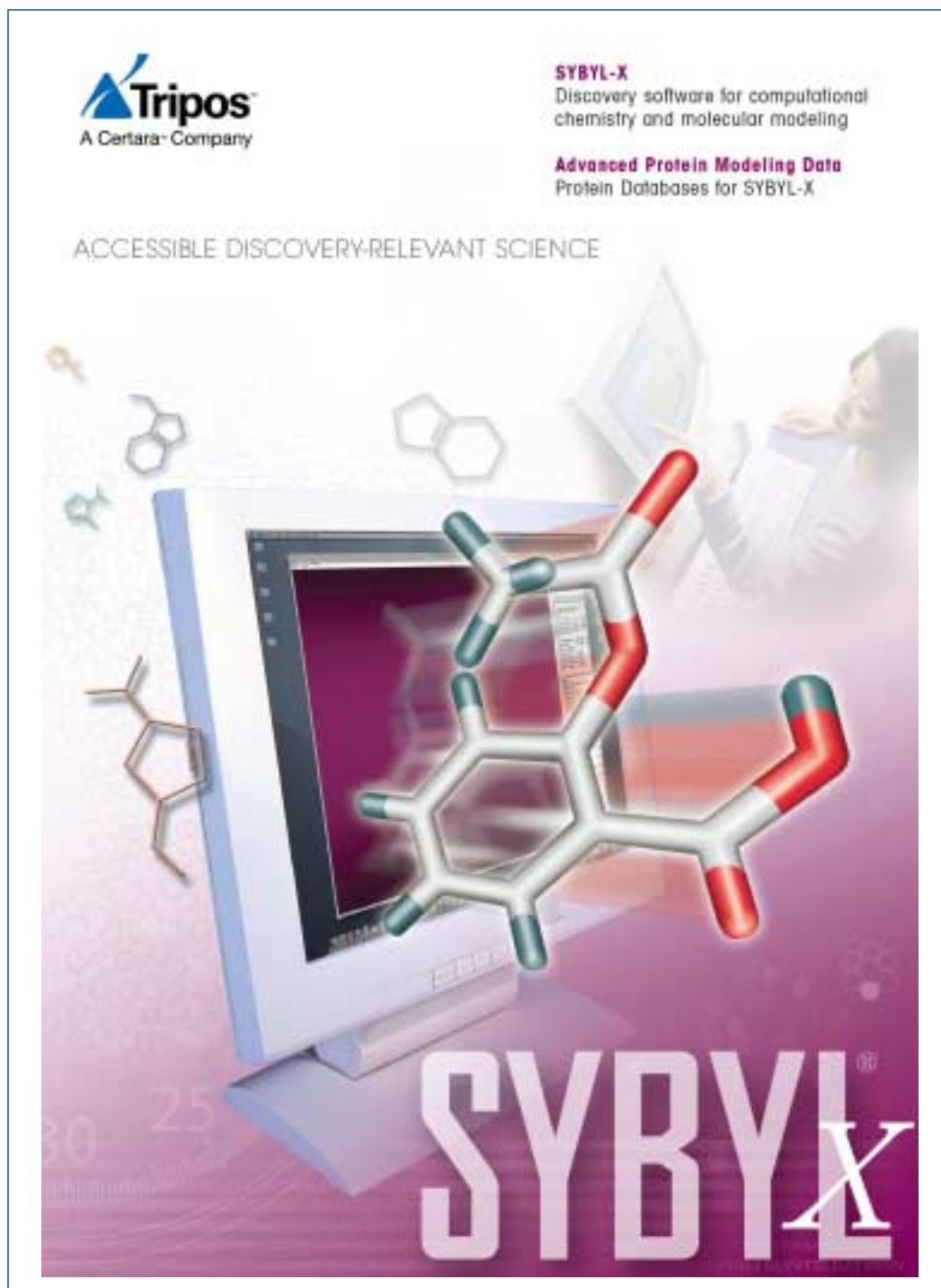# SYBYL®-X 2.1.1

Discovery Software for Computational Chemistry and Molecular Modeling

Installation Instructions for Mac OS X 10.6

Hardware Requirements

SYBYL-X 2.1.1.1 is optimized for the following:

- OS: Mac OS X 10.6.7 (Snow Leopard)
- Memory: 2 GB or greater
- Screen Resolution: 1280x1024 or greater

The following amounts of space are needed:

- Software Installation: 1.3 GB
- Database Installation:
  Prodat: 1.3 GB
  Advanced Protein Modeling: 14 GB

