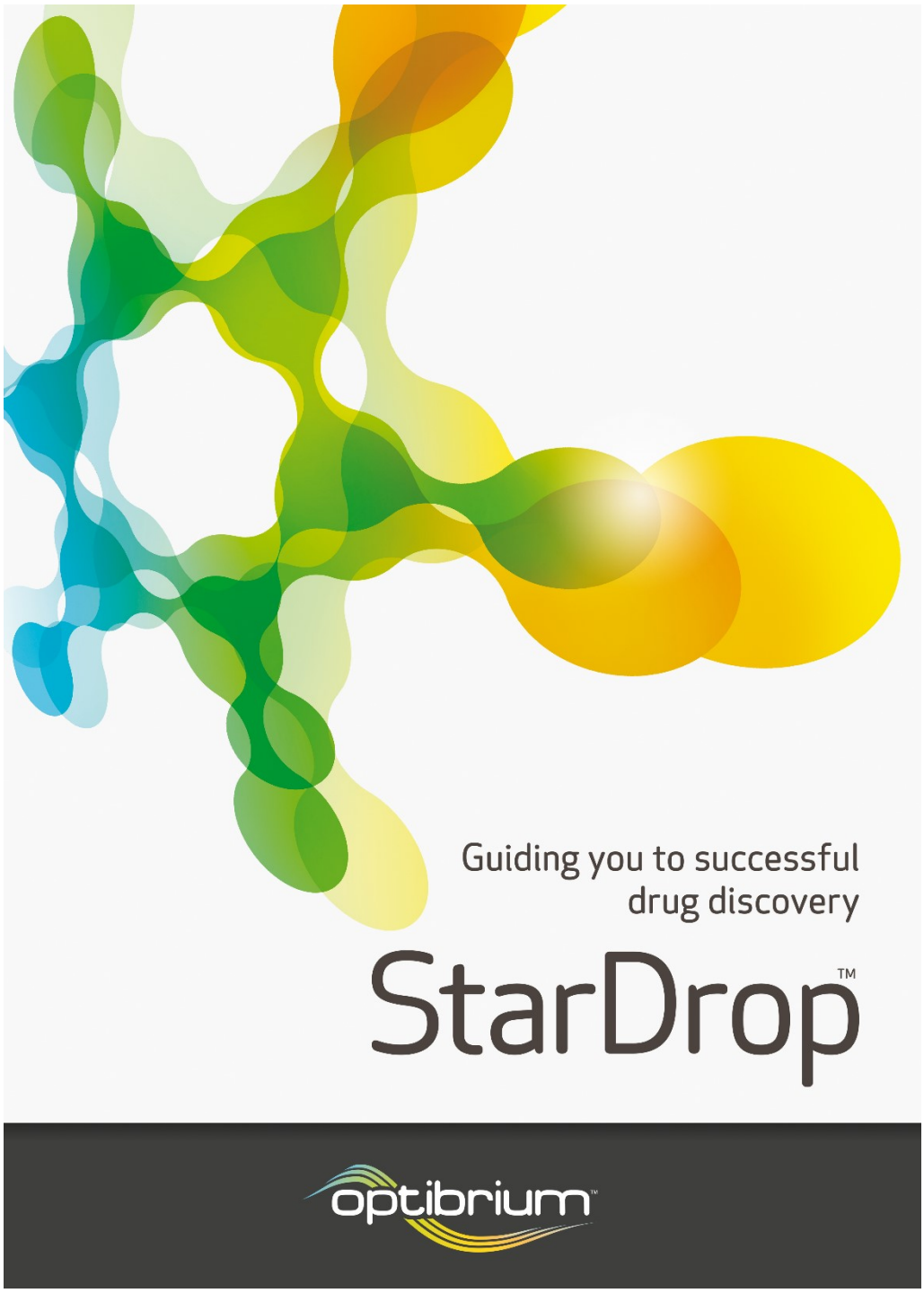
StarDrop™ System and Installation Guide

Version 7.0



Contents

1 Introduction

This document gives an overview of the StarDrop system and its installation. It is intended to be used as a technical guide for the installation, maintenance and support of StarDrop.

2 Prerequisites

2.1 Hardware

For the Windows[1] or macOS[2] operating systems, the recommended minimum hardware is as follows:

- 4 GB RAM
- 2 GB hard disk space

To install all the servers (ADME QSAR, P450, Auto-Modeller™ and License) and the Derek Nexus™ web service on a single Linux machine, the following minimum hardware is recommended:

- 4 GB RAM
- 4 GB hard disk space

Please note that the memory requirements for the Auto-Modeller server can be significantly higher when modelling data sets with many thousands of data points. For advice on system configuration please contact stardrop-support@optibrium.com.

2.2 Operating Systems

The **StarDrop client** is supported on the following **64-bit** operating systems:

- Windows 10
- macOS 10.15 (Catalina) and 11 (Big Sur)

The **StarDrop servers** are supported on the following **64-bit Linux** operating systems:

- Red Hat Enterprise Linux 6, 7 and 8[3]
- CentOS 6, 7 and 8[3]

If installing a new Linux operating system, we suggest you select the option to include "developer tools". For further advice please contact stardrop-support@optibrium.com.

2.3 System Configuration

Domain name resolution (DNS) must be properly configured on both server and worker machines. This must return the correct IP addresses for the machine names for the server and worker machines entered during the installation process. This can be tested using

nslookup <machine name>

Furthermore, the IP address of the local machine should be present in the file /etc/hosts associated with the fully qualified name and hostname of the machine. Here is an example /etc/hosts file:

```
127.0.0.1     localhost.localdomain    localhost
::1           localhost6.localdomain6  localhost6
192.168.1.117 tom.jerry.co.uk          tom
```

[1] Windows is a registered trademark of Microsoft Corporation in the United States and/or other countries.
[2] macOS is a registered trademark of Apple Inc. in the United States and/or other countries.
[3] Red Hat, Enterprise Linux and CentOS are registered trademarks of Red Hat, Inc.

The final line has been added which maps the machine name, 'tom' in this example, to the IP address 192.168.1.117. The 'hostname' and the 'ip addr' commands can be used to obtain the hostname and IP address respectively. Note that you may need to ensure your network adaptor is activated. Also, the machine name, e.g. 'tom', should *not* map onto the loopback address 127.0.0.1.

