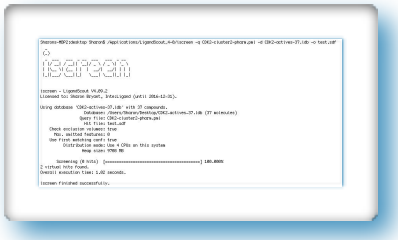
LigandScout Command Line Tools

- **LigandScout** software suites are outfitted with command line tools to enable you to run jobs, such as, creating structure-based and ligand-based pharmacophores, create and manage libraries for virtual screening, perform virtual screening and generate ROC curves, manage jobs on a compute cluster and many other useful tasks in the background without using the graphical user interface.
- The command line executables are located in the LigandScout installation directory and function on Mac, Windows and Linux operating systems.
- This document summarizes the available command line tools in LigandScout versions 4.4 and later.



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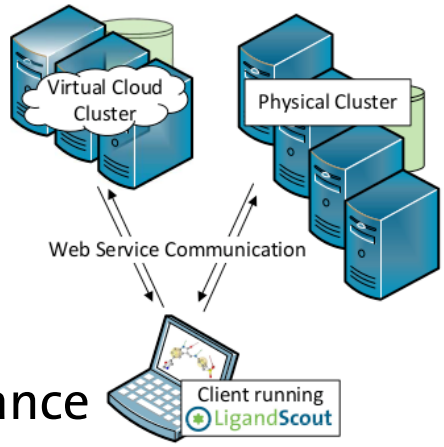
Summary of Command Line Tools

Name of Executable	Function
iaffinity	Binding affinity estimation
ialign	Align binding sites, ligands and/or pharmacophores.
ipharmgen	Generate a structure-based pharmacophore model
idbgen	Multi-conformational virtual screening library generation (LDB)
idbextract	Extract compounds from a database (LDB) file by name.
iscreen	Virtual screening
espresso	Ligand-based pharmacophore modeling
icluster	Cluster compounds based on their pharmacophore features
iconfgen	Create multi-conformational (SDF) files (Generate conformations of molecules)
irocplotter	Create receiver operating characteristic (ROC) curves
idbmerger	Merge LigandScout database (LDB) partitions
idbinfo	Retrieve information about a LigandScout database
libpos	Saves start position of compounds for idbgen (speeds up processes for compute cluster)
libsize	Obtain the total number of compounds in a library
ligandscout_activation	LigandScout license Activation
ligandscout_sysid	Generate information needed for offline LigandScout license activation
iworker	Use computing resources of other computers on a network

Support for multi-cpu clusters- 2020

LigandScout Remote



- Run LigandScout iscreen & idbgen on a high performance compute cluster (HPC remote server)

  https://docs.inteligand.com/ls-remote/

- Run LigandScout iscreen & idbgen on Amazon Web Services (AWS)

  https://docs.inteligand.com/ls-remote/working-with-aws/

Also support for multi-cpu clusters- 2020

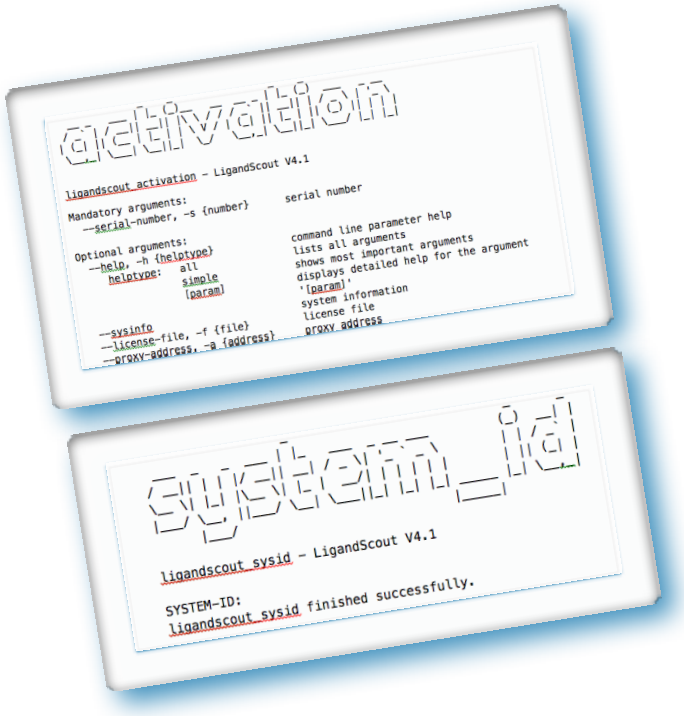
LigandScout License Activation

- License activation.