SYBYL-X 2.1.1 Installation

Download the Software if Necessary

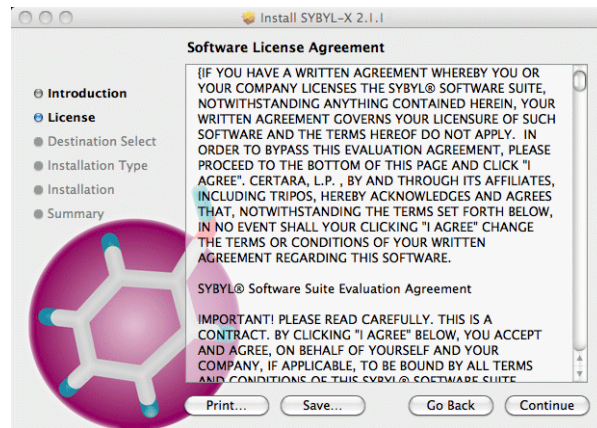If you are installing from a DVD skip to "Install SYBYL-X 2.1.1."

1. Download **SYBYL-X2.1.1-Darwin.pkg** from the Tripos website.

2. Store the downloaded file on the machine where you will perform the installation and in a directory that you can access.
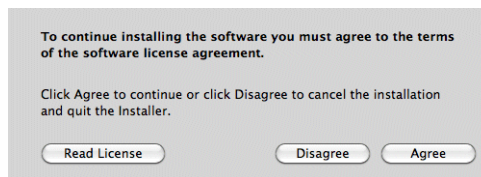
Install SYBYL-X 2.1.1

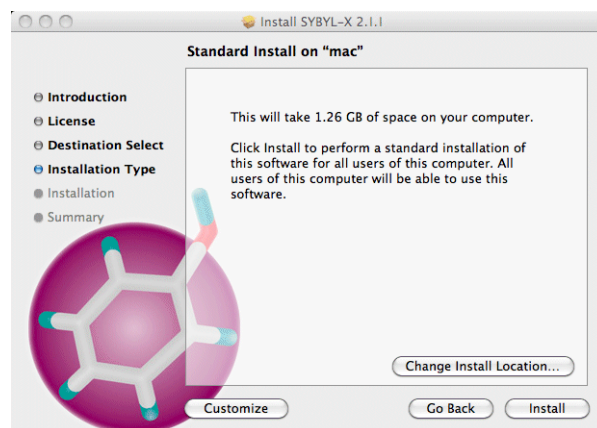3. Double-click on the file **SYBYL-X2.1.1-Darwin.pkg**.

4. Click **Continue**.

5. Read the license agreement and click **Continue**.

6. To accept the terms of the license agreement click **Agree**.

7. Click **Change Install Location...**

How the software will be installed depends on whether you have administration privilege on this computer.

- If you do, select **Install for all users of this computer**.
- If you do not, select **Install for me only**.
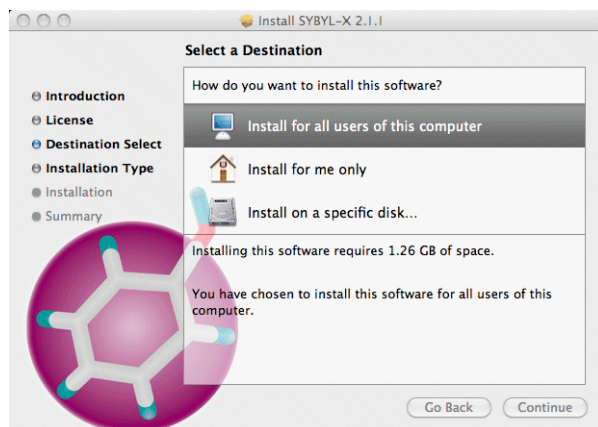
8. After selecting the appropriate destination, click **Continue**.
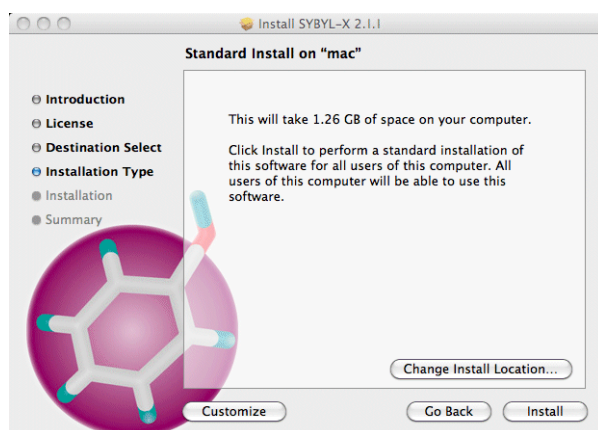
9. Click **Install** to proceed with the installation.