The firewall option must be disabled or configured to allow access to the required ports for inter-process communication. Also "SELinux" (secure Linux) must be disabled. It is assumed that the server will be installed behind a company firewall so that firewalls are not required on individual machines. Furthermore, the StarDrop servers should not be run on a machine that is accessible from the internet. If this is not the case, please contact stardrop-support@optibrium.com for further assistance.

One of Python 2.3 through 2.7 is required to run the servers' installation script.

2.4 System Overview

A schematic describing the components of the StarDrop system and their interaction is given in Figure 1.

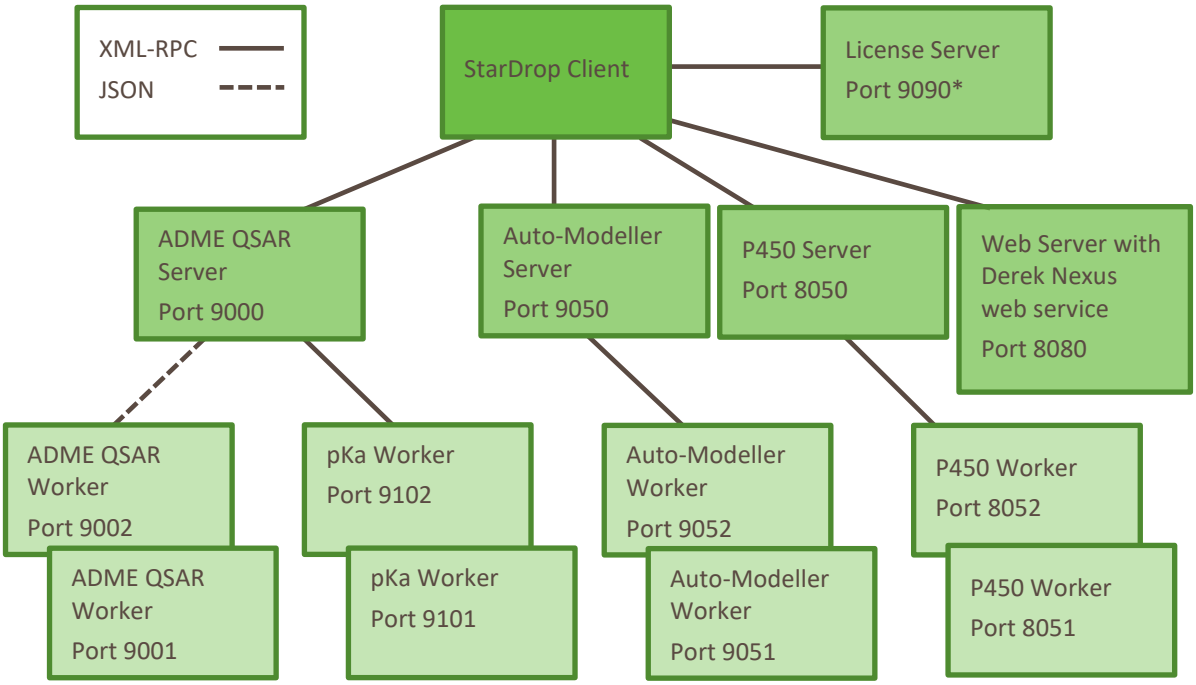


Figure 1. A schematic representation of the components of the StarDrop system and their interactions. The default ports for communication are shown (these can be changed during installation).

There are up to 10 principal software components:

- **The StarDrop Client**
- **Auto-Modeller Server**
  A server for generating models, required as part of the 'Auto-Modeller' module; responsible for receiving requests from the Client, distributing these to worker processes, collecting the results and returning these to the Client.
- **Auto-Modeller Worker(s)**
  Worker processes for generating models. Requests for model generation are created by the Auto-Modeller server and results are returned to the server.
- **ADME QSAR Server**
  A server for running high-throughput predictive ADME models as part of the ADME QSAR module; responsible for receiving requests, distributing these to worker processes, collecting the results and returning these to the client. This server may also be configured to run third-party models via Python scripts (see the StarDrop Scripting and Customisation guide for details).
- **ADME QSAR Worker(s)**

Worker processes for calculating high-throughput predictive ADME model results. Requests for these are generated by the ADME QSAR server and the results are returned to the server.

- **pKa Worker(s)**
  Worker processes for calculating pKa model results. Requests for these are generated by the ADME QSAR server and the results are returned to the server.
- **P450 Server**
  A server for running P450 metabolism models as part of the P450 module; responsible for receiving requests from the Client, distributing these to P450 worker processes, collecting the results and returning these to the Client.
- **P450 Worker(s)**
  Worker processes for calculating the results of the P450 metabolism models. Requests for these are generated by the P450 server and results are returned to the server.
- **Derek Nexus web service**
  The Derek Nexus web service sits on a web server and runs Derek Nexus toxicity predictions; responsible for receiving requests from the Client, calculating results and returning them.
- **License Server**
  A server for issuing floating licenses to users; responsible for holding a list of available licenses, receiving requests from users when StarDrop is started and issuing or denying licenses as appropriate.

All servers are commonly installed on a single machine although this is not a requirement. The P450, Auto-Modeller and Derek Nexus web service servers should only be installed once each. Only one instance of each will be executed on system start-up. The ADME QSAR server can be installed on multiple machines. This is only recommended when there is a requirement to serve distinct sets of custom models and in many situations a single ADME QSAR server will be sufficient.

The ADME QSAR, P450 and Auto-Modeller workers may be installed on as many machines as required (subject to license conditions). To maximize performance, by default, one process will be executed per CPU (or virtual CPU for processors supporting hyper-threading). Worker processes may be set up on the same machine as the servers. This is the recommended configuration that maximizes interactive performance and minimizes potential for disruption due to networking problems.

Optionally, a License server may be installed which supports floating licenses for StarDrop clients.

The StarDrop Scripting and Customisation Guide document describes developing custom model plug-ins for the ADME QSAR server.

3 Installation

3.1 Location

You can specify any location during the installation process, but the default location is:

/usr/local/StarDrop64

In this guide, example installation paths are shown. In all the examples this guide uses the default location, but you will need to alter this when following the examples if you have chosen your own installation location.

The web server for hosting the Derek Nexus web service can be installed in any location of your choice.

