

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			

LigandScout Pre-computed 3D Libraries for Screening

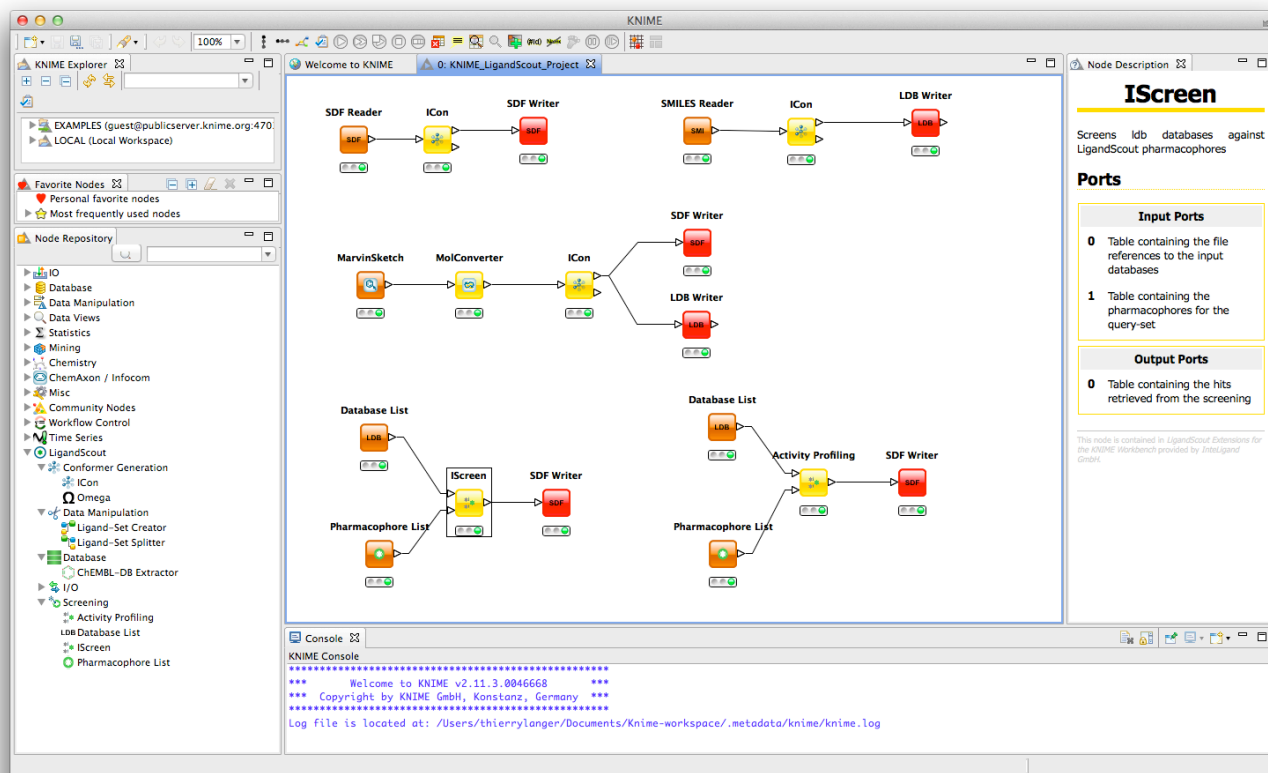
This molecular 3D multiconformational in silico screening library package contains approximately 6 million molecules selected from the ZINC database (preferred suppliers that are able to deliver compounds within a short delay) and from the eMolecules compound procurement service. The download consists 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.



The screenshot displays the KNIME software interface with a workflow for database screening. The workflow consists of several nodes connected in a sequence:

- SDF Reader** (sdf) → **ICon** → **SDF Writer** (sdf)
- SMILES Reader** (sm) → **ICon** → **LDB Reader** (ldb)
- MarvinSketch** → **MolConverter** → **ICon** → **SDF Writer** (sdf) and **LDB Writer** (ldb)
- Database List** (ldb) → **IScreen** → **SDF Writer** (sdf)
- Pharmacophore List** → **IScreen** → **SDF Writer** (sdf)
- Database List** (ldb) → **Activity Profiling** → **SDF Writer** (sdf)
- Pharmacophore List** → **Activity Profiling** → **SDF Writer** (sdf)

The **Node Description** panel on the right shows details for the **IScreen** node:

- IScreen**: Screens ldb databases against LigandScout pharmacophores
- Ports**:
 - Input Ports**:
 - 0 Table containing the file references to the input databases
 - 1 Table containing the pharmacophores for the query-set
 - Output Ports**:
 - 0 Table containing the hits retrieved from the screening

The console at the bottom shows the following output:

```

KNIME Console
*****
*** Welcome to KNIME v2.11.3.0046668 ***
*** Copyright by KNIME GmbH, Konstanz, Germany ***
*****
Log file is located at: /Users/thierry.langer/Documents/Knime-workspace/.metadata/knime/knime.log
  
```