

Schrödinger Product Installation on Linux

The instructions below are for a new installation of Schrödinger Suite 2012 Update 2 software on a typical Linux platform. If you need more details or encounter problems, refer to the [Installation Guide](#), which is included at the top level of the DVD or the download along with these instructions.

Checking your system

1. Check that your system has sufficient disk space:

```
df -h
```

To install all products, at least 8 GB is needed for each architecture (32 bit or 64 bit). 25 GB is required for the PDB and BLAST databases for Prime.

2. Check that your system version is adequate:

```
uname -r
```

For recent Linux distributions, the version reported should be at least 2.6.12.

Installing the software

3. If installing from DVD, mount the product DVD.

You must have a DVD-ROM drive or a DVD-R Read/Write or DVD+/-R Read/Write drive. DVD+R Read/Write drives cannot read our DVDs.

If installing from a download, extract the tar file:

```
tar -xvf Schrodinger_Internet_Download.tar
```

4. Change to the top-level directory on the DVD or the download:

```
cd topleveldir
```

For a download this directory should be the subdirectory Schrodinger_Internet_Download in the directory you extracted the tar file.

5. Run the install script:

```
sh ./INSTALL
```

Using sh is sometimes necessary when installing from DVD.

6. Enter the information requested by the INSTALL script.

The installation directory must not contain a previous Schrödinger software release. It is created if it does not exist. See [Section 3.3](#) of the *Installation Guide* for details.

7. Set the SCHRODINGER environment variable to the installation directory:

```
bash:      export SCHRODINGER=installdir
csh/tcsh: setenv SCHRODINGER installdir
```

8. Set the SCHRODINGER_PYTHONPATH environment variable if PYTHONPATH is defined:

```
bash:      export SCHRODINGER_PYTHONPATH=" "
csh/tcsh: setenv SCHRODINGER_PYTHONPATH
```

Setting up access to remote hosts

9. Edit the file `$SCHRODINGER/schrodinger.hosts` and add entries for all hosts or batch queues on which the software will be run. Do not remove the `localhost` entry.

See [Section 7.1](#) and [Section 7.3](#) of the *Installation Guide* for details. The minimum required for a host entry is
`name: hostname`

10. Set up passwordless `ssh` access between all hosts on which the software will be run.

See [Section 7.2](#) of the *Installation Guide* for details.

11. Perform any necessary cluster configuration (see [Section 7.5](#) of the *Installation Guide*).

Setting up licensing

12. Log on to the license server host (if you are not already logged on to it).

13. Run the `machid` script to obtain information for the license:

```
$SCHRODINGER/machid > machid.out
```

14. Send the output of `machid` to `help@schrodinger.com` to obtain a license.

15. When you receive the license information, which is sent as an attachment, save it as `$SCHRODINGER/license`. You can overwrite the existing file, which is a placeholder.

16. On the license server host, start the license server, and check that it is running.

```
licadmin SERVERUP  
licadmin STAT
```

See [Chapter 6](#) of the *Installation Guide* for details.

Checking the installation

17. Run the installation checker:

```
$SCHRODINGER/installation_check
```

18. Start Maestro to ensure that it is correctly installed.

```
$SCHRODINGER/maestro &
```

19. Choose `Help` → `Manuals Index` to ensure that the PDF viewer is working correctly from Maestro.

20. Choose `Help` → `Online Help` to ensure that the browser is working correctly from Maestro.