Installing ADMET Predictor on Linux OS

Prerequisites:

1. A 64-bit Linux workstation with standard user accounts.
2. A running Flexera License Server (FLS), either on the corporate intranet, or locally on the workstation itself. Please check with your IT Department first. The FLX Linux programs, *lmcomposite* and *lmgrd*, are included in the installation folder. They are used to generate the composite ID of the computer and to manage the license, respectively on a Linux computer.
3. The Linux machine must have the Linux Standard Base (LSB) Core packages installed. For Ubuntu and similar systems, a command such as "sudo apt-get install lsb-core" would be used to install this package. Other versions of Linux would use analogous commands.

Before starting the installation, contact your IT Department regarding the Flexera License Server. ADMET Predictor will not work without a valid license, thus you must take care of this before anything else.

Step 1. Obtain "ADMET_Predictor_v11.tar.gz" install package from Simulations Plus Inc.
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 "ADMET_Predictor_v11" directory:
```
$ tar –zxvf ADMET_Predictor_v11.tar.gz
```
Make sure that all authorized users also have "write" permissions to this directory. The program needs to periodically update the model databases "ModelProperties.inp" and "TooltipsAndFormats.inp", as well as create and update error logs.
Step 4. Obtain information necessary to create your license file. Change the working directory to ADMET_Predictor_v11 and run the HostID Utility "lmcomposite":
```
$ cd ADMET_Predictor_v11
$ ./lmcomposite
```
Step 5. Copy the output of lmcomposite and e-mail it to licensing@simulations-plus.com (required for license creation).
Step 6. Obtain your license file (License.lic) from email correspondence with licensing@simulations-plus.com.
Step 7. Provide your IT Department or Flexera administrator with the following items and information. This is required to configure the Flexera license server.
   a. License file obtained via e-mail correspondence
   b. The vendor daemon executable ("simplus") located in the ADMET_Predictor_v11 directory
   c. Note: "simplus" should reside in the same directory as Flexera daemon "lmadmin" or "lmgrd".
   d. Note: the license sever is usually started using the command "./lmgrd -c <full_path_to_license_file>"
Step 8. Modify the "RunAP.sh" shell script found in the ADMET_Predictor_v11 directory. The following two variables ADMET_PREDICTOR_PATH and SIMPLUS_LICENSE_FILE need to be modified according to the commented instructions contained in the script. For enhanced security, you may move both the shell script "RunAP.sh" and the executable file, "ADMET_Predictor", to another read-only directory (e.g., /usr/local/bin). Make sure that the PATH variable for all users contains this location.
Step 9. Once the license is active, perform the following test run inside the ADMET_Predictor_v11 directory:

```
$ ./RunAP.sh –t QMD –d 2D Demo2D.qmd
```
> Observe the standard output, examine the output file "Demo2D.dat", and the contents of "ADMET_Predictor_Errors.log." Please call Simulations Plus at (661) 723-7723 if unable to determine the cause of any errors.

Remarks:

1. You may need to install one or more dependencies in order for ADMET Predictor to run successfully. The dependencies include the following: libstdc++6 and g++-11. If installing these dependencies is not possible, you can try running the statically-linked version of ADMET Predictor (ADMET_Predictor_static), which has these dependencies built in. Simply modify the RunAP.sh file to call ADMET_Predictor_static rather than ADMET_Predictor.
2. It is possible to run ADMET Predictor inside of a docker container. This approach allows you to install the various dependencies without interfering with the main system. Note that you should always use the dynamic version of ADMET Predictor when running inside of a docker container (see Remark 1 above).
3. The Linux version of ADMET Predictor is limited to batch mode runs from the command line with the results output as a tab-delimited file *.dat or other machine-readable formats. Consult the section titled "*Command Line*" in the ADMET Predictor manual for details. The "RunAP.sh –h" command displays the command line options.
4. The Linux version does not have the functionality to generate 2D atomic coordinates. Thus, RDF and SDF outputs may have all atomic coordinates equal to zero. The exceptions are Bayer workflows (option –w) generated using SDF input: in this case the input coordinates are passed into the output file.
5. Users should always use the RunAP.sh script to execute the program rather than the ADMET_Predictor executable. The script accepts the same options as described in the Manual and Tutorial.
6. ADMET Predictor can be incorporated into Pipeline Pilot workflows in the Linux environment. Pipeline Pilot components and subprotocols are included in the "ADMET Predictor component for Pipeline Pilot.zip" archive.

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, you should follow the following steps:

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. You may need to install the dependency libssl1.1 in order for the service to run successfully. If installing this dependency is not possible, you can try running the statically-linked version, called ADMETPredictorService_static, which has the dependency built in.