LigandScout 4.4 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			✔

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Mariahilferstrasse 74B/11
1070 Wien/Vienna
Austria, Europe

www.inteligand.com
office@inteligand.com
Fax +43 1 8174955 1371