3.2 Servers

StarDrop servers can be installed on a PC running Linux. Section 2.2 lists the supported Linux distributions. The guidelines described in section 2.3 should be followed before running the installer.

The installation process will check dependencies, remove any existing installations, install the requested servers and start the servers.

StarDrop servers are installed by running the python **install script** found in the StarDrop server bundle. This script can be run using one of Python 2.3 through 2.7 (Note: you may need to install Python 2 on Red Hat Enterprise Linux 8 and CentOS 8 using the command '*yum install python2*'). To run the installer:

1. Download the bundle **StarDrop-7.0-server-installer.tar** from the Optibrium web site (using the credentials emailed to you)
2. Login as root or using an account with sudo privileges
3. Untar the bundle

   tar xvf StarDrop-7.0-servers-installer.tar

4. Change to installer directory

   cd servers_installer

5. Run the installation script:

   python install_stardrop_servers.py

The installer will prompt with a number of questions. You can type 'yes' or 'no' as appropriate followed by pressing **Enter.** Alternatively, you can simply press **Enter** to accept the default option which is indicated in brackets. For example, a default 'yes' answer is indicated by [yes]. The following sections describe the various installation options and prompts that you may see.

Dependency Check

The installer will perform a dependency check and report any missing libraries. If system libraries are missing, and if 'yum' is available, the installer will give the option to find packages that provide the missing libraries with the following prompt:

Would you like to find packages that provide these missing libraries? [No]:

If you type **Yes,** then the installer will use the yum 'whatprovides' and yum 'install' commands to find and install the necessary packages. This step may take a long time to complete. Alternatively, you can cancel the installation by typing **No** and install the required packages yourself or consult your system administrator before installing packages. If 'yum' is not available, then you will need to find an alternative means of installing the libraries.

The libraries that are present on a Linux distribution can depend on the options chosen when Linux is installed.

License Agreement

The installer will confirm that you agree to the license terms:

Do you agree to the license terms? [Yes]:

To agree, press **Enter**. Typing *No* will abort the installation process.

Default or Custom Installation

The installer will prompt for a *default* or *custom* installation

Please select default or custom installation

default: *Provides a default installation directory*
Sets a default number of worker processes
Sets default server and worker port addresses
Servers will be started automatically

custom: *Allows customisation of all installation parameters*

Please type 'default' or 'custom' [default]:

Press **Enter** to select a default installation. Type *custom* followed by **Enter** to select a custom installation. If you wish to install servers and workers on separate machines, manually set the installation directory or manually set port numbers then you must select a custom installation.

Confirm server Installation

The installer will ask for confirmation before installing each of the four server types:

1. ADME QSAR server
2. Auto-Modeller server
3. P450 server
4. License server.

For example, the installer will ask:

Would you like to install the ADME QSAR server? [yes]:

To agree, press **Enter**. Typing *No* will skip the installation for that server, and you will be asked if you wish to install the next server**.**

For the case of the license server:

Would you like to install the License server? [yes]:

If you have a **floating license**, then please confirm installation by pressing **Enter**. The license server is required in order to install and use floating licenses.

Removing Existing Installations

In order to proceed with an installation any existing installation must first be removed. If an existing installation is detected the installer will confirm the removal. For example:

An existing installation has been detected
In order to proceed this must first be removed
All currently installed models will be preserved
You are about to remove the ADME QSAR server. Do you wish to continue? [yes]:

Press **Enter** to remove the existing server. Typing *No* will skip the server installation and you will be asked if you wish to install the next server. The uninstall process will preserve some files. For example, ADME QSAR models files, license files, cached data used by the P450 and Auto-Modeller servers will be preserved and reinstated.

Specify the Installation Directory

By default, StarDrop servers will be installed in the directory /usr/local/StarDrop64. If you run a **custom installation** you can explicitly set the base installation directory:

Please specify an installation directory [/usr/local/]:

To accept the default value, press **Enter**. To install into a different directory, type in the full path of the base directory and press **Enter**. Note that the installer will always create a single directory called 'StarDrop64' within the directory you have specified.

For the ADME QSAR server, you will be prompted to provide information about where to install new custom model extensions. This is only necessary when adding custom models to the server and further information on this is available in the StarDrop Scripting and Customisation Guide.

Secure server communication

For a **custom installation**, you can choose whether to configure secure communication between the StarDrop servers and client (i.e., HTTPS). If you choose secure communication, then you can either specify your own certificate or use a default self-signed certificate.

Configuring servers and workers

If you select a **default installation**, then servers and their workers will be configured with default options and you will not be prompted. One worker will be configured for each CPU (or virtual CPU) on the computer and the server and workers will be assigned default port numbers. A default installation will also assume that all servers and their workers are to run on the same machine.

Selecting a **custom installation** allows you to explicitly set the number of workers and set the port numbers. You can also specify machine URIs for any workers that are installed on separate machines. For systems with several processors, it may be better to not create one worker per processor per server, but to divide up the available processors between the co-hosted servers and their workers. For assistance in setting up installations over multiple machines contact stardrop-support@optibrium.com

A custom installation prompts for the following configuration options:

a. Configuring *this* computer:

   How do you wish to configure this computer?
   1. *Configure to run server and worker processes*
   2. *Server only – choose only if you intend to setup your workers on other machines*
   3. *Worker only – choose only if you intend to setup a server on another machine*

   Choose (1 2 3) [1]:

   You should only select options 2 or 3 if this installation is to be part of a larger cluster. If this is the only machine onto which you are installing this server, type **1** and press **Enter**. For assistance in setting up installations over multiple machines contact stardrop-support@optibrium.com.

b. The installer will prompt for the number of worker processes. For example:

   Please specify the number of ADME QSAR workers to configure [1]:

   The default number given in brackets will be the number of CPUs (or virtual CPUs) available on the machine. To accept this default value, press **Enter**. To install a smaller number of worker processes, type the required number and press **Enter**. (E.g., you may wish to set up a number of workers that is less than the number of CPUs in order to reserve CPUs for other tasks.)

c. The installer will confirm the port numbers to use for each worker process. This question will be repeated for each worker:

   Please specify a port for worker #1 [9001]:

   To accept the default value, press **Enter**. To use a different port number, type the desired number and press **Enter**.

