SER11 LEU12 GLU13 ASP14 LYS14A THR14B GLU14C ARG14D GLU14E LEU14F LEU14G VAL14H SER14 THR14A SER14B SER14C VAL17 GLU18 GLY19 SER20 ASP

No Protein Selected 1 message

Clicking on any heavy atom of the target structure enables you to edit the residue side chain or the component.

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Mode Overview

Rotate

Current Edit State
Z2FF_1

Flip
Next Interchange Option
Flip Sites

Unresolved Segments

N-Term	Unresolved
1 THR_H_147	WTIANVGK GLV_H_150

Proteins (# 1)

Filename	Description
Z2FF	Exploring Thrombin S1-pocket

2D

RNC(=O)C[C@H](c1ccc2c(c1)c[nH]2)R

Target View Control

Show Binding Site Only Change Visibility of Residues

1	5	10	15	20	25	30
GLUC	ALAT	ASPA	CYS1	GLY2	LEU3	ARG4
PRO5	LEU6	PHI7	GLU8	LYS9	LYS10	SER11
LEU12	GLU13	ASP14	LYS14A	THR14B	GLU14C	ARG14D
GLU14E	LEU14F	LEU14G	GLU14H	SER14I	THR14J	LEU14K
LEU14L	LEU14M	VAL17	GLU18	GLY19	SER20	ASP

No Protein Selected

1 message

Clicking on a bond allows you to rotate it for rotamer exploration. Use the clashes visualization to check for reasonable conformations.

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Mode Overview

The screenshot displays a molecular modeling software interface. On the left, there are panels for 'Current Edit State' (showing 'Z2FF_1'), 'Unresolved Segments' (listing '1 THR_H_147' and 'GLY_H_150'), and 'Proteins (# 1)' (listing 'Z2FF Exploring Thrombin S1-pocket'). Below these is a '2D' panel showing a chemical structure of a peptide backbone with a benzimidazole-like side chain. The main window shows a 3D ribbon representation of a protein structure in blue, with a ligand molecule in orange and red. A red box highlights a toolbar at the top with icons for copy, paste, and delete. A green callout box with an arrow points to the protein structure, containing the text: 'You can also edit the molecular structure in the same way as in the **Molecule Editor**. Use hotkeys for elements or the supporting toolbar.' At the bottom, there is a 'Target View Control' panel with a sequence viewer showing residues from 1 to 30, including GLYC, ALA18, ASP14, CYS1, GLY2, LEU3, ARG4, PRO5, LEU6, PHE7, GLU8, LEU9, LEU10, SER11, LEU12, GLU13, ASP14, LEU15, THR16, GLU17, ARG18, LEU19, LEU20, VAL21, SER14, THR16, SER16, VAL17, GLU18, GLY19, SER20, and ASP21.

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Mode Overview

The screenshot displays the YASARA software interface. On the left, a panel titled "7649_1 - Extract Your Ligand" shows a table of hetero groups:

Hetero Groups	LOI	Name	Estimated Affinity
1	<input type="checkbox"/>	Do not extract a ligand	
2	<input type="checkbox"/>	MES_A_901	
3	<input checked="" type="checkbox"/>	YPO_A_902	
4	<input type="checkbox"/>	CLA_A_907	
5	<input type="checkbox"/>	MDL_B_1	

The main window shows a 3D ribbon representation of a protein (blue) with a ligand (orange and green) bound in its active site. A histogram window titled "C16 - C19, YPO_A_902" displays a torsion distribution with a peak at -5°. The bottom of the interface features a "Target View Control" panel with a sequence viewer showing residues 1 through 30.

11.1 Energy Minimization

The YASARA module is a third-party integration that enables you to perform structure refinement of your target of interest or complex.

Important note:
To run the energy minimization a valid YASARA license for SeeSAR is required.

