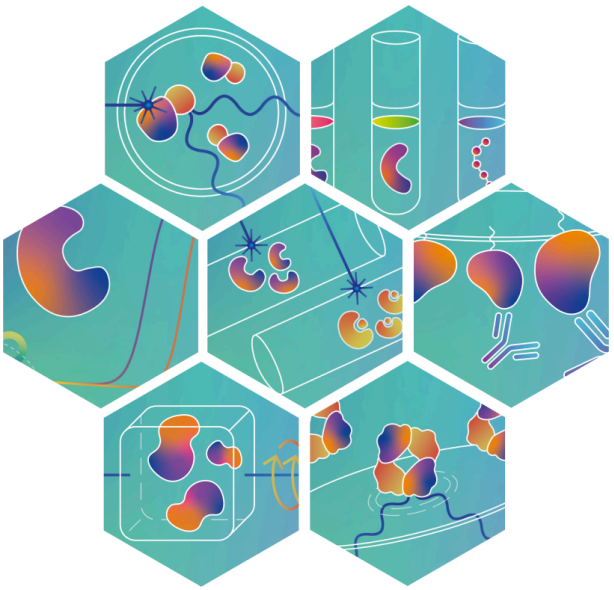
Running the eSPC tools on Linux

February 2026



1. Install the Docker Engine

a. Go to the official Docker website: https://docs.docker.com/engine/install/ubuntu/
b. Follow the instructions and install the Docker engine
c. Verify that it works by running this command in the **Terminal**:

   $ sudo docker run hello-world

2. Pull the docker image and run it

a. Open a **Terminal** and run:

   i. For **ThermoAffinity**:

```
$ docker pull emblspc/thermoaffinity_espc:1.0
$ docker run -p 3838:3838 emblspc/thermoaffinity_espc:1.0
```

ii. For **MoltenProt**:

```
$ docker pull emblspc/moltenprot_espc:1.1
$ docker run -p 3838:3838 emblspc/moltenprot_espc:1.1
```

iii. For **FoldAffinity**:

```
$ docker pull emblspc/foldaffinity_espc:1.0
$ docker run -p 3838:3838 emblspc/foldaffinity_espc:1.0
```

iv. For **ChiraKit**:

```
$ docker pull emblspc/chirakit_espc:1.0
$ docker run -p 3838:3838 emblspc/chirakit_espc:1.0
```

v. For **PhotoMol**:

```
$ docker pull emblspc/photomol_espc:2.0
$ docker run -p 3838:3838 emblspc/photomol_espc:2.0
```

vi. For **KinGenie**:

```
$ docker pull emblspc/kingenie_espc:1.0
$ docker run -p 3838:3838 emblspc/kingenie_espc:1.0
```

vii. For **Raynals**:

```
$ docker pull emblspc/raynals_espc:1.0
$ docker run -p 3838:3838 emblspc/raynals_espc:1.0
```

3. Open the tool

a. Open any Browser and go to http://0.0.0.0:3838/

Congratulations! The tool should be open and ready for use.