Installing ADMET Predictor on Linux OS

Prerequisites:

1. A 64-bit Linux workstation with standard user accounts.
2. A running Reprise License Server or valid license file. Please check with your IT department for guidance.

Before starting the installation, contact your IT department regarding the ADMET Predictor licensing requirements. The instructions below assume that you already have either a running Reprise License Server (local, network or cloud) or a valid license file.

Step 1. Obtain an installer file appropriate for your operating system. For example, on Ubuntu 24 you would obtain the file ADMET_Predictor_v13_ub24.tar.gz. If your operating system is not found, choose the one you think is the closest match.

Step 2. Select/create a directory where the ADMET Predictor files will reside. For example, it may be a user's home directory (for single user) or a global directory accessible to each authorized user.

Step 3. Using the terminal window unzip and extract the contents of the installer file. For example use: tar -xzf ADMET_Predictor_v13_rhel8.tar.gz. Note that the extracted folder name will have the form ADMET_Predictor_v13_xyz, where xyz denotes the operating system (e.g., ub24 or rhel8). In the steps below we simply refer to this folder as ADMET_Predictor_v13.

Step 4. **Make sure that all authorized users have "write" permissions to the ADMET_Predictor_v13 directory**. The program needs to periodically update the model databases "ModelProperties.inp" and "TooltipsAndFormats.inp", as well as create and update error logs.

Step 5. Modify the "RunAP.sh" shell script found in the ADMET_Predictor_v13 directory. The two variables ADMET_PREDICTOR_PATH and SIMPLUS_LICENSE_FILE need to be modified according to the commented instructions contained in the script.

Step 6. Perform the following test run inside the ADMET_Predictor_v13 directory:

```
$ ./RunAP.sh -t QMD Demo2D.qmd
```
Make sure the "-t" uses a regular (ASCII) hyphen character. Observe the standard output, examine the output file "Demo2D.dat", and the contents of "ADMET_Predictor_Errors.log." Please see the Command Line section of the ADMET Predictor manual for details about all valid command-line arguments.

Remarks:

1. There are two separate ADMET Predictor binaries: ADMET_Predictor and ADMET_Predictor_qt. The second one links with Qt libraries provided in a directory called "lib"; this version is required if you want the functionality to create image files

(e.g., images of pKa microstates, metabolite trees, etc.). The RunAP.sh script invokes the binary ADMET_Predictor by default; you must modify the last line in this file if you wish to use ADMET_Predictor_qt.

2. The Qt-enabled version may require the installation of dependencies. On Debian (Ubuntu) you will likely need the packages libgl1, libegl1, libfontconfig1 and libxkbcommon0. On Fedora (Red Hat) you will likely need the packages mesa-libGL, mesa-libEGL, fontconfig and libxkbcommon.
3. Clients should always use the RunAP.sh script to execute the program. This is important for setting required environment variables. The script accepts the same options as described in the manual.
4. ADMET Predictor can be incorporated into Pipeline Pilot and KNIME workflows in the Linux environment. Pipeline Pilot components and subprotocols are included in the "ADMET Predictor component for Pipeline Pilot.zip" archive. The KNIME node is named ADMET_Predictor.knwf.

ADMET Predictor Service

The ADMET Predictor Service (REST API) is described in the manual entitled ADMETPredictorService.pdf. If you would like to run the service on Linux, please follow the steps below. We strongly recommend that before running the service you first complete a successful run of ADMET Predictor from the command line, as described earlier. This will ensure that licensing requirements have been satisfied.

Step 1. Modify the unit file ADMETPredictorService.service so that the paths are correct. You will need to replace <admet_predictor_folder> with the path to your ADMET Predictor installation on Linux.
Step 2. Modify the configuration file ADMETPredictorService.cfg. See the ADMET Predictor Service manual for further details.
Step 3. Place the unit file in the folder /etc/systemd/system
Step 4. Start the service using the command:
```
$ systemctl start ADMETPredictorService
```
Step 5. To stop the service, use the command:
```
$ systemctl stop ADMETPredictorService
```

Remarks:

1. There are two separate service binaries: ADMETPredictorService and ADMETPredictorService_qt. These are analogous to the two separate ADMET Predictor binaries described earlier.
2. The binaries above can be run from the command line rather than as a service (daemon). See the API manual for instructions. We recommend that you try this first, because the console output facilitates troubleshooting.