   Please ensure that all ports selected are available through the local network firewall.

d. The installer will now confirm the port number to use for the server process:

   Please specify a Port for server [9000]:

   To accept the default value, press **Enter**. To use a different port number, type the desired number and press **Enter**.

   Please ensure that the port selected is available through the local network firewall.

e. Specify additional workers on other machines. The installer will ask:

   Have you installed workers on other machines that you would like the server to use? [no]

   If no additional workers have been installed, then press **Enter** to accept the default response. If you do have additional workers installed on other machines, then type *Yes*. Additional workers are specified by their machine name URI and port number. The installer will first prompt for the machine name:

   Please specify machine name and port numbers for additional worker(s)
   The machine name is the fully qualified domain name 'mymachine.mydomain.com'
   Please enter a machine name. Press 'Enter' when you have no more to add:

   Enter the machine name by typing the full URI (e.g., mymachine.mydomain.com) and press **Enter.** The installer will then prompt for the port number for this additional worker:

Port [9001]:

Enter the port number and press **Enter**. You will then be asked again for a machine name. If you have no more workers to add, then press **Enter** without specifying a machine name to finish this process.

f. For the P450 server, if you select a **custom installation** then you will also be prompted to confirm whether you wish SMILES strings to be canonicalized:

Do you want all smiles strings to be canonicalised before processing? [yes]

Starting the servers

If you select a **default installation**, then the StarDrop servers will be started automatically. In addition, the servers will be configured to start each time the machine is restarted.

If you select a **custom installation** you can choose whether or not the servers start at the end of the installation and whether they are configured to start automatically when the machine is restarted. For example, the installer will ask:

a. Starting the server.

Do you wish to start the ADME QSAR server (StarDrop_modelserver service) now? [Yes]:

Pressing **Enter** will start the server.

b. You can also indicate whether servers should start automatically when the machine is restarted. For example:

Do you wish the ADME QSAR server to start automatically each time you restart this machine? [Yes]:

Unless you wish to configure the start-up process manually, press **Enter**.

c. You can indicate whether the Model Server REST Service should start automatically when the machine is restarted. This is not necessary for StarDrop but can be used by other systems to access StarDrop Model Server predictions (see StarDrop Scripting and Customisation Guide). For example:

Do you wish the Model REST Service to start automatically each time you restart this machine? [Yes]:

Unless you wish to configure the start-up process manually, press **Enter**.

The installer will report whether the server start was successful. For example:

Starting service: /etc/init.d/StarDrop_modelserver start
Starting Model Server: [OK]

Section 4.5 describes how to start and stop the servers manually.

Tracking license usage

If you select a **custom installation** and install the license server (which manages floating licenses) then the installer will ask whether you wish to track license usage.

Would you like to be able to track license usage? [yes]

If you select 'yes' then license usage data will be recorded in the file <installation directory>/sls/var/run/sls-usage.log. See section 4.4

Floating License timeout

If you install the floating license server, you will be asked to set a timeout in hours

Timeout (between 0.25 and 24 hours) [1]:

A floating license limits the number of concurrent users to the number of seats that have been purchased. A user will take up one seat when they connect to the server. That seat is released and made available to someone else by disconnecting from the server.

Sometimes a seat can be taken but the user is not actively using the server and is not available to release the seat. To cater for this scenario the license server has a timeout. This is the time, in hours, after which an inactive seat will automatically become available for anyone to use.

The timeout value is written to the configuration file: /etc/sysconfig/StarDropLicenseServer_conf.py

3.2.1 Installation log

At the end of the installation, an installation log is saved in the file <installation directory>/StarDropInstall.log.

3.3 Floating License

If you have a floating license, then you will need to initialise the StarDrop license server with the necessary license information.

To obtain a license file, email the results of the command:

ip addr show

to stardrop-support@optibrium.com and you will receive a license file called sls.conf in return.

Copy the license file (sls.conf) to /usr/local/StarDrop64/sls/var/run. When the file is in place, (re)start the license server service:

/etc/init.d/StarDrop_sls restart

3.4 Derek Nexus Web Service

The Derek Nexus web service can be installed on a PC running Linux. Section 2.2 lists the supported Linux distributions. The guidelines described in section 2.3 should be followed before running the installer.

The Derek Nexus web service must be installed on a web server using a supported Java Development Kit (JDK). The 64-bit JDK version of the Java distribution must be installed and not just the runtime environment.

The following instructions describe installing an appropriate Java environment and web server and include all the necessary URLs and instructions for obtaining these (please note that an internet connection may be required for downloading the necessary components). If these are already available, then some of the steps may be omitted, but for advice on running the Derek Nexus web service alongside other web applications please contact stardrop-support@optibrium.com.

1. Install a 64-bit Java 1.8 with development kit bundle:
    a. Create a directory in which a java bundle can reside and change to that directory:

    ```
    mkdir /opt/stardrop
    cd /opt/stardrop
    ```

    b. Download the Java 8 development kit (you may need to create an Oracle account) from

    http://www.oracle.com/technetwork/java/javase/downloads/java-archive-javase8-2177648.html

    Note: You should download the file called jdk-8uXXX-linux-x64.tar.gz (at the time of writing XXX was version 152)

    c. Extract the java bundle with the command (replacing XXX as appropriate):

    ```
    tar -xzf jdk-8uXXX-linux-x64.tar.gz
    ```

2. Install an Apache Tomcat[4] server:
    a. Download Apache Tomcat 8.0.36 using the command (all one line):

    ```
    wget "https://archive.apache.org/dist/tomcat/tomcat-8/v8.0.36/bin/apache-tomcat-8.0.36.tar.gz"
    ```

    b. Extract the server with the command:

    ```
    tar -xzf apache-tomcat-8.0.36.tar.gz
    ```

[4] Apache Tomcat and Tomcat are trademarks of the Apache Software Foundation.

c. Rename the folder to 'tomcat' using the command:

```
mv apache-tomcat-8.0.36 tomcat
```

3. Download the file **DerekNexus.tar** from the Optibrium web site (using the credentials emailed to you) and copy it to the /opt/stardrop directory
   a. Extract the Derek Nexus web service and start-up script using the command:

```
tar -xvf DerekNexus.tar
```