  ligandscout_activate -s <serial_number>

- License activation - offline.

  ligandscout_sysid



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Create SB-Pharmacophore ipharmgen

- Create a structure-based pharmacophore with ipharmgen

  ipharmgen -i macromolecule.pdb -o SB-pharm.pml

- To see all ipharmgen executable command options.

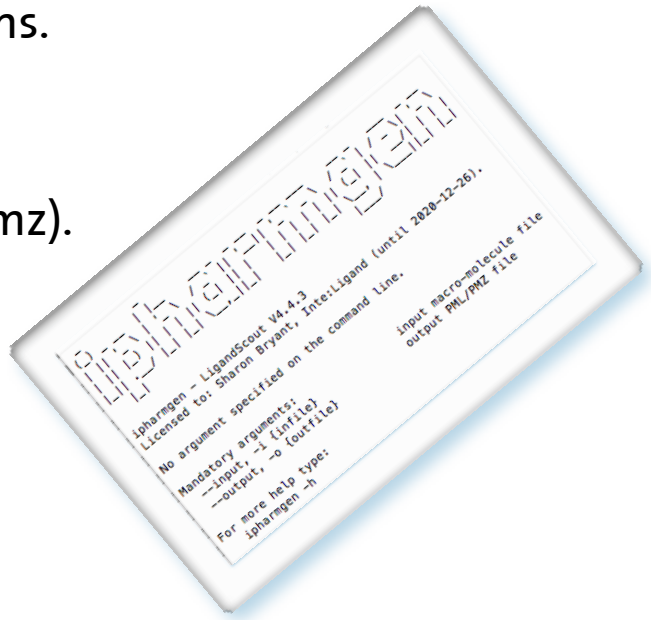
  ipharmgen -h all

- Designate input macromolecules -i...(pdb, pml, pmz).

  ipharmgen -i macromolecule.pdb

- Designate output file -o...output file (pml, pmz).

  -o SB-pharm.pml



Estimate Binding Affinity with iaffinity

- Estimate binding affinity with iaffinity

  iaffinity -i library.smi - a active-site.pdb -o library.sdf

- To see all iaffinity executable command options.

  iaffinity -h all

- Designate input library or molecule file -i...(smi, sdf, ldb, dwar, mol2).

  iaffinity -i library.smi

- Designate active site file -a...(pml, pmz, pdb)

  iaffinity -a active-site.pdb

- Designate output -o...Output File (sdf, mol2, ldb).

  -o output-file.sdf

- Options for minimization (ligands, side-chains, all).

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Create Databases with idbgen

- Create LigandScout compound databases for Virtual Screening.

  idbgen -i library.smi -o database.ldb

- To see all idbgen executable command options.

  idbgen -h all

- Designate input library file -i...(smi, sdf, ldb, mol2, dwar).

  idbgen -i library.smi

- Designate output library file -o...Output Database (ldb).

  -o database.ldb

* *A stand-alone application with its own GUI is also in the installation directory.*

idbgen-gui.app

Virtual Screening with iscreen

- Virtually screen database(s) with one or more pharmacophores.

  iscreen -q pharmacophore.pmz -d database.ldb -o hitlist.sdf

- To see all iscreen executable command options.

  iscreen -h all

- Designate query pharmacophore(s) (pmz).

  iscreen -q pharmacophore.pmz

- Designate database(s) for screening (ldb).

  -d database.ldb

- Designate output hit-list file (sdf, ldb).

  -o hitlist.sdf

Create ROC Curves with irocplotter

Create receiver operating characteristic (ROC) curves from the command line.

irocplotter -i hits.sdf -o rocplot.png -a actives.sdf -d decoys.sdf

irocplotter -i hits.sdf -o rocplot.png -a 37 -d 1291

-a ... Specifies the actives file(s) or total number of actives.

