

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

You will be sent instructions in an email message for obtaining and installing the license. If you do not receive an email message with instructions about your license, contact help@schrodinger.com.

Checking the installation

12. Run the installation checker:

```
$(SCHRODINGER)/installation_check
```

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

```
$(SCHRODINGER)/maestro &
```

14. Choose **Help** → **Manuals Index** to ensure that the PDF viewer is working correctly from Maestro.
15. Choose **Help** → **Online Help** to ensure that the browser is working correctly from Maestro.