Schrödinger Utilities

This document contains a complete list of the utilities stored in `$SCHRODINGER/utilities` in the Schrödinger Suite 2012 distribution, with a brief description and links to command syntax and fuller descriptions. Some utilities are general-purpose utilities, others are specific to a product. Most utilities are intended for general use, others are only used internally and are marked as such. For utilities that have a full description elsewhere, you can click the utility name to go to the full description in the source document.

The following documents provide a description of command syntax for selected utilities:

Phase Command-Line Database Tasks
Phase Command-Line Pharmacophore Modeling

Utility	Product	Description
canvas_app	Canvas	Run a Canvas job.
canvasBayes	Canvas	Builds Bayes model from binary or continuous training data.
canvasConvert	Canvas	Converts between different molecular file formats.
canvasCSV2FPBinary	Canvas	Converts a CSV file into a Canvas fingerprint binary file.
canvasCSV2PW	Canvas	Generates a binary pairwise similarity or distance matrix using CSV input.
canvasCSVMatrix	Canvas	Generates a distance matrix based on delimited input data (CSV).
canvasDBCS	Canvas	Dissimilarity based compound selection
canvasFPBinary2CSV	Canvas	Converts a Canvas fingerprint binary file to a CSV file.
canvasFPCombine	Canvas	Combines fingerprints for distinct or overlapping sets of molecules.
canvasFPGen	Canvas	Generates fingerprints for molecules in a structure file.
canvasFPHist	Canvas	Generates histogram of nearest-neighbor similarites for diversity analysis.
canvasFPMatrix	Canvas	Generates a pairwise similarity or distance matrix using binary or scaled fingerprints from one or two sets of molecules.
canvasHC	Canvas	Performs full hierarchical clustering and reports details for a specific number of clusters.
canvasHCBuild	Canvas	Performs full hierarchical clustering.
canvasHCSelect	Canvas	Reports details for a specific level of clustering.
canvasJob	Canvas	Does setup and cleanup for jobs associated with a Canvas project.
canvasKMeans	Canvas	Performs K-means clustering.
canvasKPLS	Canvas	Builds and tests kernel-based partial least squares regression models.
canvasLC	Canvas	Performs leader-follower clustering.
canvasLibOpt	Canvas	Fill holes in a library with a set of structures and optimize structure properties
canvasMCS	Canvas	Finds the maximum common substructure among a given set of molecules.
canvasMDS	Canvas	Multi-dimensional scaling driver.
canvasMLR	Canvas	Builds and tests multiple linear regression models.
canvasMolDescriptors	Canvas	Calculates molecular descriptors.
canvasNnet	Canvas	Builds and tests an ensemble model of neural networks.

Utility	Product	Description
canvasPCA	Canvas	Direct principal components generation without intermediate analysis.
canvasPCAGen	Canvas	Principal components generation.
canvasPCAProj	Canvas	Projects data along one or more principal components generated by canvasPCAGen.
canvasPCAReg	Canvas	Builds and tests principal component analysis regression models.
canvasPharmFP	Canvas	Generates fingerprints from 3D pharmacophores.
canvasPLS	Canvas	Builds and tests partial least squares regression models.
canvasProjectDB	Canvas	Creates or updates a Canvas project database.
canvasPW2CSV	Canvas	Generates a CSV matrix file from a binary pairwise similarity or distance matrix.
canvasRP	Canvas	Build and test recursive partitioning trees for an input CSV file.
canvasSDMerge	Canvas	Merges CSV data with an existing SD file into a new SD file.
canvasScaffold	Canvas	Decompose a set of structures into all possible ring-containing fragments.
canvasSearch	Canvas	Searches a list of target molecules against a set of queries
canvasSOM	Canvas	Creates a Kohonen self-organizing map (SOM) from scaled (real) values.
canvasSOMBits	Canvas	Creates a Kohonen self-organizing map (SOM) from binary data.
canvasTreeDraw	Canvas	Draws dendrograms.
cg_active_plot	CombiGlide	Opens the Active Plot panel as a standalone panel.
cg_add_chem_features	CombiGlide	Adds chemical features to CombiGlide reagent files that lack them.
cg_chem_features	CombiGlide	Opens the Chemical Features panel as a standalone panel.
cg_chsr	CombiGlide	Run ligand-based core-hopping job.
cg_combine_bld	CombiGlide	
cg_interactive_enum_dock	CombiGlide	Opens the Interactive Enumeration and Docking panel as a standalone panel.
dump_sqlite	CombiGlide	Used internally.
libselector	CombiGlide	Performs library selection.
mae_to_sqlite	CombiGlide	Used internally for conversions between Maestro and SQLite database formats.
make_comb_sqlite	CombiGlide	Used internally for SQLite databases.
protocore_prep	CombiGlide	Performs preparation of protocore molecules.
reagentprep	CombiGlide	Prepares reagent files. Not for general use.
vcsprep	CombiGlide	Not for general use.
core_pareto	Core Hopping	Not for general use.
corefinder	Core Hopping	Extract cores for use with ligand-based core hopping.
adj_fep_pots	Desmond	Not for general use.
multisim	Desmond	Runs multiple Desmond simulations.
solvate_pocket	Desmond	Solvates buried pockets in a protein structure.

