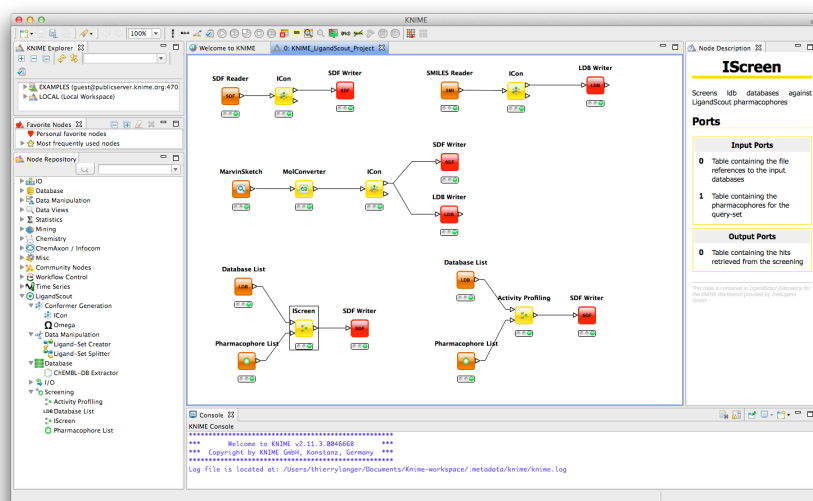




# LigandScout Expert Knime Extensions

The LigandScout Expert Knime Extensions nodes 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 Expert Knime Extensions**, simply include the URL below in the *Help* dropdown menu: *Install New Software...* within the Knime platform.

<http://www.inteligand.com/knime-nodes>

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](http://www.knime.org) website.

- LigandScout
  - Alignment
    - Pharmacophore/Molecule Alignment
  - Clustering
    - Pharmacophore/Molecule Clustering
  - Conformer Generation
    - ICoN Conformer Generator
    - Omega Conformer Generator
  - Data Manipulation
    - Ligand-Set Creator
    - Ligand-Set Splitter
  - Database
    - ChEMBL-DB Extractor
    - LDB Database List
    - Database Merger
  - Docking
    - AutoDock 4
    - AutoDock Vina
  - Filtering
    - Library Filter
  - I/O
    - LDB Database List
    - 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
  - Molecular dynamics
    - DCD Pharmacophore Creator
    - DCD DCD Reader
  - Molecule Property
    - Chirality Enumerator
    - Fingerprint Calculator
    - Fingerprint Similarity Calculator
    - Property Appender
    - Standard Properties
  - Pharmacophore
    - Espresso – Ligand-based Pharmacophores
    - Merged Pharmacophore Creator
    - Shared Pharmacophore Creator
    - Structure-based Pharmacophore Creator
  - Screening
    - Activity Profiling
    - IScreen
  - Tautomerization
    - Tautomer Generation