Schrödinger Product Installation on Windows

This document describes how to install Schrödinger Suite 2012 Update 2 software for use on a single Windows machine. If you need more details or encounter problems, refer to Chapter 4 of the *Installation Guide*, which is included at the top level of the download along with these instructions. If you want to run jobs on remote hosts, or perform any other nondefault installation tasks, see the *Installation Guide*.

It is assumed that you have downloaded the software into your Downloads folder.

Installing the software

- 1. Open your Downloads folder:
 - Windows 7/Vista: Start → Documents, then click Downloads in the side bar.
 - Windows XP: Start → My Documents, then double-click Downloads.
- 2. Right-click on the downloaded zip file (the name starts with Schrodinger Suite) and choose Extract All.

A panel opens so you can choose the destination where the extracted files will go.

Windows 7/Vista:

- a. Leave the destination at the default.
- b. Ensure that Show extracted files when complete is selected.
- c. Click Extract.

Windows XP:

- a. Click Next.
- b. Leave the destination at the default.
- c. Click Next.
- d. Select Show extracted files, and click Finish.
- 3. Double-click the folder that starts with Schrodinger Suite (there should be only one folder).
- 4. Double-click setup, and click Run in the Open File Security Warning dialog box.
- 5. Click Next in the installer.
- 6. In the Destination folder step, click Next to accept the default location and user. (You will not see this step if you are installing an update rather than a new release.)
- 7. In the Setup Type step, leave the selection at the default, and click Next.
- 8. In the Product Selection folder, check Select All and click Next.

If you want to install only some products, check the boxes for those products instead of checking Select All.

- 9. In the File Types step, click Next.
- 10. In the Profile Selection step, click Next.
- 11. Click Start to start the installation.
- 12. If your virus checker objects to any executables, allow the executable to be used.
- 13. When the installation finishes, click Next.

- 14. In the Software Activation step, click Next. (Software activation is dealt with below.)
- 15. Deselect View Release Notes and click OK.

Obtaining and installing a license

If you obtained Maestro under the Maestro Academic Campaign, the license is included with the software and is installed automatically. You can skip this section.

Otherwise, follow the instructions below.

16. Send a request for a license with the file schrodinger_machinfo.txt, which is placed on your Desktop, to licensing@schrodinger.com to obtain a license.

The license file is sent as an attachment to an e-mail message that contains further instructions.

17. Save the attachment as license.txt in the installation folder.

You can overwrite the existing file, which is a placeholder.

18. Follow the instructions in the message to start using your license.

Checking that the software and documentation is working

19. Choose Start \rightarrow All Programs \rightarrow Schrodinger-2012 \rightarrow Diagnostics.

The Diagnostics panel opens and runs various diagnostic tests.

- 20. In the Server Status tab of the License tab, click Start License Server.
- 21. Double-click the Maestro icon on your desktop to start Maestro.
- 22. Choose Help → Manuals Index to ensure that the PDF viewer is working correctly from Maestro.
- 23. Choose Help → Online Help to ensure that the browser is working correctly from Maestro.