4. Set up the start-up script:
   a. Place the tomcat startup script in directory /etc/init.d and move to that folder:

```
cp /opt/stardrop/DerekNexus/tomcat /etc/init.d/.
```

   b. Open the tomcat script in a text editor. Change the line starting with "export JAVA_HOME=" to point to the installed jdk directory: "/opt/stardrop/jdk1.8.0_XXX" (replacing XXX as appropriate)
   c. Set the script to run at start-up using the commands:

```
chkconfig --add tomcat
chkconfig --level 234 tomcat on
```

5. Install the Derek Nexus web service:
   a. Copy the file **derekwebservice.war** into the **webapps** directory in the Apache Tomcat installation.
   b. Start the tomcat server using the command:

```
service tomcat start
```

   c. You should see a **derek** directory created in the Apache Tomcat installation directory alongside the webapps directory.
6. Install the Derek Nexus web service license and update the configuration:
   a. In the **derek** directory, inside the **configuration** subdirectory is a text file called:

```
org.lhasalimited.ws.derek.config.properties
```

   open this file in a text editor.
   b. Find the line which starts "LOGIN_KEY =" and change **defaultKey** to **StarDrop**
   c. Save and close the file
   d. From the email sent to you by StarDrop support, copy the attached license file **License.lxt** into the **licensekeys** subdirectory of the **derek** directory. (Please note that this key will be moved when the service is started)
   e. Restart the Apache Tomcat service by using the commands:

```
service tomcat restart
```

7. Test the installation from a StarDrop client (after completing the steps in Section 3.6 below)
   a. Start StarDrop (ensuring that you have installed the client license keys provided by StarDrop support) on a PC which has network connectivity with the PC on which you installed the Derek Nexus web service
   b. From the **File** menu in StarDrop choose **Preferences…**
   c. On the **Derek Nexus** tab (at the far right) add the name or IP address of the Derek Nexus server
   d. Click the **Test** button
   e. If the result of the test was **Success** then, when you **OK** the preferences, you should see a Derek Nexus branch on the main **Models** tab in the StarDrop client under which the different toxicity endpoints are listed

3.5 Server Tests

You can test that the servers are running correctly by running a python script called 'server_tests.py'.

1. Change to servers_installer directory. The directory would have been created by extracting **StarDrop-7.0-server-installer.tar** during the server installation. Refer to Section 3.2 if you can't locate the directory.
2. Run the test script:

   python server_tests.py

Tests are performed for each installed server. For example, if all server types are installed and all tests pass, then the server_tests.py output will look similar to this:

Loopback address test [OK]
p450 testWorker http://servername.optibrium.com:8051 [OK]
p450 queueSMILES test: [OK]
p450 retrieveXML test: [OK]
AMG amg_testserver test: [OK]
Model Server test-ping server: [OK]
Model Worker instance test: [OK]
Model Server test-meta: [OK]
License server sls_checkserver logged in users test [OK]
License server sls_checkserver license info test [OK]

Test are run only if the servers are running. The test script will report any servers that are not running. For example:

"AMG tests not run. No server running".

Section 4.5 describes how to stop and start the servers.

A test log file is written to /tmp/StarDropServerTests.log. If any tests do fail then please contact support@optibrium.com and attach this test log file to the email.

3.6 StarDrop Client

3.6.1 Installation - Windows

To install the StarDrop client for all users you must be logged into the PC using an account with administrator privileges. If you do not have administrator privileges, then you can still install StarDrop for yourself. Please note that if StarDrop has previously been installed by an administrator then it must first be uninstalled (again, by an administrator) before you can install StarDrop using an account without administrator privileges.

To install as an administrator:

1. Run **StarDrop-7.0-installer.msi**.
2. Once you have accepted the terms in the License Agreement click **Install**.

To install StarDrop as a non-administrator:

1. Run **StarDrop-7.0-installer.msi**.
2. Once you have accepted the terms in the License Agreement click **Advanced**.
3. Choose **Install just for you** and click **Next**.
4. Click **Install**.

3.6.2 Installation – macOS

On macOS double-click the image file called **StarDrop-7.0.dmg**.

3.6.3 Licensing and Configuration

1. Once the installation is complete, start StarDrop. The first time you run StarDrop, or when there isn't a valid license key, it will start in **Viewer mode.** While in viewer mode you will be able to view previously saved files, but all major functionality will be disabled. Once a valid key has been installed, all licensed functionality will be restored.
2. From the **Help** menu choose **Manage Licenses**.

3. To obtain a license key click the **Request License Key** button and send the automatically generated email to stardrop-support@optibrium.com, filling in the remaining details.
   A license key will be issued (license agreement permitting) and sent back to you.
4. When you have received your new license key, open the **Manage Licenses** dialogue again, click the **Add** button and then copy & paste the license key into the box, then click **OK**.
5. Click **OK** to complete the process.
6. If you are using StarDrop's P450 or Auto-Modeller modules, server settings for these can be configured in the preferences from the **File** menu by selecting **Preferences**. A dialogue box will appear.
7. On each of the **P450, Auto-Modeller** and **Derek Nexus** tabs, as appropriate, enter the name and port for the server. If you do not know the correct settings, please contact your local StarDrop administrator.
8. Now click the **Test** button. A message will appear telling you whether StarDrop could successfully contact the server. If this is not the case, please contact your local StarDrop contact to confirm the server details.
9. Click the **OK** button to save these preferences and installation is complete.
10. If you wish to re-distribute the server details to others without their needing to edit the preferences, you can find the server settings saved in the "serverconfig.xml" file in the StarDrop folder within a user's home directory. It contains entries used to initialise StarDrop on start-up:

```
<?xml version = "1.0" encoding = "UTF-8"?>
<StarDropServerSettings>
        <AmgSettings>
                <Server>MyAutoModellerServerName</Server>
                <Port>9050</Port>
        </AmgSettings>
        <ModelSettings>
                <Servers/>
        </ModelSettings>
        <RegioSettings>
                <Server>MyP450ServerName</Server>
                <Port>8050</Port>
        </RegioSettings>
        <DerekNexusSettings>
                <Server>MyDerekNexusServerName</Server>
                <Port>8080</Port>
        </DerekNexusSettings>
</StarDropServerSettings>
```

4 StarDrop Server and Worker Files

4.1 /usr/local/StarDrop64/modelserver

This contains the executables and configuration files for the ADME QSAR server and worker.

var/log/model_server.log: This is the log file for the ADME QSAR server. It will only be present on the designated ADME QSAR server machine.

var/log/model_worker_*.log: This is the log for a ADME QSAR worker. It will only be present on a machine running an ADME QSAR worker process.

var/cache: This directory is where all the ADME QSAR results are cached.