Utility	Product	Description
system_builder	Desmond	Builds a model system.
para_epik	Epik	Obsolete; use epik instead to run in distributed mode.
applyhtreat	General	Adds or removes hydrogen atoms, dummy atoms, and lone pairs.
checkupdates	General	Checks Schrödinger web site for software updates.
chem_features	General	Lists the chemical feature types present in the input structures
generate_2d_report	General	Creates a PDF or HTML file of 2D structure images
getpdb	General	Retrieves PDB files from local mirror of the PDB database.
ligand_interaction_diagram	General	Create a diagram of receptor-ligand interactions as an image file.
ligfilter	General	Filter a structure file based on criteria for structure properties.
m2iotov11	General	Converts all blocks in a Maestro format file into a format that can be read by Maestro 7.0 (file format version 1.1).
maesubset	General	Selects a subset of the structures present in a Maestro format file.
maevalidate	General	Validate the format of a Maestro file and filter out badly formed structures.
md5util	General	Used internally.
merge_duplicates	General	Merge one or more sets of structures, eliminating duplicates.
mol2convert	General	Converts between Mol2 and Maestro file format.
pdbconvert	General	Converts between PDB and Maestro or MacroModel format.
postmortem	General	Create an archive file containing information from given jobs and installation information. Useful for sending to technical support.
prepwizard	General	Runs the protein preparation wizard.
propfilter	General	Filters structures in Maestro format file based on properties. Superseded by ligfilter.
proplister	General	Lists properties in Maestro format files.
protassign	General	Assign chi angles in residues and orientation of waters.
python	General	Python interpreter.
randsub	General	Selects a random subset of lines from a file and writes them to another file. (Distributed with Phase.)
rmsdcalc	General	Computes the RMSD between each structure in a given file and a corresponding reference structure from a second file. (Distributed with Phase.)
sdconvert	General	Converts between MDL SD, Maestro, and MacroModel format files.
sdsubset	General	Extracts a subset of structures from an SD format input file.
seqconvert	General	Converts between different sequence and alignment formats.
structcat	General	Concatenate structure files into a single file, with format conversion.
structconvert	General	Converts between Maestro, MDL SD, PDB, Sybyl Mol2, SMILES, and MacroModel format files.
uffmin	General	Cleans up structures by geometry minimization with a universal force field.
unique_names	General	Creates unique entry names and titles for all structures in a Maestro file.

Utility	Product	Description
uniquesmiles	General	Generates Unique SMILES strings for the input structures.
visdump	General	Wrapper for h5dump, a utility for manipulating visualization (.vis) files
ziputil	General	Utility for creating and extracting zip archives.
idle	General/Python	Python IDE.
glide_ensemble_merge	Glide	Merges sorted Glide pose viewer files into one or more output files sorted by GlideScore, with optional offsets for each file.
glide_merge	Glide	Merges sorted Glide pose viewer files from a para_glide run.
glide_rescore	Glide	Replaces the docking score properties in Glide pose output files with different values, so that the -best-by-title option of glide_sort can be used to combine different screens.
glide_sort	Glide	Re-ranks Glide poses by custom criteria or combines job outputs into one file.
impref	Glide	Runs the refinement stage of protein preparation. There is little need to run impref directly.
jagconvert	Jaguar	Reads and writes Jaguar input (.in) files, BioGraf (.bgf) files, XMol (.xyz) files and Maestro (.mae) files. Reads Gaussian9x (.g9x) files and MacroModel (.dat) files but does not write them.
jaguar_pka	Jaguar	Recalculates pKa values using parameters for a specified functional group.
makedafs	Jaguar	Creates dealiasing functions for all elements in the specified basis.
makegrids	Jaguar	Creates grids for all elements in the specified basis.
makejbasis	Jaguar	Converts basis from Gaussian format to Jaguar basis set format.
mpich	Jaguar	Starts and manages MPICH secure servers.
elim.schrodinger	Job Control	Checks availability of licenses for LSF queues. Not for direct use.
flexlm_sensor.pl	Job Control	Checks availability of licenses for SGE queues. Not for general use.
jnanny	Job Control	Check for and recover stuck jobs.
jserver	Job Control	Job Control file server.
jserver_log_parser	Job Control	Report on file transfer activity as recorded in jserver log files.
lictest	Job Control	Not for general use.
licutil	Job Control	Sets up license checking for queues.
pbs_lic_sensor.pl	Job Control	Checks availability of licenses for PBS queues. Not for direct use.
desalter	LigPrep	Eliminates all molecules except the molecule with the largest number of atoms in each structure.
guardian	LigPrep	Not for general use.
ionizer	LigPrep	Produces multiple structures for each input structure, with different combinations of ionized states based on the ionizable groups present.
ionizer_guard	LigPrep	Associated with ionizer. Not for general use.