-d ... Specifies the decoys file(s) or total number of decoys.

-i ... Specifies a previously created hit list file.

(This should be a LigandScout hit list. If not, the score property needs to be defined using the -s option).

-o ... Specifies the image output file to save an image of the ROC curve .

(The default size of the image is 630 x 600. This can be changed using the -p option).

Manage Resources for idbgen & iscreen

- Set memory and CPU settings with command line options for **idbgen** and **iscreen** executables.
- Define maximum memory size.

  -M … designate memory size (in GB)
- Define number of CPU cores to use (default: all cores).

  -C … designate the number of cores
- Example:

  idbgen -M4 -C 8 …

  iscreen -M4 -C 8 …

*__Important note__: There is no space between “M” and “4”, but insert a space between “C” and “8”

Merge Database Partitions with idbmerger

- Merge database partitions created by **idbgen**.

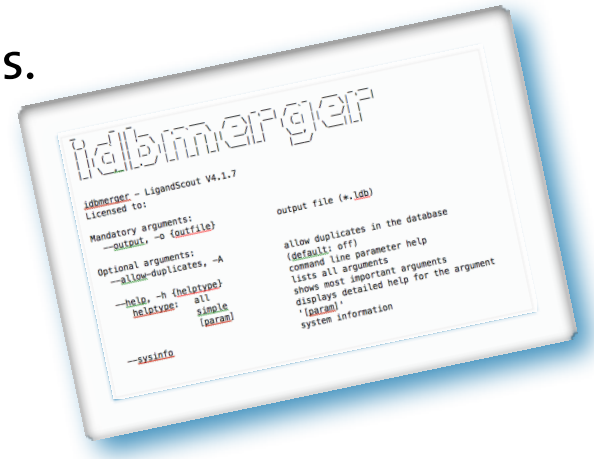
  idbmerger -o db_merged.ldb db_part*.ldb

- To see all idbmerger executable command options.

  idbmerger -h all

- Concatenate hit list partitions created by **iscreen**.

  cat hitlist_part*.sdf > hitlist_merged.sdf



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Manage Compound Libraries

- 3D Multi-conformational compound database merging.

  idbmerger

  idbmerger -o merged.ldb chunk*.ldb

- LigandScout database information retrieval.

  idbinfo

  idbinfo -d database.ldb

- Extract compounds from an LDB file by name

  idbextract executable

- Obtain information about a compound library.

  libsize library.sdf (number of compounds in library).

  libpos -i library.sdf -o library.pos

Extract Compounds from LDB Files

- Extract compounds from a screening library (LDB) by name

  idbextract -i drugbank.ldb -n Sorafenib -o sorafenib.ldb

- To see all **idbextract** executable command options.

  idbextract -h all

- Designate input database -i...(LDB).

  idbextract -i drugbank.ldb

- Designate name of compound for extraction -n...

  -n Sorafenib

- Designate output file -o...(sdf, ldb).

  -o sorafenib.ldb

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Ligand-Based Modeling with espresso

- Create ligand-based pharmacophore models from training set.

  espresso -t training-set-ligands.sdf -o pharmacophore.pml (or pmz)

- To see all espresso executable command options.

  espresso -h all

- Designate input library file -i...(smi, sdf, or ldb or .lsd).

  espresso -t training-set-ligands.smi

  espresso -i training-set-ligands.lsd

- Designate output sdf file -o...Output File (sdf, mol2, ldb, smi, lsd).

  -o output-file.sdf

Generate Conformations with iconfgen

- Generate conformations and create multi-conformational sdf files.

  iconfgen -i library.smi -o library.sdf

- To see all iconfgen executable command options.

  iconfgen -h all

- Designate input library file -i...(smi, sdf, ldb, dwar, mol2).

  iconfgen -i library.smi

- Designate output sdf file -o...Output File (multiconf sdf).

