**S.1.: SEBOS installation Instructions:**

Steps of acquiring the prerequisites for a clean installation using the install\_molpher.sh script :

conda , gcc , g++ ,cmake , molpher, linux/wsl.

Creates a conda environment with all module prerequisites.

* **Step 1 :** Install miniconda :

$wget <https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh>

$bash Miniconda3-latest-Linux-x86\_64.sh

Activate conda :

$~/miniconda3/bin/conda init

$source ~/.bashrc

* **Step 2 :** Check/install for C and C++ compilers and cmake .
* xtract and Navigate to the SEBOS directory.
* **Step 4. :** Download and compile molpher python module library. create a conda envaroment that access the library :

$./install\_molpher.sh

Add the following envaromental variable to your ~/.bashrc or ~/.zshrc as instructed by the script.

Example (replace xxx and yyy based on your installation)

export LD\_LIBRARY\_PATH=/xxx/molpher-lib/dist/lib/:/yyy/miniconda3/envs/molpher-lib-build/lib/

export PYTHONPATH=/xxx/molpher-lib/dist/lib/python3.9/site-packages/mol:/xxx/molpher-lib/dist/lib/python3.9/site-packagesmolpher-0.0.0b4.dev1-py3.9-linux-x86\_64.egg

Activate the molpher environment

$conda activate molpher-lib-build

Copy Source files to a running directory :

* Run SEBOS python code:

$python SEBOS.py

Note please be sure that the LD\_LIBRARY\_PATH and PYTHONPATH envaromental variables is set correctly. Those are set during initial setup but have to be manualy added in .bashrc of set at every terminal. You can use the set\_env.sh script to add the appropriate PYTHONPATH environment variable . You can use either the comments

$. set\_env.sh

or

$ source set\_env.sh

* Use an interactive environment to View and analyses results at a Post process stage:

$jupyter-notebook inter\_graph.ipynb

Note : The necessary postprocess files can be found in the directory postpros/

In no browser has been installed use localhost:8888

Select to open the inter\_graph.ipynb file , and run using shift+enter on the cell with the code:

Use Cytoscape and the additional futures provided in the ipynb file to analyze the resulting network.

* How to remove the environment (xxx the path used to install the molpher library during step 4):

$conda env remove --name molpher-lib-build

$rm -rf /xxx/molpher-lib/

jupyter-notebook inter\_graph.ipynb

**SEBOS installation Instructions including Autodock vina support:**

Run build\_all.sh,instead oftheinstall\_molpher.sh that runs as part of the build\_all.sh **(and press Enter / select yes in the prompts. )**

**$** **./build\_all.sh**

**This will automatically create 3 conda environments including the** molpher-lib-build , download all necessary files and create an executable Vina\_doc (using pyinstaller) that has to be pleased in the working directory where the python code runs.

**Copy the Vina\_dock executable to your working directory.**

**List of the conda environments created during the installation process :**

**Remove environments :**

$conda env remove --name mgltools\_env

$conda env remove --namevina\_env

$conda env remove --name molpher-lib-build

manually delete the molpher-lib directory : $rm -rf /xxx/molpher-lib/

remove/reset environmental variables in the .bashrc (if manual changes have been made)

**Note :** An optional step in the workflow involves using PyInstaller to create standalone executables. PyInstaller itself is licensed under the GNU General Public License v2 (GPLv2).

🔹 No PyInstaller-generated binaries are distributed as part of this project.

🔹 Users are responsible for generating executables locally using their own PyInstaller installation.

If you choose to create and redistribute executables produced with PyInstaller, you must ensure that you comply with the terms of the GPLv2 license for any such distributed binaries.