

# Schrödinger Product Installation on Linux

The instructions below are for a new installation of Schrödinger's Release 2015-2 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 6 GB is needed. 25 GB is required for the PDB and BLAST databases for Prime.

2. Check that your operating system is supported.

## Installing the software

1. 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
```

2. 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.

3. Run the install script:

```
sh ./INSTALL
```

Using `sh` is sometimes necessary when installing from DVD.

4. Enter the information requested by the `INSTALL` script.

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

5. Set the `SCHRODINGER` environment variable to the installation directory:

```
bash:      export SCHRODINGER=installdir
```

```
csh/tcsh: setenv SCHRODINGER installdir
```

6. 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

1. 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*

2. Set up passwordless `ssh` access between all hosts on which the software will be run, if you have not done this previously.

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

3. Perform any necessary cluster configuration (see [Section 7.9](#) of the *Installation Guide*).

### Setting up licensing

If you obtained the free version of Maestro as an academic user, or if you have a node-locked license, the license is included with the software and is installed automatically.

Otherwise, you will be sent an email message with information about obtaining and installing the license. If you do not receive a message, go to <http://www.schrodinger.com/licensing> for instructions.

If you do not have access to a license server on another machine, start one locally, as follows.

1. Open the Diagnostics panel.

```
$(SCHRODINGER)/diagnostics
```

2. In the Server Status tab of the License tab, click Start License Server.

### Checking the installation

1. Open the Diagnostics panel, which runs checks and reports the results.

```
$(SCHRODINGER)/diagnostics
```

2. Start Maestro to ensure that it is correctly installed and licensed.

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

3. Choose Help → Documentation Index in Maestro and click on a link to ensure that the manuals open in your PDF viewer.