



LigandScout 4.5 Functionality Comparison

Features	LigandScout Essential	LigandScout Advanced	LigandScout Expert
Structure-based Pharmacophore Modelling			
Ligand-based Pharmacophore Modelling			
Screening Library Generation			
Virtual Screening			
Model Validation (automated ROC curve)			
Extended Table Filtering & Export			
High Speed 3D Conformer Generator			
Tautomer Generator			
Pharmacophore-based Alignment & Clustering			
2D Molecular Editor			
Interactive Molecular Property Graphs			
Protein Binding Pocket Finder			
Interactive Molecular Docking			
Interactive Ligand Binding Affinity Estimation			
Automated Apo-Site Pharmacophore Generator			
Molecular Dynamics Trajectories Import			
Interactive MD Trajectories Analysis Graphs			
Inte:Ligand Knime Extensions			
Remote Cluster or Amazon Cloud Computing			
Pre-computed 3D Libraries for Screening			