Utility	Product	Description
ligparse	LigPrep	Characterizes molecular databases, selects molecules meeting certain criteria, eliminates molecules meeting certain criteria, or selects subsets of the molecules present possessing certain statistical characteristics.
lp_filter	LigPrep	Not for general use.
lp_labeler	LigPrep	Not for general use.
lp_noredund	LigPrep	Not for general use.
neutralizer	LigPrep	Neutralizes functional groups where possible by adding or removing protons.
para_ligprep	LigPrep	Obsolete, same as ligprep. Use ligprep to run in distributed mode
ring_conf	LigPrep	Finds low-energy conformations for the flexible ring systems within a structure.
ring_templating	LigPrep	Creates templates for flexible ring systems of a set of structures.
smiles_to_mae	LigPrep	Converts a SMILES file to a Maestro format file. Only for use by LigPrep.
stereoizer	LigPrep	Labels stereochemical features or generates structures based upon the chiral properties of the chiral atoms in the structure.
tautomerizer	LigPrep	Generates probable tautomeric states.
autoref	MacroModel	Performs a restrained minimization of a protein-ligand structure using MacroModel. Can be used for the refinement stage of protein preparation.
maemmod	MacroModel	Converts Maestro format file to MacroModel format.
mmio_convert	MacroModel	Compresses or uncompresses MacroModel files
mmodmae	MacroModel	Converts MacroModel format file to Maestro format.
mmodmol	MacroModel	Converts MacroModel file to Sybyl Mol2 format.
molmmod	MacroModel	Converts Sybyl Mol2 file to MacroModel format.
para_bmin	MacroModel	Obsolete, same as bmin. Use bmin to run in distributed mode
premin	MacroModel	Prepares multi-ligand structure files for use in Glide and other applications.
queue_bmin	MacroModel	Legacy script for running MacroModel jobs sequentially. Use of a queuing system is encouraged instead.
serial_split	MacroModel	Splits up the output of a MacroModel serial job.
project_convert	Maestro	Converts Maestro projects to the current project format.
project_extract	Maestro	Extracts usabe information from a corrupted Maestro project.
autopert	MCPRO+	Automatically generate FEPs. Not for general use.
autozmat	MCPRO+	Automates the generation or modification of a Z-matrix for MCPRO.
ffld_server	MCPRO+	Not for general use.
mcpro_convert	MCPRO+	Not for general use.
mcpro_zmat	MCPRO+	Generate or update MCPRO+ model system.
align_hypoPair	Phase	Aligns one hypothesis to another.
cluster_matrix	Phase	Performs hierarchical, agglomerative clustering on a similarity or distance matrix.