10. Click **Close** to complete the installation step.

Licensing

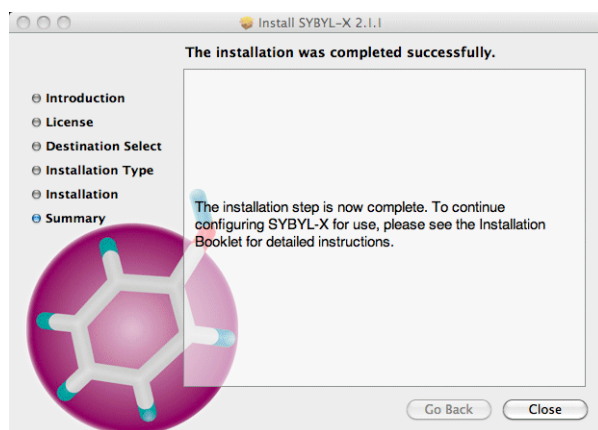Choose only one of the following options:

- Step 11: You have SYBYL-X 1.3
- Step 12: You have SYBYL 8.1, but not SYBYL-X 1.3
- Step 13: You do not have SYBYL-X license keys

11. If you have SYBYL-X 1.3 your existing license file will continue to work. Proceed to "License Manager Configuration: Autostart at Reboot" on page 6.

12. If you have SYBYL 8.1 but not SYBYL-X 1.3, simply copy your existing license file to the SYBYL-X 2.1.1 installation.

    A. From the **Finder**'s **Go** menu select **Computer**, then navigate to the directory where SYBYL 8.1 is installed. Navigate to **AdminTools11.6** then **tables**. Select the file named **license_file** and drag it to your desktop.

    B. From the **Finder**'s **Go** menu select **Computer**, then navigate to the directory where SYBYL-X 2.1.1 is installed (by default, **tripos**) at the top level of your hard drive if you installed as administrator or within your home directory if you installed as an individual user. Navigate to **AdminTools11.6** then **tables**. Drag the file named **license_file** from your desktop to this location.

    C. Proceed to "Starting the License Manager" on page 6.

13. If you do not yet have SYBYL-X license keys, you must obtain them from Tripos.

    A. The information used to obtain your license keys, now or at the time of your license renewal, is stored in **keyfile.txt** within the directory where SYBYL-X 2.1.1 is installed.

    B. Copy the text in this file and email it to **keys@tripos.com** along with your name, the name of your organization, your email address, and a phone number where you can be contacted.

14. The email you will receive from Tripos includes your keys as an attached file. Perform the following steps to install your license keys:

    A. Save the license key file to your desktop and name it **license_file**.

    B. From the **Finder**'s **Go** menu select **Computer**, then navigate to the directory where SYBYL-X 2.1.1 is installed (by default, **tripos**) at the top level of your hard drive if you installed as administrator or within your home directory if you installed as an individual user. Navigate to **AdminTools11.6** then **tables**.

    C. Copy the file named **license_file** from your desktop to this location.

    D. It is good practice to keep a backup copy of your license file in a location outside of your SYBYL-X installation.

Starting the License Manager

Before you can launch SYBYL-X 2.1.1 after installation you must start the license manager.

15. If you installed "for all users": In the **Finder**'s **Go** menu select **Applications**, then **SYBYL-X 2.1.1**, then **Utilities**.
    If you installed "for me only": In the **Finder**'s **Go** menu select **Home**, then **bin**, then **SYBYL-X 2.1.1**, then **Utilities**.

16. Double-click on **Startup Local License Manager**.

    This will take about a minute. The license manager involves two processes, triposlm.exe and lmgrd.exe.

License Manager Configuration: Autostart at Reboot

To configure your license manager to start automatically when the machine is rebooted, do the following.

17. Log in as root.

18. Copy the following file from your SYBYL-X 2.1.1 installation:

    sybylx2.1.1/tables/darwin/DarwinStartup.tar
    to your computer's **/Library/StartupItems**

19. Extract the file in that location by typing:

    tar -xvf DarwinStartup.tar

20. Verify that:
    - All extracted files and directory are owned by root and that the group name is "wheel".
    - Permissions on all directories and executables are 755.
    - Permissions on all other files are 644.

21. If you did not install SYBYL-X 2.1.1 "for all users":

    A. Go to **/Library/StartupItems/Triposlm**

    B. Edit the definition of TA_LICENSE on line 14 of the file **Triposlm**
        export TA_LICENSE=/tripos/AdminTools11.6

        Replace tripos with the path to the AdminTools11.6 directory in your installation.

