



LigandScout 4.4

Version 4.4 greatly expands LigandScout's capabilities in the field advanced molecular design: It introduces a convenient 2D molecular editor as well as a new pharmacophore feature type, namely Halogen Bonding. With the addition of new interactive data analysis plots (Scatter Plot, Radar Plot, and the Parallel Coordinates Diagram), the library view has received an upgrade, too: All plots can now be resized and de-attached into separate screens.

LigandScout 4.4 Advanced and Expert versions have received an update of their analysis capabilities of molecular dynamics trajectories: Pharmacophores for the entire trajectory, or for a subset can be calculated with a single click. Producing such a huge amount of data requires advanced techniques for analyzing and understanding them. To achieve this goal, LigandScout 4.4 offers various user interactive and highly customizable plots (e.g. MD Pharmacophores Plots) - with more to come.

Furthermore, LigandScout 4.4 Expert introduces a completely new set of features summarized under the term Remote Execution. It is now possible to screen large compound libraries on remote High Performance Computing (HPC) clusters directly from within the graphical LigandScout user interface. Similarly, conformer generation can be done remotely. In order to use LigandScout's remote execution features, a server software running on the requested HPC cluster is required. Please visit the Inte:Ligand support website (<https://docs.inteligand.com>) for more details and installation instructions. It is also possible to run the software with virtual clusters in the Amazon Web Services Elastic Compute cloud.

Finally, with LigandScout 4.4, the search functionality in this manual has been overhauled and is now able to search for arbitrary words and terms.

Installation

The installers for the following operating systems: Linux 64bit, Windows 64bit, and macOS. They are available from our website, for obtaining the download links, please contact office@inteligand.com.

After starting LigandScout, it will prompt you for a license serial number. Enter the serial number provided per mail to you. You should be connected to the internet to activate your license. In some cases a security firewall may require offline activation. Please follow the guided instructions if LigandScout prompts you for offline activation. Alternatively, or for activation on a compute cluster, please insert the serial number into a file called 'serial' and place the file into the LigandScout installation directory. Upon first start of the software, the license file will be generated (internet connection necessary).



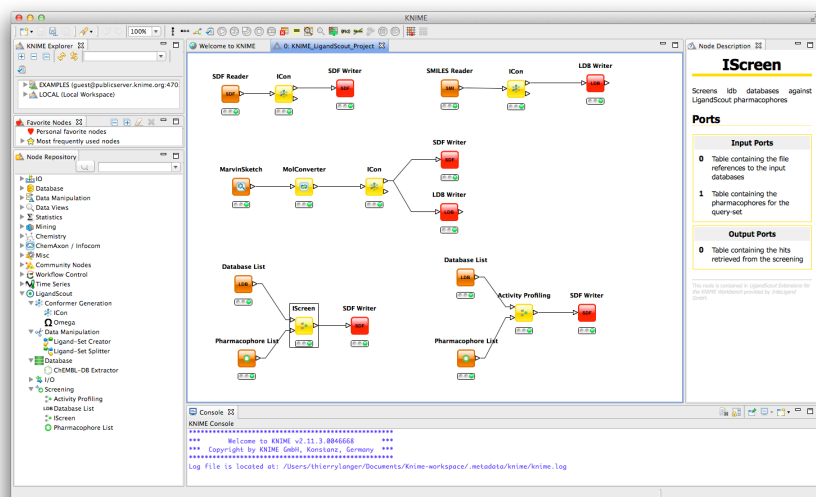
LigandScout Functionality Comparison

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 Clustering			
Pharmacophore-based Alignment			
Interactive Molecular Property Graphs			
Protein Binding Pocket Finder			
Interactive Molecular Docking			
Ligand Binding Affinity Estimation			
Automated Apo-Site Pharmacophore Generator			
Molecular Dynamics Trajectories Import			
Interactive MD Trajectories Analysis Graphs			
Inte:Ligand Knime Extensions			
Remote Cluster and Amazon Cloud Computing			
Pre-computed 3D Libraries for Screening			



Inte:Ligand Knime Extensions

The innovative Inte:Ligand Knime Extensions now combine cutting edge LigandScout algorithms, optimized for design of molecules and analysis of big data with the pipelining workflows of Knime. We developed more than 40 ready to use LigandScout nodes, available for designing customized workflows to support early molecular discovery research.



Use our pre-made workflows or create your own for automated processes, such as structure- and ligand-based pharmacophore generation, virtual screening and ligand activity profiling, data clustering, physicochemical property calculations and filtering, molecular docking, conformation generation, strain energy minimization, diastereomer and tautomer enumeration, fingerprint similarity analysis, pharmacophore-based alignment and molecular dynamics trajectory analysis based on pharmacophore analysis. Our nodes support input and output from and to various essential file formats.

Easy Installation

To install the **LigandScout Knime Extensions**, simply search for the Inte:Ligand LigandScout Extensions in the KNIME 4.0 partner area using the *Help* dropdown menu: *Install New Software...*

Knime is available as open source workflow platform and needs to be installed previously to installing the LigandScout Expert Knime Extensions. Download is available via the knime.org website.

- ▼ LigandScout
 - ▼ Alignment
 - Pharmacophore/Molecule Alignment
 - ▼ Clustering
 - Diversity Picker
 - Fingerprint Clustering
 - Pharmacophore/Molecule Clustering
 - ▼ Conformer Generation
 - ICon
 - ▼ Data Manipulation
 - Ligand-Set Creator
 - Ligand-Set Splitter
 - ▼ Database
 - ChEMBL-DB Extractor
 - LDB Database List
 - Database Merger
 - Patent
 - ▼ Docking
 - AutoDock 4
 - AutoDock Vina
 - ▼ Filtering
 - Duplicate Remover
 - Library Filter
 - ▼ I/O
 - LDB Database List
 - GRO Reader
 - LDB LDB Reader
 - LDB LDB Writer
 - LSD LSD Reader
 - LSD LSD Writer
 - MOL Mol Reader
 - MOL Mol Writer
 - MOL2 Mol2 Reader
 - MOL2 Mol2 Writer
 - PDB PDB Reader
 - PDB PDB Writer
 - PMZ Pharmacophore Reader
 - PMZ Pharmacophore Writer
 - SDF SDF Reader
 - SDF SDF Writer
 - SMI SMILES Reader
 - SMI SMILES Writer
 - ▼ Minimization
 - MMFF94 Library Minimizer
 - MMFF94 Minimizer
 - ▼ Models
 - IL-Carcinogenesis-Models
 - IL-DILI-Models
 - IL-MAO-Models
 - IL-Tox-Models
 - IL-hERG-Models
 - ▼ Molecular dynamics
 - AMBER Trajectory Reader
 - CHA Filter
 - CHA Re-Score
 - DCD DCD Trajectory Reader
 - MD Pharmacophore Creator
 - TRR TRR Trajectory Reader
 - XTC XTC Trajectory Reader
 - ▼ Molecule Property
 - Chiralator
 - Fingerprint Calculator
 - Fingerprint Similarity Calculator
 - InChI Generator
 - Property Appender
 - Standard Properties
 - ▼ Pharmacophore
 - Ligand-based Pharmacophore Creator
 - Merged Pharmacophore Creator
 - Shared Pharmacophore Creator
 - Structure-based Pharmacophore Creator
 - ▼ Screening
 - Activity Profiling
 - IScreen
 - ▼ Tautomerization
 - Tautomer Generation
 - ▼ Tools
 - 3D Viewer
 - ChartView
 - Table Merger

inte:ligand

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

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