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Mode Overview

The screenshot displays a molecular docking software interface. On the left, a panel titled "7G49 - Extract Your Ligand" contains a table of hetero groups. A red box highlights the "7G49" dropdown menu (1), a green play button (2), and the "YPO_A_902" row in the table (3). Below the table is a 2D chemical structure of YPO_A_902. The main window shows a 3D ribbon representation of a protein (blue) with a ligand (green and orange spheres) bound in its pocket. A small window titled "C16 - C19, YP0_A_902" displays a histogram of torsion angles for the C16-C19 bond, with a vertical line indicating a value of 63°. The bottom of the interface shows a "Target View Control" bar with residue numbers and names.

Hetero Groups	LOI	Name	Estimated Affinity
			µM
1		Do not extract a ligand	
2		MES_A_901	
3		YPO_A_902	
4		CL_A_907	
5		MOL_B_1	

In order to perform an energy minimization, we will load PDB 7G49. This complex contains a ligand with an unfavorable torsion.

Load the PDB and select YPO_A_902 as the ligand to define the binding site.

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Mode Overview

Right-click on the structure you would like to refine and select 'Add to Protein Editor'.

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Mode Overview

N-Term	Unresolved	C-Term
1 LYS_A_463	--- PSGK	① --- CYS_A_468
2 GLU_A_573	--- PK	② --- ASN_A_576

Proteins (# 1)

Filename	Description
7G49_1	one of our Antiviral In proteins with R.P.

Target View Control

1 5 10 15 20 25 30

all 7G49_1 TRPS TRSD ALAD TRSD SERPS GLVPS SERP CYSB LYSB GLVQ ARG1 CYSQ PHEB GLI6A LEI6S GLN6G GLI6T VAL6B GLV6B PRO70 PRO71 ASP72 CYS73 ARG74 CYS75 ASP76 ASN77 LEU78 CYS79 LYS80 SER81 TYR82 SER83

No Protein Selected

Unresolved segments are displayed in the corresponding table and, if the necessary information is available in the structure file, are automatically added. They are then completed automatically during energy minimization.

If this information is unavailable (e.g., for in-house structures), it can be entered manually.

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Mode Overview

Current Edit State
7G49_1

Unresolved Segments

N-Term	Unresolved	C-Term
1 LYS_A_463	--- PSGK	① --- CYS_A_468
2 GLU_A_573	--- PK	② --- ASN_A_576

Proteins (# 1)

Filename	Description
7G49	Crystal Structure of rat Autotaxin in complex with 8-2...