    C. Save the file.

SYBYL-X Shortcuts

22. The following shortcuts are available:

- **SYBYL-X** — Starts SYBYL-X and displays its graphical interface window.
- **Utilities**
    - **Bookshelf** — Starts the online help independently of the SYBYL-X application.
    - **Shutdown Local License Manager** — Shuts down the locally running license manager for all versions of SYBYL-X.
    - **Startup Local License Manager** — Starts the local license manager for all versions of SYBYL-X.
    - **SYBYL-X Command Line** — Starts SYBYL-X without graphics and displays its command console only.
    - **SYBYL-X Environment Shell** — Does not start SYBYL-X, but opens a system shell in which the SYBYL-X environment has been defined. This provides easy access to SYBYL-X's standalone applications.
    - **SYBYL-X Plus Console** — Starts SYBYL-X, displays its graphical interface window, and opens a separate system console that will receive a small amount of information produced by some SYBYL-X 2.1.1 operations.

23. For the convenience of one-click access to SYBYL-X, drag the SYBYL-X icon to your Dock.

Optional Protein Database: Prodat

Tripos supplies a binary protein database, Prodat, for use with SYBYL-X 2.1.1.

Note: The contents of the Prodat database have not changed since the SYBYL-X 1.3 release. If this database is already installed in a directory parallel to your SYBYL-X installation(s), SYBYL-X 2.1.1 will locate it automatically.

You may choose to:

- "Install the Protein Database" on page 8.
- "Configure SYBYL-X 2.1.1 to Use a Customized Protein Database" on page 8.
- Skip this option and proceed to "Optional Databases for Advanced Protein Modeling" on page 8.

Install the Protein Database

The Protein Database (Prodat) is installed via a separate installer.

24. If you are installing from DVD skip to step 25. Otherwise, download the necessary file.

   A. Download **Prodat-1009-X2.1-Darwin.pkg**.

   B. Place it in a location where it can be accessed to perform the installation.

25. Double-click on the file **Prodat-1009-X2.1-Darwin.pkg**.

   Prodat_1009 will be installed in a directory parallel to your SYBYL-X 2.1.1 installation.

26. Proceed to "Optional Databases for Advanced Protein Modeling" on page 8.

Configure SYBYL-X 2.1.1 to Use a Customized Protein Database

27. If you have a local, customized, version of Prodat you must configure SYBYL-X 2.1.1 to access it. To do so use a text editor.

   A. Navigate to the location where you installed SYBYL-X 2.1.1 and go to the **lib** directory.

   B. In the **environment** file edit the definition of TA_PDBTABLES to use the path to the directory containing your existing Protein Database.

Optional Databases for Advanced Protein Modeling

Tripos supplies several databases for use with FUGUE™ and ORCHESTRAR™.

Note: The contents of the Advanced Protein Databases have not changed since the SYBYL-X 1.3 release. If these databases are already installed in a directory parallel to your SYBYL-X installation(s), SYBYL-X 2.1.1 will locate them automatically.

You may choose to:
   • "Install the Advanced Protein Modeling Databases" on page 8.
   • "Configure SYBYL-X 2.1.1 to Use Existing Databases" on page 9.

Install the Advanced Protein Modeling Databases

The Advanced Protein Modeling Databases are installed via a separate installer.

28. If you are installing from a DVD skip to step 29. Otherwise, download the files.

   A. Download **orchestrar_db_1009-X2.1-Darwin.pkg** and place it in a location where it

can be accessed to perform the installation.

    B. Download **orchestrar_db_1009_1.dat** and **orchestrar_db_1009_2.dat** and place them in the same location as the installation package.

29. Double-click on the file **orchestrar_db_1009-X2.1-Darwin.pkg**.

The Advanced Protein Modeling Databases will be installed in a directory parallel to your SYBYL-X 2.1.1 installation. Expect the installation to take 20 to 30 minutes.

Configure SYBYL-X 2.1.1 to Use Existing Databases

30. If you have a local, customized, version of the Advanced Protein Modeling Databases you must configure SYBYL-X 2.1.1 to access them. To do so use a text editor.

    A. Navigate to the location where you installed SYBYL-X 2.1.1 and go to the **lib** directory.

    B. In the **environment** file edit the definition of TA_ORCHESTRAR_DB to use the path to the directory containing your existing advanced protein modeling databases.

Where to Turn for Assistance

If you encounter any problems, please contact your local support office. For a complete listing of support offices, go to: **http://www.tripos.com/support**.

We thank you for your interest in Tripos software products and we look forward to serving you again in the future.

11/2013