  -o output-file.sdf

Cluster Compounds with icluster

- Cluster compounds based on their pharmacophore features.

  icluster -i library.sdf -o library.sdf

- To see all icluster executable command options.

  icluster -h all

- Designate input library file -i...(smi, sdf, mol2 or ldb).

  icluster -i library.smi

- Designate output sdf file -o...Output File (sdf, mol2 or ldb).

  -o output-file.sdf

Align Molecules/Pharmacophores with ialign

- Align molecules and or pharmacophores (pharm) with ialign

  ialign -i molecule1.sdf -r molecule2.sdf -o molecule1-aligned.sdf

  ialign -i pharm1.pml -r pharm2.pml -o pharm1-aligned-to-pharm2.pml

  ialign -i molecule1.sdf -r pharm2.pml -o molecule1-aligned-to-pharm2.sdf

- To see all ialign executable command options.

  ialign -h all

- Designate input molecule/pharm -i...(sdf, smi, ldb, dwar, mol2, pml, pmz).

  ialign -i molecule1.pml

- Designate reference molecule or pharmacophore -r...(sdf, smi, ldb, dwar, mol2, pml, pmz)

  ialign -r molecule2.pml

- Designate output file -o...output file (pml, pmz).

  -o aligned.pml

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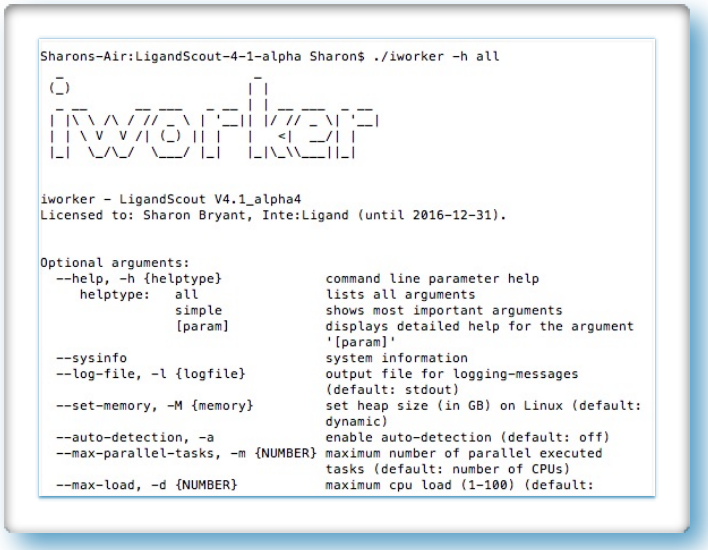
Network Distribution with iworker

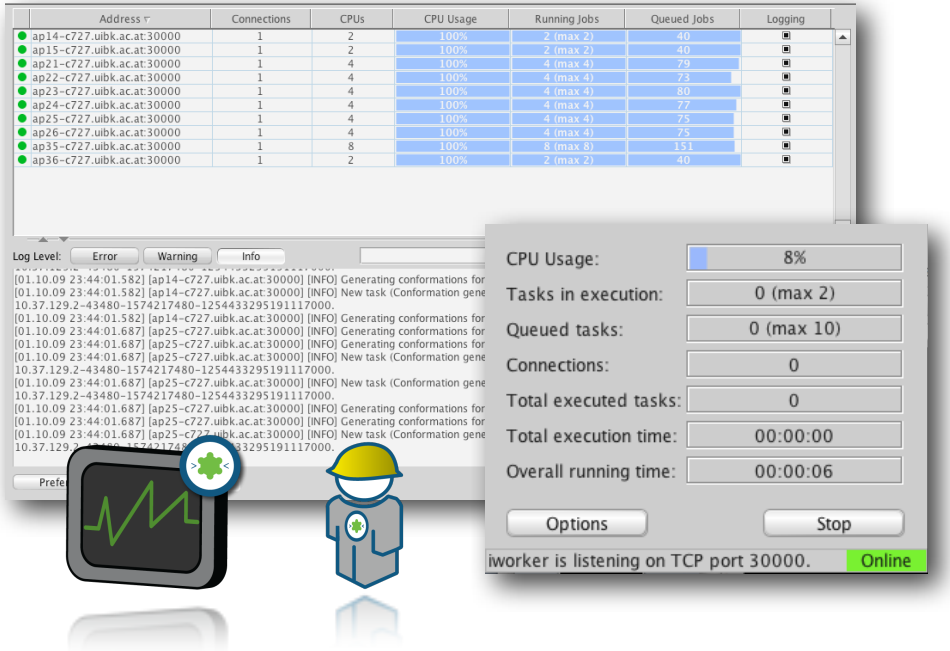
- Use computing resources of other computers on a network.