4.2 /usr/local/StarDrop64/p450

This contains the executables and configuration files for the P450 server and worker.

var/log/p450.log: This is the log for the P450 server and P450 worker processes. It will be present on all machines running a P450 server and/or P450 worker processes.

var/cache/P450: This is where all P450 results are cached.

4.3 /usr/local/StarDrop64/amg

var/log/amg.log: This is the log file for the Auto-Modeller server. It will only be present on the designated Auto-Modeller server machine.

var/log/amg_worker*.log: This is the log for an Auto-Modeller worker. It will only be present on a machine running an Auto-Modeller worker process.

var/cache/AMG: This is where all completed Auto-Modeller sessions are stored

4.4 /usr/local/StarDrop64/sls

var/log/sls.log: This is the log file for the StarDrop License server, containing basic debug information about the server operation. It will only be present on the designated server machine.

var/run/sls-usage.log: This is the operation log file for the StarDrop License server. An entry is added for each interaction of the server with a client. The information in this file can be extracted in a more usable form by running:

python /usr/local/StarDrop64/sls/bin/sls_getloginfo.pyc

4.5 /etc/init.d

The auto-start scripts for all the server processes are placed in this directory. These scripts are:

StarDrop_modelserver: Start, stop and restart the ADME QSAR server and worker processes. The ADME QSAR server will only be executed on the machine selected as the server during installation.

StarDrop_p450: Start, stop and restart the P450 server and P450 worker processes. The P450 server will only be executed on the machine selected as the server during installation.

StarDrop_amg: Start, stop and restart the Auto-Modeller server and Auto-Modeller worker processes. The Auto-Modeller server will only be executed on the machine selected as the server during installation.

StarDrop_sls: Start, stop and restart the StarDrop License server process. The StarDrop License server will only be executed on the machine selected as the server during installation.

During installation, the option to automatically start these services at specified run-levels will be given. It is recommended that the services be automatically started at the default run-level to automatically recover the server and worker processes in the event of an unexpected reboot.

4.6 /etc/sysconfig

The environment configurations for the ADME QSAR, Auto-Modeller and P450 processes are contained in this directory.

StarDrop_modelserver: This contains the configuration for the installation directory and whether a log file should be maintained for the ADME QSAR server and workers.

StarDrop_p450: This contains the environment configuration for the P450 server and P450 workers, including the ports used and cache directory.

StarDrop_amg: This contains the environment configuration for the Auto-Modeller server and workers, including the ports used.

StarDrop_sls: This contains the environment configuration for the StarDrop License server, including the port used.

One additional configuration file per server and worker is used for process specific settings.

5 Uninstalling

This section describes how to uninstall individual servers. Note that you do not need to uninstall individual servers before running the installer. The installer will automatically uninstall any existing installations as required.

5.1 ADME QSAR Server and Workers

The uninstall script will:

- Stop any running services
- Remove the services and any auto-start entries
- Remove all installed files

When uninstalling the ADME QSAR server model files stored in the 'models' directory will be preserved by being copied to /tmp. A prompt will also ask about preserving the ADME QSAR cache. Subsequent installation will reinstate these model files and any preserved cache.

To uninstall the ADME QSAR server and workers the following steps must be performed:

1. Login as root or using an account with sudo privileges
2. Untar the bundle

   tar xvf StarDrop-7.0-servers-installer.tar

3. Change to installer directory

   cd servers_installer

4. Run the uninstall script:

   python uninstall_modelserver.py

5. Answer the necessary questions.

5.2 P450 Server and Workers

The uninstall script will:

- Stop any running services
- Remove the services and any auto-start entries
- Remove all installed files

When uninstalling the P450 server a prompt will ask whether or not to preserve the cache of previously run molecules. The cache will be copied to /tmp/P450. The cache is stored in an encrypted form and the results saved here can only be accessed by running the P450 server and using the StarDrop client.

To uninstall the P450 server and workers the following steps must be performed:

1. Login as root or using an account with sudo privileges
2. Untar the bundle

   tar xvf StarDrop-7.0-servers-installer.tar

3. Change to installer directory

   cd servers_installer

4. Run the uninstall script:

   python uninstall_p450.py

5. Answer the necessary questions.

5.3 Auto-Modeller Server and Workers

The uninstall script will:

- Stop any running services
- Remove the services and any auto-start entries
- Remove all installed files

When uninstalling the Auto-Modeller server a prompt will ask whether or not to preserve the cache of previously run sessions. The cache will be copied to /tmp/AMG. The cached sessions can then be accessed if the server is reinstalled by copying them to the var/cache/AMG folder in the install directory.

To uninstall the Auto-Modeller server and workers the following steps must be performed:

1. Login as root or using an account with sudo privileges
2. Untar the bundle

   tar xvf StarDrop-7.0-servers-installer.tar

3. Change to installer directory

   cd servers_installer

4. Run the uninstall script:

   python uninstall_amg.py

5. Answer the necessary questions.

5.4 License Server

The uninstall script will:

- Stop any running services
- Remove the services and any auto-start entries
- Remove all installed files

When uninstalling, the license configuration file sls.conf will be backed-up to /tmp.

To uninstall the StarDrop License server the following steps must be performed:

1. Login as root or using an account with sudo privileges
2. Untar the bundle

   tar xvf StarDrop-7.0-servers-installer.tar

3. Change to installer directory

   cd servers_installer

4. Run the uninstall script:

python uninstall_sls.py

5. Answer the necessary questions.

5.5 Derek Nexus Web Service

The Derek Nexus web service can be removed by stopping the web server and deleting the Derek Nexus web service files.

1. If the web server is Apache Tomcat server described in the installation steps (Section 3.4) then this can be stopped using the command:

   service tomcat stop

2. To remove the Derek Nexus web service files, navigate to the Apache Tomcat installation (from installation steps this will be in /opt/stardrop/tomcat)
3. Delete the folder named **derek**
4. In the **webapps** folder, delete the folder name **derekwebservice** and the file **derekwebservice.war**

5.6 StarDrop Client

The StarDrop client can be uninstalled by opening the 'Control Panel' and going to the 'Add or Remove Programs' section or selecting ‘Uninstall a program’.