Target View Control

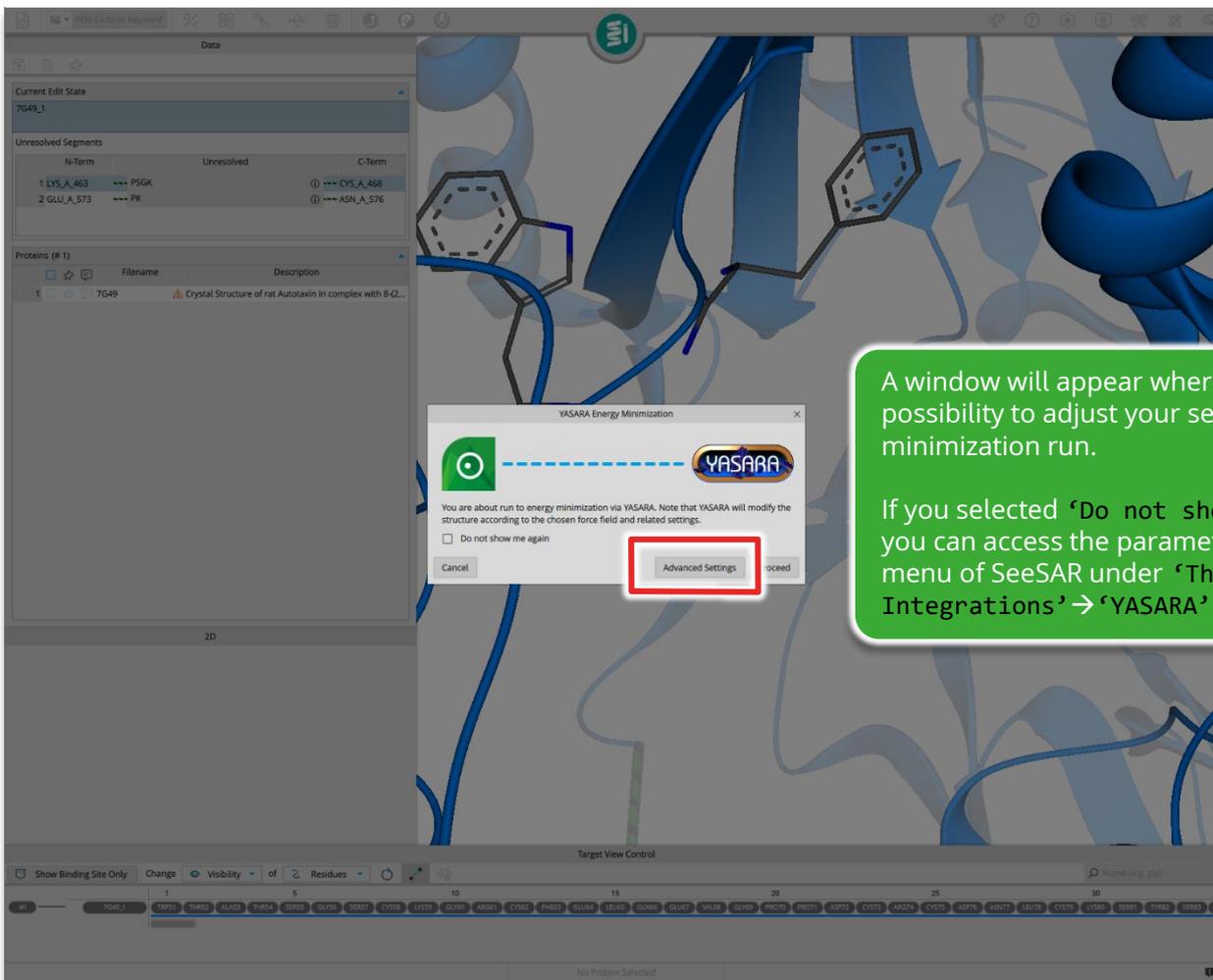
1 5 10 15 20 25 30

all 7G49_1 TRPS TRPSD ALA33 THRS4 SER55 GLY76 SER57 CYS58 LYS59 GLY60 ARG61 CYS62 PHE63 GLU64 LEU65 GLN66 GLI67 VAL68 GLY69 PRO70 PRO71 ASP72 CYS73 ARG74 CYS75 ASP76 ASN77 LEU78 CYS79 LYS80 SER81 TYR82 SER83

To start the minimization, click on 'Energy minimize and save to table'.

