inte:ligand

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LigandScout 4.0 Functionality Comparison

Features	LigandScout Essential	LigandScout Advanced	LigandScout Expert/Knime
Structure-based Pharmacophore Modelling	✓	✓	✓
Ligand-based Pharmacophore Modelling	✓	✓	✓
Virtual Screening	✓	✓	✓
Model Validation (automatic ROC curve)	✓	✓	✓
Extended Table Filtering & Export	✓	✓	✓
High Speed 3D Conformer Generator	✓	✓	✓
Tautomer Generator	✓	✓	✓
Pharmacophore-based Clustering	✓	✓	✓
Pharmacophore-based Alignment	✓	✓	✓
Free Energy of Binding Estimation		✓	✓
Molecular Docking		✓	✓
Apo-Site Pharmacophore Modelling		✓	✓
Molecular Dynamics Trajectories Import		✓	✓
Pre-computed 3D Libraries for Screening			✓
Knime LigandScout Extension			✓

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LigandScout Pre-computed 3D Libraries for Screening

This molecular 3D multiconformational in silico screening library package contains approximately 6 million molecules selected from the ZINC database (preferred suppliers that are able to deliver compounds within a short delay) and from the eMolecules compound procurement service. The download consists of two compressed files. The LigandScout databases are in ldb format and present as chunks of 500k or 750k compounds each, ready for parallel in silico screening.

On request, other databases can be computed and made available for download free of charge.

Knime LigandScout Extensions

The Knime LigandScout Extensions contain nodes using cutting edge LigandScout technology, optimized for the usage of big data packages within Knime. Nodes are available for I/O operations (smiles reader and writer, sdf reader and writer, mol2 reader and writer, ldb reader and writer), conformer generation, and database screening (both hit screening and hit activity profiling available).

Future releases (Q4.2015) will contain additional nodes for structure- and ligand-based pharmacophore generation, standard molecular physicochemical property calculation, pharmacophore-based clustering, and molecular docking.