Phase Command-Line Database Tasks

Database management tasks can be run in the foreground or submitted as a single-CPU job to any host that has access to the database directory. Site creation and database search jobs can be run on multiple processors. When you create the database, make sure that it is on a file system that is accessible to all hosts that need access to the database. For details on the commands and options, see Chapter 13 of the *Phase User Manual*.

On Linux, you should prepend the command with `$SCHRODINGER/`. On Windows, you can run the command in a Schrodinger Command Prompt window, which you open from the Start menu.

To create a new database:

```
phase_database database import [jobName] -i structFile [-new [-fd fdFile]]
    [-multi [-connect] [-stereo]] [-title propName] [-blimit maxRec] [-unique]
```

To add molecules to an existing database:

```
phase_database database import [jobName] -i structFile [-multi [-connect] [-stereo]]
    [-title propName] [-blimit maxRec] [-unique]
```

To restart a failed database creation or molecule addition:

```
phase_database database import [jobName] -i structFile -RESTART
```

To delete molecules from a database:

```
phase_database database delete [jobName] -isub subset
```

To competely remove a database:

```
[sh] rm -rf database
```

To generate conformers and pharmacophore sites:

```
phase_database database revise [jobName] [-sites] [-confs {auto|all}] [-max maxConfs]
    [-sample {rapid|thorough}] [-amide {orig|vary|trans}] [-ewin deltaE] [-bf numPerBond]
    [-skip maxRot] [-append]]
```

To restart a conformer and site generation job:

```
phase_database database revise [jobName] -RESTART
```

To create a subset from the structures in a hit file:

```
phase_database database subset [jobName] -hits hitfile -osub subset
```

To create a subset from a logical operation on two existing subsets:

```
phase_database database subset [jobName] -isub1 subset1 -logic {AND|OR|NOT} -isub2 subset2
    -osub subset
```

To create a subset based on presence of conformers and sites:

```
phase_database database subset [jobName] -has {confs|sites} [false] -osub subset
```

To create a subset of structures with specified titles:

```
phase_database database subset [jobName] -titles fileName -osub subset
```

To export structures from a database to a (compressed) file:

```
phase_database database export [jobName] -ofmt base [-get maxConfs] [-limit maxStruct]
    [-quota Gbytes] [-isub subset]
```

To add properties to a database:

```
phase_database database revise [jobName] [-props] [-isub subset]
```

To extract properties from a database into the SQLite table:

```
phase_database database extract [jobName] [-append] [-stats] [-map]
```

To query properties extracted from a database:

```
phase_database database query [jobName] {-where condition | -file propFile | -smarts string }
```

To convert a database:

```
phase_database database convert [jobName] -source sourceDb [-new [-fd fdFile]] [-blimit maxRec]
    [-nosites] [-isub subset]
```

To search for matches in a database, files, or command-line pharmacophore project:

```
phase_find_matches source hypoID jobname [[-distinct] | [-connect] [-stereo]] [-title propName]
    [{-flex|-refine} [-sample {rapid|thorough}] [-max numConfs] [-bf numPerBond] [-ewin deltaE]
        [-amide {vary|orig|trans}] [-skip maxRot] [-append]]
    [-d deltaDist] [-match minSites [-ex]] [-t timeLimit] [-inplace] [-nosort | -keep maxHits]
    [-report n] [-isub subset] [-sites|-noindex] [-noref] [-notol] [-nocnst] [-nomask]
    [-norules] [-noqsar] [-noxvol] [-noivol] [-atypes] [-aw alignWeight] [-ac alignCutoff] [-hard]
    [-ap alignPenalty] [-vw vectorWeight] [-vc vectorCutoff] [-volw volumeWeight] [-volc volumeCutoff]
    [ivolw ivolWeight] [ivolc ivolCutoff] [-verbose]
```

To screen a database (or files) by molecular shape:

```
$SCHRODINGER/shape_screen -screen screenSource -shape shapeFile -JOB jobname [job-options] [-NOJOBID]
    {-CHECKPOINT|-RESTART path|-NO_CHECKPOINT} [-NSUB m] [-split] [-title propName] [-v|-nv]
    [-distinct] [-norm 1|2|3|4] [-filter minSim] [-sort [-keep maxKeep]] [-best]
    [-report n [-redun tol]] [-table] [-align smartsFile] [-xvol xvolFile] [-hydrogens]
    [-atomTypes {mmod|element|pharm} [-dual]] [-atomWeights propName]
    [-pharm [-fd fdFile] [-rad radFile]] [-flex [-flexSearchMethod {rapid|thorough}]
    [-flexMaxConfs maxConfs] [-flexConfsPerBond numPerBond]
    [-flexMaxRelEnergy energy] [-flexAmideOption {vary|orig|trans}] [-flexAppend] ]
    [-limit <numConfs>] [-scoreInPlace] [-isub dbSubIn] [-osub dbSubOut]
```

In the commands above, *job-options* represents the standard Job Control options and other job options:

`-HOST` *host*	Run the job on the specified host.
`-LOCAL`	Run the job in the current directory, rather than in a temporary scratch directory.
`-TMPDIR` *tmpdir*	Use *tmpdir* for temporary files.
`-WAIT`	Do not return control to the shell until the job finishes.
`-INTERVAL` *n*	Interval in seconds between output updates.
`-NICE`	Run the job at reduced priority.