

# Quick Start Guide StarDrop 7.1



A complete platform for small molecule design, optimisation and data analysis



We are delighted to introduce the exciting new features offered by StarDrop 7.1. If you are new to StarDrop or would like more detailed descriptions of the new features, please see the StarDrop User Guide or contact [info@optibrium.com](mailto:info@optibrium.com)

## New Surfex eSim3D™ Module

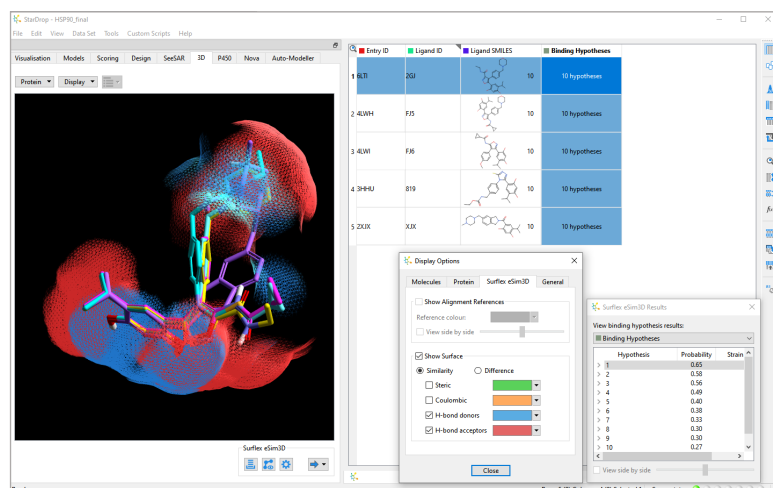
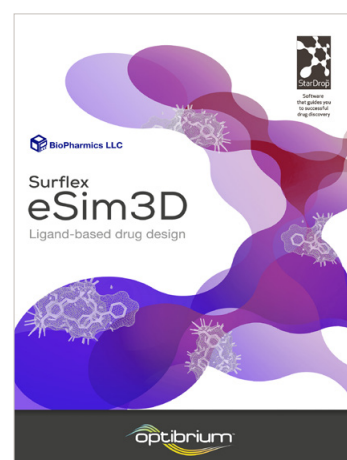
### Enhanced 3D ligand-based design

The new Surfex eSim3D module provides industry-leading 3D ligand-based design methods, enabling you to identify and optimise novel active compounds, even with little or no target structure information.

Underpinned by rigorously validated science, Surfex eSim3D offers unprecedented accuracy and performance to help you;

- Find novel potent compounds with 3D virtual screening against known actives
- Understand 3D structure-activity relationships to guide further optimisation of your compounds' potency with rigorously validated pose prediction
- Generate binding mode hypotheses by alignment of multiple known actives
- Get a complementary perspective to docking where you have 3D structures of your target to improve the performance of virtual screening

Developed in collaboration with BioPharmics LLC, Surfex eSim3D compares compounds based on molecular shape, electrostatic fields and directional hydrogen bonding preferences.



You can [watch a quick video](#) of Surfex eSim 3D in action or [contact us](#) for a free evaluation to try it yourself.

## Upgrading from torch3D™ to Surfex eSim3D

If you license the torch3D module, you'll receive an automatic upgrade to Surfex eSim3D when installing StarDrop 7.1, giving you access to many new capabilities above and beyond torch3D, including;

- Align multiple active compounds to generate binding model hypotheses. These can be used as a target for the alignment of novel compounds, increasing the robustness of your virtual screens over a single reference compound
- Generate ensembles of 3D conformations for your compounds using the fast and rigorous ForceGen method
- Perform virtual screens on an unlimited number of compounds, removing the 500-compound limit of torch3D

Furthermore, Surfex eSim3D brings StarDrop's 3D ligand-based design support back to the latest macOS version.

If you don't already license torch3D and would like to explore the enhanced capabilities of Surfex eSim3D, [contact us](#), and we'd be delighted to provide a free trial license.


## Improvements to the SeeSAR View Module User Interface

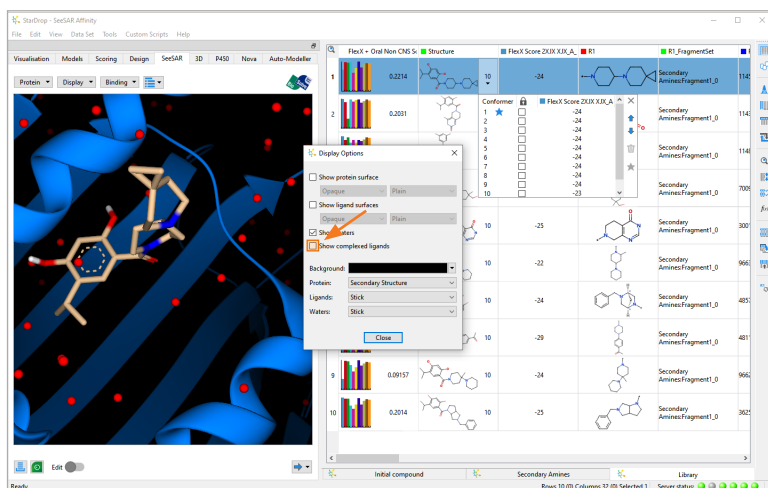
### Choose poses for inspection directly in Table View

To simplify your interactions with multiple poses of the same compound in SeeSAR View, you can now access them directly in Table View. Click on the number of conformations shown next to the compound structure to view a dropdown showing all poses, whether generated with the SeeSAR Pose module or your preferred docking platform via StarDrop's Pose Generation Interface. This change harmonises the user interface for conformations in the SeeSAR modules and the new Surfex eSim3D module.

### Handling co-crystallised ligands in SeeSAR View

If you wish to hide ligands co-crystallised with your targets, you can now access this option from Display Options under the Display menu above the 3D viewer in the SeeSAR area. Just untick the Show complexed ligands checkbox.

You can also easily focus the view back on the co-crystallised ligand using the  button above the 3D viewer area.



If you have any questions or would like any additional information about StarDrop 7.1, don't hesitate to get in touch with us at [info@optibrium.com](mailto:info@optibrium.com)