# 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	inte-ligar

Support for multi-cpu clusters- 2020

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# 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.







# **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).

-• ... 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).



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# 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





# **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



# **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



### **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

		Address 🗸	Connections	CPUs	CPU Usage	Running Jobs	Queued Jobs	Logging	
		ap14-c727.uibk.ac.at:30000	1	2	100%	2 (max 2)			
	ap15-c727.uibk.ac.at:30000	1	2	100%					
Sharons-Air:LigandScout-4-1-alpha Sharon\$ ./iworker -h all		ap21-c727.uibk.ac.at:30000	1	4	100%				
_		ap22-c727.uibk.ac.at:30000	1	4	100%		73		
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orker - LigandScout V4.1_alp	ha4								
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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.





### **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.



Command lines tools information is located in the Appendix of the

user manual.







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### www.inteligand.com