Utility	Product	Description
combine_hits	Phase	Combines hit files from a database search.
combine_matches	Phase	Combines match files from a database search.
compare_featureDefs	Phase	Compares two sets of feature definitions
convert_hypoDistToXYZ	Phase	Creates a hypothesis .xyz file from a file containing intersite distances.
convert_hypoXYZToDist	Phase	Creates a hypothesis intersite distance file .dist from an .xyz file.
convert_hypoFeatures	Phase	Converts feature definitions for a hypothesis using a new feature definition file.
convert_ivolToMae	Phase	Converts an included volumes file to a file in Maestro format.
create_hypoConsensus	Phase	Creates a consensus hypothesis from a set of pre-aligned ligands.
create_hypoFiles	Phase	Creates the .def, .mae, .xyz and .tab hypothesis files from a single reference ligand structure and a feature definition file.
create_hypoSDFile	Phase	Creates an SD file to help visualize hypotheses that have no reference ligand.
create_hypoTabFile	Phase	Creates the .tab file for a hypothesis that does not have one.
create_ivolShape	Phase	Creates an included volumes file to represent the positive image of a ligand or the negative image of a receptor.
create_molSites	Phase	Creates a CSV file that contains the Phase features and associated atom numbers for the structure in the input Maestro file.
create_shapeConsensus	Phase	Creates a consensus shape query from a set of queries.
create_xvolClash	Phase	Creates excluded volumes where only inactives would have steric clashes.
create_xvolReceptor	Phase	Creates excluded volumes from a receptor structure.
create_xvolShell	Phase	Creates excluded volumes that surround the reference ligand for a hypothesis.
flex_align	Phase	Performs flexible alignment of ligands to a flexible reference structure.
pharm_align_mol	Phase	Does setup/cleanup for the job that aligns project ligands or new molecules to a hypothesis.
pharm_archive	Phase	Preserves project data in a tar archive.
pharm_buffer_struct	Phase	Not for general use.
pharm_build_qsar	Phase	Does setup/cleanup for the job that builds QSAR models.
pharm_cluster_hypotheses	Phase	Does setup/cleanup for the job that clusters hypotheses by geometric similarity.
pharm_cluster_modes	Phase	Creates a text file to help visualize clusters of ligands and hypotheses that represent potential binding modes.
pharm_create_sites	Phase	Does setup/cleanup for the job that creates pharmacophore sites.
pharm_data	Phase	Performs various operations on the pharmacophore model project data.
pharm_find_common	Phase	Does setup/cleanup for the job that identifies common pharmacophores.
pharm_help	Phase	Prints a summary of the command line pharmacophore model workflow.
pharm_project	Phase	Creates a new command line pharmacophore model project or add molecules to an existing project.
pharm_score_actives	Phase	Does setup/cleanup for the job that scores hypotheses with respect to actives.
pharm_score_inactives	Phase	Does setup/cleanup for the job that scores hypotheses with respect to inactives.
phase_cluster_hits	Phase	Cluster the hits according to the sites that were matched.
phase_complex	Phase	Construct a pharmacophore model from a receptor-ligand complex.

Utility	Product	Description
phase_fqsar	Phase	Construct a pharmacophore model from a receptor-ligand complex.
phase_hypoSimCalc	Phase	Computes a similarity matrix for a set of pharmacophore hypotheses.
phase_qsar_stats	Phase	Extracts statistics from Phase QSAR models and from hit files that contain QSAR predictions.
phase_volCalc	Phase	Calculates the volume overlap for structures in a file.
phasedb_check	Phase	Checks database integrity.
phasedb_confsites	Phase	Generates conformations and create sites in a Phase 3D database.
phasedb_convert	Phase	Converts Phase 3D database between storage and version formats.
phasedb_count_records	Phase	Counts records in a Phase 3D database subset.
phasedb_export	Phase	Exports structures from a Phase 3D database to a file.
phasedb_fetch_hits	Phase	Not for general use.
phasedb_findmatches	Phase	Finds matches to a hypothesis in a Phase 3D database.
phasedb_index	Phase	Creates indices on certain tables in Phase database.
phasedb_manage	Phase	Manages a Phase 3D database.
phasedb_match_keys	Phase	Prescreens a Phase 3D database using the 3D key information.
phasedb_props	Phase	Uses properties in Phase 3D database for screening or subsets.
phasedb_split_records	Phase	Distributes structures across processors for Phase 3D database search.
phasedb_subset	Phase	Creates subsets of a Phase 3D database.
qsarVis	Phase	Visualizes QSAR models.
align_binding_sites	Prime	Align multiple proteins on selected residues near the binding site.
hetgrp_ffgen	Prime	Generates parameter files for ligands. Not for general use.
rsync_pdb	Prime	Creates or updates a local mirror of the PDB.
secstruc	Prime	Assigns secondary structure.
SkaParser	Prime	Parses SKA results.
SkaResultsViewer	Prime	Graphical viewer for structural alignment (SKA) results.
structalign	Prime	Aligns two or more protein structures using SKA.
update_BLASTDB	Prime	Updates BLAST databases from the web.
ccp42cns	PrimeX	Convert a CCP4 map file to CNS format.
mtzprint	PrimeX	Print the contents of an .mtz reflection file.
refconvert	PrimeX	Convert between reflection file formats.
mkqsinput	QSite	Converts input files from previous versions to QSite 4.0 format.