

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



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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
- OpenBabel/Pybel (<http://openbabel.org>)
 - Chemical/Biological file format transformations.

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](#)

Funded...

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- EU FP7 GRANATUM project, *"A Social Collaborative Working Space Semantically Interlinking Biomedical Researchers, Knowledge and data for the design and execution of In Silico Models and Experiments in Cancer Chemoprevention"*, contract number ICT-2009.5.3.
- www.granatum.org
- lisis.cs.ucy.ac.cy



Cross Linked...

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- EU FP7 Linked2Safety project, *“A Next-Generation, Secure Linked Data Medical Information Space For Semantically-Interconnecting Electronic Health Records and Clinical Trials Systems Advancing Patients Safety In Clinical Research”*, contact number 288328.
- www.linked2safety-project.eu



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