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Mode Overview

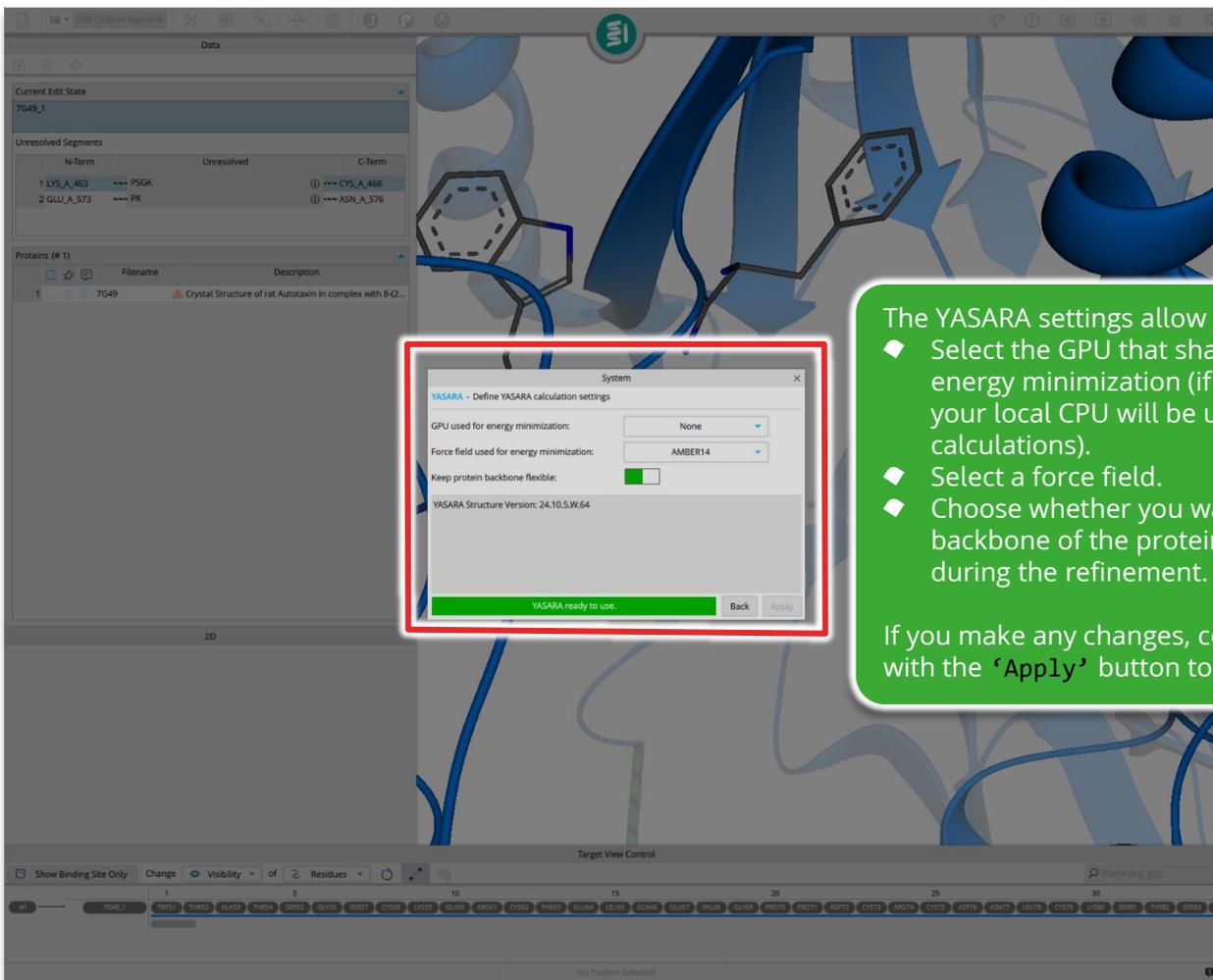


A window will appear where you will have the possibility to adjust your settings or start the minimization run.

If you selected 'Do not show me again', then you can access the parameters in the 'System' menu of SeeSAR under 'Third-Party Integrations' → 'YASARA'.

