

LiSIs: a Galaxy-based platform for Life Sciences Informatics Research



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What is LiSIs?

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- Scientific Workflow platform for Virtual Screening.

LiSIs: Input Layer

UPLOAD DATA FILES

- [Upload File](#) from your computer

- [GRANATUM File Loader](#)

PARSE DATA FILES

- [SDF File Reader](#)

- [SMI File Reader](#)

- [Property File Reader](#)

LiSIs: Pre-processing Layer

COMPOUND PRE-PROCESSING TOOLS

- [Compound Fragmenter](#)

- [Descriptor Calculator](#)

- [Fingerprint Calculator](#)

DOCKING PRE-PROCESSING TOOLS

- [Coord Calculator](#)

- [Protein Cleaner](#)

LiSIs: USER processing Layer

FILTERS

- [Chemical Properties Filter](#)

- [GRANATUM Ro5 Filter](#)

- [Lipinski Ro5 Filter](#)

- [Similarity Filter](#)

- [Diversity Filter](#)

- [Substructure Filter](#)

USE AN EXISTING PREDICTIVE MODEL

- [Property Predictor](#) Predict a biological or chemical property of compounds using one of the existing Predictive Models

DOCKING MODEL PREDICTORS

- [Vina Predictor](#)

LiSIs: Post-processing Layer

- [Output Reformatter](#)

- [Binary File Merger](#)

LiSIs: EXPERT processing Layer

BUILD AND EVALUATE A PREDICTIVE MODEL USING ANY OF THE FOLLOWING ALGORITHMS

- [Linear SVM](#)

- [Decision Trees](#)

- [Random Forest](#)

- [k-Nearest Neighbors](#)

DOCKING MODEL BUILDER:

- [Dock Vina Builder](#)

LiSIs: Output Layer

WRITE DATA FILES

- [SMI Writer](#)

- [SDF Writer](#)

- [CSV Writer](#)

- [TAB Writer](#)

SENT DATA FILES

- [GRANATUM File Writer](#)

Powered by...

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- Galaxy (galaxyproject.org)
 - Scientific Workflow Management System
- RDKit (www.rdkit.org)
 - Cheminformatics Toolkit
- R (www.r-project.org)
 - Statistical environment for data mining, machine learning and statistics
- AutoDock Vina (vina.scripps.edu)
 - Molecular Docking Prediction

Funded by...

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- www.granatum.org
- lisis.cs.ucy.ac.cy



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