

# 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\_v102.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\_v102” directory:

```
$ tar -zxvf ADMET_Predictor_v102.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 “ADMET\_Predictor\_Errors.log” and “Troubled\_SMILES.txt”.

Step 4. Obtain information necessary to create your license file. Change the working directory to ADMET\_Predictor\_v102 and run the HostID Utility “lmcomposite”:

```
$ cd ADMET_Predictor_v102
```

```
$ ./lmcomposite
```

Step 5. Copy the output of *lmcomposite* and e-mail it to [licensing@simulations-plus.com](mailto:licensing@simulations-plus.com) (required for license creation).

Step 6. Obtain your license file (License.lic) from email correspondence with [licensing@simulations-plus.com](mailto: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\_v102 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\_v102 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\_v102 directory:

```
$ ./RunAP.sh -t QMD -d 2D Demo2D.qmd
```

Observe the standard output, examine the output file “Demo2D.dat”, contents of “ADMET\_Predictor\_Errors.log” and “Troubled\_SMILES.txt.” Please call Simulations Plus at (661) 723-7723 if unable to determine the cause of any errors.

**Remarks:**

1. 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.
2. The Linux version does not have a capacity of generating 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.
3. 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.
4. 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.