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Mode Overview



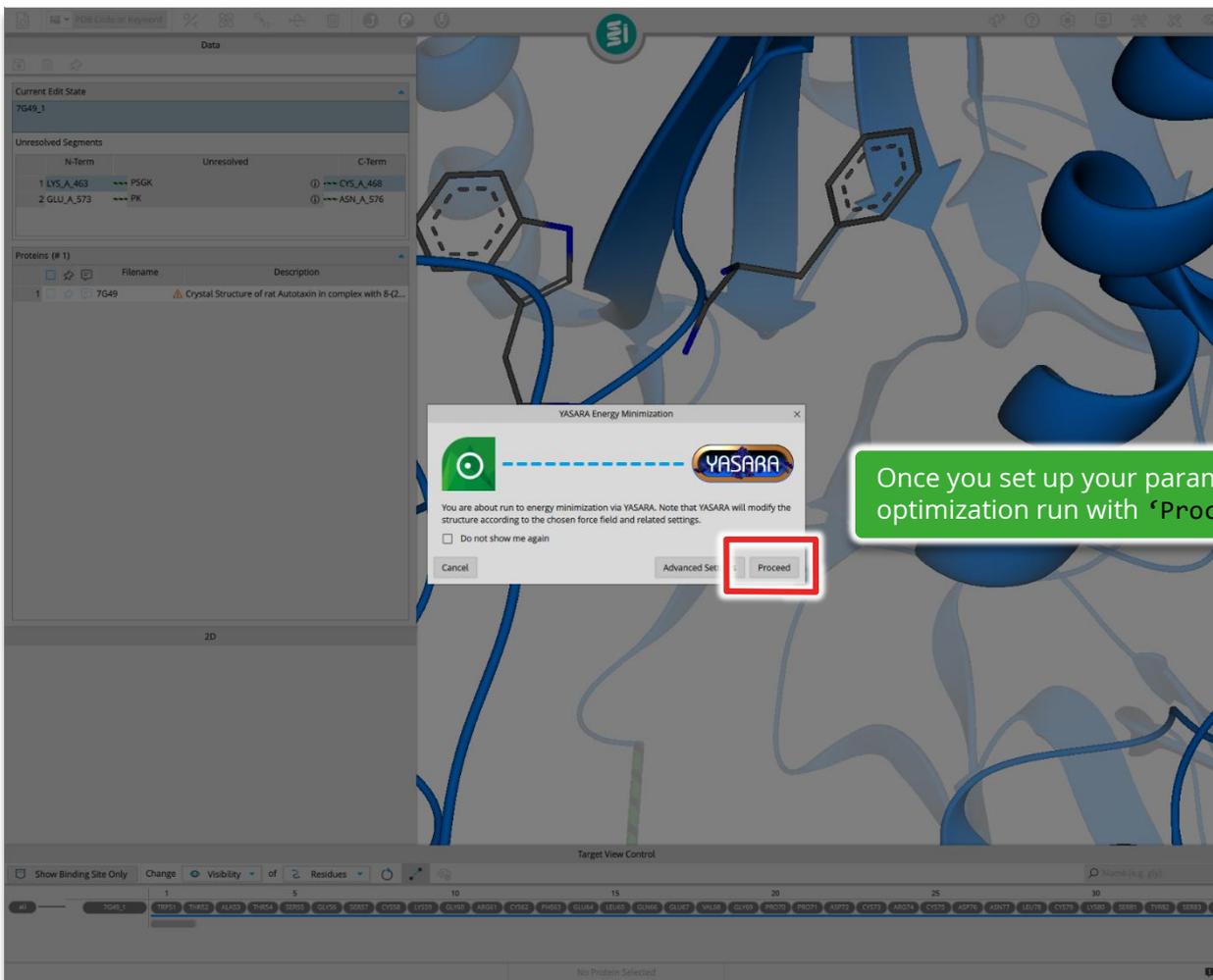
The YASARA settings allow you to:

- ◆ Select the GPU that shall be used for the energy minimization (if no GPU is selected, your local CPU will be used for the calculations).
- ◆ Select a force field.
- ◆ Choose whether you want to keep the backbone of the protein flexible or rigid during the refinement.

If you make any changes, confirm the settings with the 'Apply' button to use them.

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Mode Overview



Once you set up your parameters, start the optimization run with 'Proceed'.

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Mode Overview

The screenshot displays the Protein Editor interface. The main window shows a 3D ribbon representation of a protein structure in blue. Two specific residues are highlighted with dashed boxes: LYS_A_463 and ASN_A_576. On the left, a 'Data' panel is visible, containing a table of unresolved segments and a list of proteins.