5.7 Legacy Servers

The ADME QSAR uninstall process will also remove any previous model running servers shipped with earlier versions of StarDrop.

6 Non-root Access to StarDrop Servers

If you wish to configure the StarDrop servers that you have installed to be manageable by a user other than root, you should complete the following steps. In this example, the user ‘sys_stardrop’ is a non-root user given access to control the servers and access their logs.

1. Stop the StarDrop servers.

   /sbin/service StarDrop_modelserver stop

   /sbin/service StarDrop_p450 stop

   /sbin/service StarDrop_amg stop

   /sbin/service StarDrop_sls stop

2. Use the *chown* command to change the owner associated with all the StarDrop files in the following directories (replacing sys_stardrop with the appropriate user):

   a. /usr/local/StarDrop64

   cd /usr/local/StarDrop64
   *chown -R sys_stardrop: **

   b. /etc/init.d

   cd /etc/init.d
   *chown -R sys_stardrop: StarDrop_**

   c. /etc/sysconfig

cd /etc/sysconfig
*chown -R sys_stardrop: StarDrop_**

3. Login using the credentials for the user
4. Start the servers

   /sbin/service StarDrop_modelserver start

   /sbin/service StarDrop_p450 start

   /sbin/service StarDrop_amg start

   /sbin/service StarDrop_sls start

5. The user now has access to start and stop the servers, and can access log files (e.g. /usr/local/StarDrop64/modelserver/var/log)

7 ADME QSAR Server Management

To install additional models on the server, model files (with extension '.aim') and python plugin modules ('.py') must be copied to the models installation directory (usually /usr/local/StarDrop64/modelserver/models/aim or /usr/local/StarDrop64/modelserver/models/py) by the server administrator, after which the server should be restarted.

8 Troubleshooting

This section provides some simple troubleshooting suggestions should any of the following problems occur. If these steps do not solve the problem, or should you experience any other difficulties with this software, please contact stardrop-support@optibrium.com.

8.1 ADME QSAR Server

8.1.1 Client shows 'Failure' when testing server settings from the 'Models' tab in the preferences dialogue

Please note: In many cases it is not necessary to use the ADME QSAR model server because the client software can calculate models 'locally'. As such, please make sure that a server has been installed for use before attempting to connect. Should a server be available on the network and this error occur then:

- Check that the IP address/name of the server is correct in the Models tab in the Preferences dialogue. This should be the server DNS name or IP address, not a URL.
- Check that the port number associated with the server is correct.
- Check that the server name is recognised by the client machine and that the DNS settings are correct by using the command:

  nslookup <server name>

  At a command prompt where <server name> is replaced by the name of the server.

- Run the server tests described in section 3.5. If these are successful, restart the server process:

  /sbin/service StarDrop_modelserver restart

- Check the log files
  - model_server.log (default installation directory is /usr/local/StarDrop64/modelserver/var/log),
  - /tmp/StarDrop_model_server.stdout,
  - /tmp/StarDrop_model_server.stderr,
  - /tmp/StarDrop_pKa_worker<number>.stdout

- and /tmp/StarDrop_pKa_worker<number>.stderr

for any error messages and contact stardrop-support@optibrium.com if required.

8.1.2 ADME QSAR model results are never returned

If the StarDrop client shows a 'Success' message when testing the server settings in the Models tab of the Preferences dialogue, yet no results are returned, there is probably a problem with communication between the ADME QSAR server and worker processes.

- On the ADME QSAR server run the server tests described in section 3.5.
- Check that the server can resolve the IP addresses for the worker machines and vice versa. If not, correct the DNS settings.
- Check the log file model_server.log (default installation directory is /usr/local/StarDrop64/modelserver/var/log) on the failed ADME QSAR server. Ensure that the name and port numbers for the worker processes are correct. If not, correct these in /etc/sysconfig/StarDropModelServer_conf.py.
- Check the log file model_worker_9001.log (default installation directory is /usr/local/StarDrop64/ modelserver /var/log and the name of the file depends upon the port number) on the failed ADME QSAR worker. Ensure that the name and port number for the ADME QSAR server is correct. If not, correct this in /etc/sysconfig/StarDropModelWorker*_conf.py.
- After each step, restart the ADME QSAR worker processes before retesting by executing:

  /sbin/service StarDrop_modelserver restart

8.2 P450 Server

8.2.1 Client shows 'Failure' when testing server settings from 'P450' tab in the preferences dialogue or P450 panel shows 'Server Unavailable'

This is probably due to an inability of the client to connect to the P450 server.

- Check that the address of the server is correct in the Name field of the P450 tab in the Preferences dialogue. This should be the server DNS name or IP address, not a URL.
- Check that the port number of the server is correct in the Port field of the P450 tab in the Preferences dialogue.
- Check that the server name is recognised by the client machine and that the DNS settings are correct. From a command prompt try:

  telnet <P450 server name> 8050

- This should connect to the P450 server. Entering any text followed by <Enter> should return an error message in XML format.
- Check that the P450 server is running on the designated server. If not, run the following command:

  /sbin/service StarDrop_p450 start

- If the server is running, try restarting the server:

  /sbin/service StarDrop_p450 restart

- Check the log files in
  - var/log/p450.log (by default this is in /usr/local/StarDrop64/p450),
  - /tmp/StarDrop_p450.stdout,
  - /tmp/StarDrop_p450.stderr,
  - /tmp/StarDrop_p450_worker<number>.stdout
  - and /tmp/StarDrop_p450_worker<number>.stderr

  for any error messages.

8.2.2 P450 metabolism model results are never returned

If the StarDrop client shows a 'Success' message when testing the server settings in the P450 tab of the Preferences dialogue, yet no results are returned, this is probably due to a problem with communication between the P450 server and worker processes. Remember that the P450 models take a couple of minutes to run and, for larger molecules, may take even longer.

