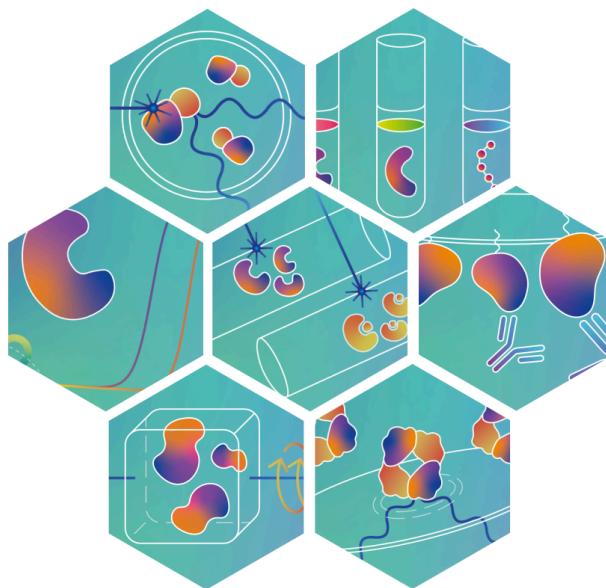

Running the eSPC tools on Linux

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.

Raynals

1. Load input

2. Analysis

3. Export

Simulation

User guide

About

Input

1. DLS files

Browse... No file selected

Set experiment parameters ☒

Select experiment test Remove

Condition	Include	Read	
carbonic anhydrase A1 12:02:17	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1
carbonic anhydrase A2 12:05:51	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1

Experiment parameters

Preprocessing

☒ (Un)select all ☐ Update

Filter by initial value 1

BQ filter

Tolerance 1.2

Time limit (µs) 100

Group by None