N-Term	Unresolved	C-Term
1 LYS_A_463	--- PSGK	① --- CYS_A_468
2 GLU_A_573	--- PK	② --- ASN_A_576

Proteins (# 2)	Filename	Description
2	7G49_1	Crystal Structure of rat Autotaxin in complex with 8-Q...

At the bottom, a 'Target View Control' bar shows a sequence of residues from 1 to 30, with the first few residues (TRPS, TRSD, ALAS3, SERSS, GLVTS, SERST, CYSB, LYSB, GLVQ, ARG1, CYSQ, PHEB, GLU4, LEU5, GLN6, GLI7, VAL8, GLV9, PRO70, PRO71, ASP72, CYS73, ARG74, CYS75, ASP76, ASN77, LEU78, CYS79, LYS80, SER81, TYR82, SER83, etc.) visible.

After the refinement calculation has finished, a new entry will be added to the **Protein Editor Mode**.

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Mode Overview

2.

N-Term	Unresolved	C-Term
1 LYS_A_463 --- P5GK		① CYS_A_468
2 GLU_A_573 --- PK		① ASN_A_576

1.

Filename	Description
7G49	Crystal Structure of rat Autotaxin in complex with 8-Q...
7G49_1	Crystal Structure of rat Autotaxin in complex with 8-Q...

From here on, you can export the refined structure or continue working with it.

For export, check the refined structure and click on 'Save checked proteins'. All checked proteins will be exported to your selected folder.

If you are working with several structures, make sure to rename them (by double clicking on the name in the 'Filename' column).

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Mode Overview

Current Edit State
7G49_2

Protein editing is paused. Click here to resume.

Unresolved Segments

N-Term	Unresolved	C-Term
1 LYS_A_463	--- P5GK	① --- CYS_A_468
2 GLU_A_573	--- PK	① --- ASN_A_576

Proteins (# 2)

Filename	Description
1 7G49	Crystal Structure of rat Autotaxin in complex with 8-2...
2 7G49	Autotaxin in complex with 8-2...

① Add to Protein Mode

To continue working on a structure, right click on it and select 'Add to Protein Mode'.

Show Binding Site Only Change Visibility of Residues

Target View Control

1 5 10 15 20 25 30

all 7G49_1 TRPS TRPSD ALAKS TRPSD SERPS GLY78 SERPS CYS78 LYS79 GLY80 ARG81 CYS82 PHE83 GLU84 LEU85 GLN86 GLU87 VAL88 GLY89 PRO70 PRO71 ASP72 CYS73 ARG74 CYS75 ASP76 ASN77 LEU78 CYS79 LYS80 SER81 TYR82 SER83

7G49_1 1 message

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Mode Overview

7G49_1 - Extract Your Ligand

Hetero Groups	LOI	Name	Estimated Affinity
			pM nM μ M mM
1	<input type="radio"/>	Do not extract a ligand	
2	<input type="radio"/>	MES_A_901	
3	<input checked="" type="radio"/>	YPO_A_902	
4	<input type="radio"/>	CLA_907	
5	<input type="radio"/>	MOL_B_1	

2D
YPO_A_902

C16 - C19, YPO_A_902
Torsion: -5°

Target View Control

Show Binding Site Only Change Visibility of Residues

7G49 YPO_A_902

You face the already known ligand selection view to define a binding site.

Here, we can check the previously red colored torsion which is green now. The energy minimization run optimized the strained torsion.