- Check if the models are running on one or more of the P450 workers. The command 'top' should show one or more 'mopac7' processes running on at least one of the workers. If this is the case, wait. If no mopac7 processes are running and the results still haven't been returned, try the next test.
- Check that the URIs of the P450 workers are correct in /etc/sysconfig/StarDropP450Server_conf.py on the P450 server machine. If not, correct and restart the P450 server by using the command:

  /sbin/service StarDrop_p450 restart

- Check that the machine names in the URIs for the P450 workers can be resolved correctly on the P450 server machine. Try:

  telnet <P450 worker name> <worker port>

  where <P450 worker name> is the name of a P450 worker machine and <worker port> is one of the configured ports, e.g. 8051. Entering any text should result in an error being returned in XML format.
- Check that the P450 worker processes are executing on the P450 worker machines. The results of the command 'ps aux' should include lines containing commands of the form

  <path>/StarDropP450Worker.py 8051

  where the path to StarDropP450Worker may vary due to the configuration options chosen during installation (by default it is /usr/local/StarDrop64/p450/bin) or be absent on some operating systems.
- If these lines are not present, start the P450 worker processes using the command:

  /sbin/service StarDrop_p450 start

- Try restarting the P450 server and P450 worker processes on the P450 server and P450 worker machines:

  /sbin/service StarDrop_p450 restart

- Check the P450 server and worker logs in var/log/p450.log (by default this is in /usr/local/StarDrop64/p450) on all P450 server and P450 worker machines for error messages.

8.2.3 An error occurred due to a software problem for a P450 calculation and now resubmitting that compound always returns 'Error'

The P450 models can occasionally return an error for a molecule due to a genuine failure of the quantum mechanical calculation in MOPAC. In these cases, many approaches to calculating the results have been attempted and all alternatives exhausted. For this reason, 'Error' results are stored in the cache to avoid repeated recalculation of an intractable compound. However, if an error occurs due to a software or configuration error, this will also be cached, resulting in an error being returned every time the compound is submitted.

This can be overcome by ticking the Force re-run of submitted molecules checkbox in the P450 tab of the Preferences dialogue in StarDrop and resubmitting the compound. This will re-run the compound and overwrite the cached error result.

8.3 Auto-Modeller Server

8.3.1 Client shows 'Failure' when testing server settings from the 'Auto-Modeller' tab in the preferences dialogue

- Check that the address of the server is correct in the Name field of the Auto-Modeller tab in the Preferences dialogue. This should be the server DNS name or IP address, not a URL.

- Check that the port number of the server is correct in the Port field of the Preferences dialogue.
- Check that the server name is recognised by the client machine and that the DNS settings are correct. At a command prompt try:

  telnet <Auto-Modeller server name> 9050

  This should connect to the Auto-Modeller server. Entering any text followed by <Enter> should return an error message in XML format.
- Check that the Auto-Modeller server is running on the designated server. If not, execute

  /sbin/service StarDrop_amg start

- If the server is running, try restarting the server:

  /sbin/service StarDrop_amg restart

- Check the log files in
  - var/log/amg.log (by default this is in /usr/local/StarDrop64/amg),
  - /tmp/StarDrop_amg.stdout
  - /tmp/StarDrop_amg.stderr,
  - /tmp/StarDrop_amg_worker<number>.stdout
  - and /tmp/StarDrop_amg_worker<number>.stderr

  for any error messages and contact stardrop-support@optibrium.com if required.

8.3.2 Auto-Modeller does not build any models

If the StarDrop client shows a 'Success' message when testing the server settings in the 'Auto-Modeller' tab of the Preferences dialogue, yet no models are built, this is probably a problem with communication between the Auto-Modeller server and the worker processes, or with multiple model generation sessions being queued on the server.

- Check that the server can resolve the IP addresses for the worker machines and vice versa. If not, correct the DNS settings.
- Run the amg_testserver.pyc command from the bin directory (default: /usr/local/StarDrop64/amg/bin) to determine whether the server is running the sessions, and the status of the worker processes. If all workers are busy, wait for them to complete. If all workers are offline, restart the server:

  /sbin/service StarDrop_amg restart

- Check the log file amg.log (default installation directory is /usr/local/StarDrop64/amg/var/log) on the failed Auto-Modeller server. Ensure that the name and port numbers for the worker processes are correct. If not, correct these in /etc/sysconfig/StarDropAMGServer_conf.py.
- Check the log file StarDrop_amg_worker*.log (default installation directory is /usr/local/StarDrop64/amg/var/log) on the failed Auto-Modeller worker. Ensure that the name and port number for the Auto-Modeller server is correct. If not, correct these in /etc/sysconfig/StarDropAMGWorker*_conf.py.
- After each of steps 2-3, restart the Auto-Modeller server and worker processes before retesting by executing:

  /sbin/service StarDrop_amg restart

8.4 License Server

8.4.1 Client reports that it is unable to obtain a license from the StarDrop License server

- Check that the name and port number for the server are correct in the Preferences dialogue.
- Verify that the server is running on the specified machine. On the server:

  cd /usr/local/StarDrop64/sls/bin

./CheckServer

and confirm that the server has the requested license available.

- Check the log files in
  - /tmp/StarDrop_sls.stdout
  - and /tmp/StarDrop_sls.stderr

for any error messages and contact stardrop-support@optibrium.com if required.

8.4.2 Releasing a locked license

There are three options for unlocking a license (all require access to the license server).

- Wait for the license to time out

The default timeout is 1 hour but this can be configured during installation. The minimum timeout is 0.25 (15 minutes). The timeout is stored in /etc/sysconfig/StarDropLicenseServer_conf.py.

- Restart the license server

/etc/init.d/StarDrop_sls restart

- Run the sls_cleanup.pyc script: (The example below assumes the default installation path)

cd /usr/local/StarDrop64/sls/bin

export LD_LIBRARY_PATH=/usr/local/StarDrop64/pycompat/lib:/usr/local/StarDrop64/lib

/usr/local/StarDrop64/pycompat/bin/python sls_cleanup.pyc

This will show the following information providing the option to log users off

There are 1 users currently logged in

Users:

Log nNQAJwAIUsername off? (y/n)y

nNQAJwAIUsername logged off

Any of these will result in that license session no longer being active enabling other users to use that license.

8.5 Derek Nexus Web Service

8.5.1 Log files

Multiple log files are generated by the Derek Nexus web service and can be useful when trouble-shooting problems.

Assuming that the Derek Nexus web service has been installed in the default location (/opt/stardrop), then logs can be found in the following locations:

/opt/stardrop/tomcat/derek/logs
/opt/stardrop/tomcat/logs (the catalina logs within here are often the most useful)

In addition, recent calculation results are stored in XML files located in:

/opt/stardrop/tomcat/derek/

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