  iworker

- Also available as a stand-alone application with its own GUI.

  iworker-gui.app





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Managing Large Jobs with LigandScout Implementation on Multi-CPU Clusters

Library generation (**idbgen**) and virtual screening (**iscreen**) can be optimized for operation on high performance compute clusters.

- Special commands & procedures for partitioning and merging LigandScout database (LDB) files (Array Job Model).
- Save start position of compounds in SDF, SMI, MOL2 formats to speed up processes for idbgen (libpos -i library.sdf -o library.pos).
- Special commands for setting & ending execution times (Time Constraints).
- Special commands for pausing and resuming jobs.
- Compound-based and task-based execution time management.

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Partitioning Jobs - Array Job Model

- Partitioning of one job (idbgen, iscreen) into multiple jobs.
- Command-line tool libsize implemented for library-size automated partitioning.
- Command-Line tool libpos to save start position of compounds for speeding up processes for idbgen.

libpos -i library.sdf -o library.pos

- Added command-line arguments to idbgen and iscreen to specify an index range for the input file.

iscreen -F 1000 -L 1999 ...

-F ... first index

-L ... last index

Time Constraints for idbgen & iscreen

- Command-line argument to set a maximum execution time.
- Command-line argument to set a process execution end time.
- Command-line argument to set a time-out on the compound level.

```
iscreen -P 1h30m ...
```

-P ... max. execution time of 1 hour and 30 minutes

```
iscreen -E '23.02.2012-17:30' ...
```

-E ... process execution end time

```
iscreen -T 10 ...
```

-T ... compound timeout 10 minutes

Resume Unfinished Jobs

- Auto-resume for unfinished jobs.
- No additional command-line arguments needed.
- idbgen & iscreen create binary resume files to store progress information.
- Binary files are deleted when jobs are complete.

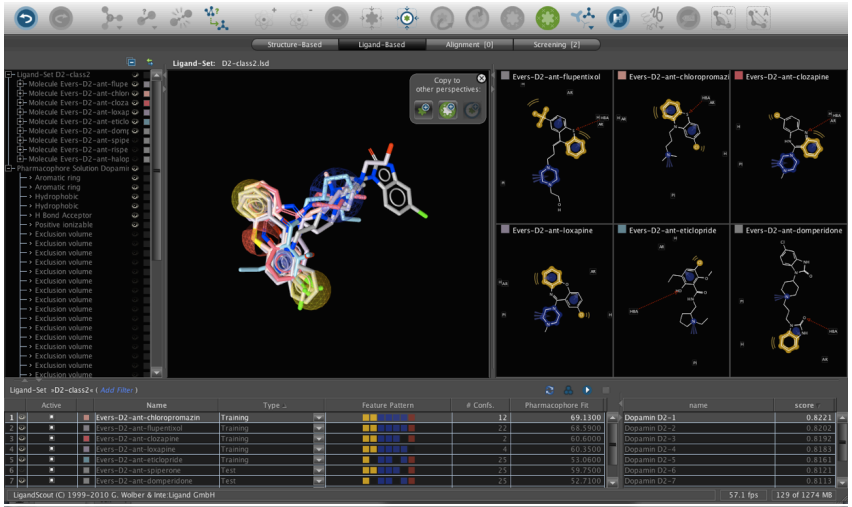
Where to Find the LigandScout Manual

1. LigandScout GUI (File pull-down menu- **Help**).
2. A printable PDF (**LigandScout_manual.pdf**) is located in the LigandScout . Installation Directory under the directory **misc.**
3. A stand-alone app with it's own GUI can be found in the installation directory and can be linked or moved to your desktop.

ligandscout-help.app

Command lines tools information is located in the Appendix of the user manual.

Questions about LigandScout?



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