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Mode Overview

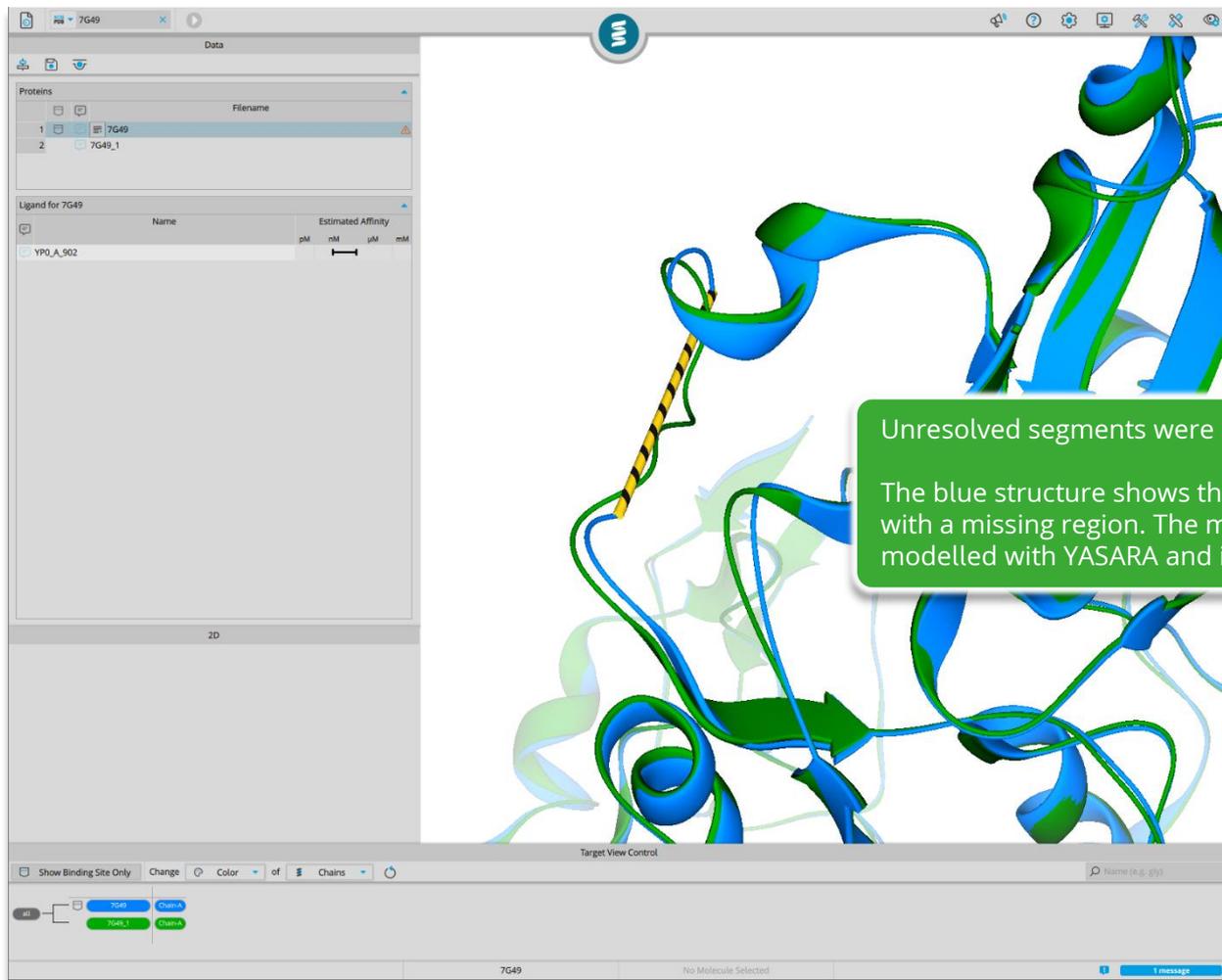


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Mode Overview



**Have fun and enjoy your
interactive drug discovery
journey with SeeSAR!**

**If you have any problems,
please reach out to us:
support@biosolveit.de**

Mode Overview



Proteins



Protein Editor



Binding Site



Analyzer



Molecule Editor



Inspirator



Docking (Local)



Similarity Scanner



Activity Spotter



Docking (Remote)



Space Docking®