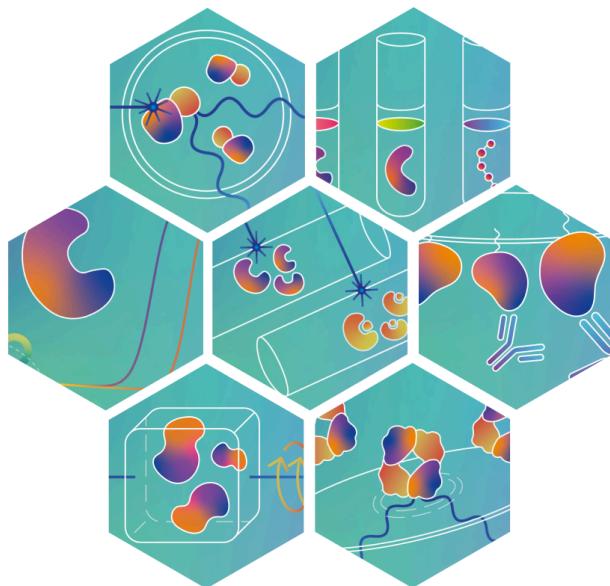


# Running the eSPC tools on Linux

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
```

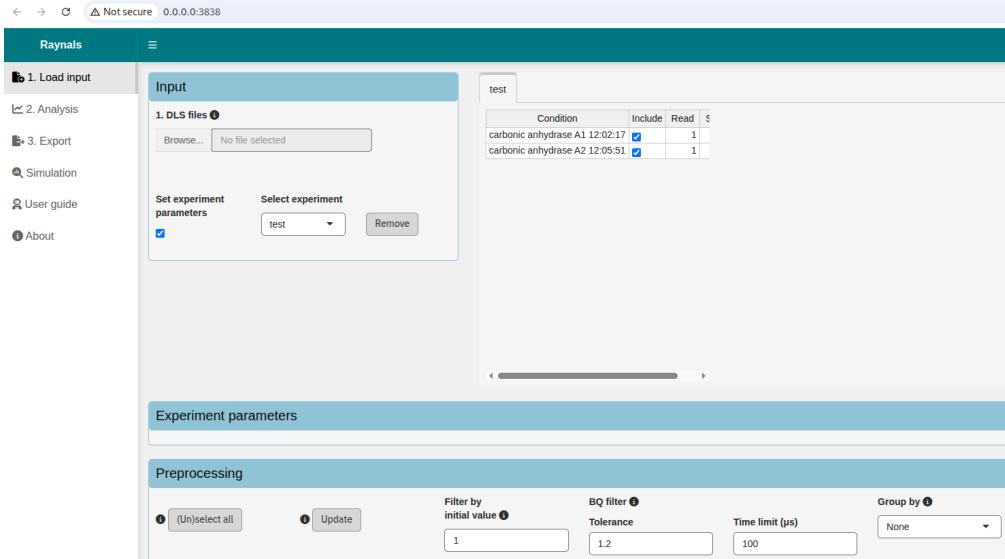
vii. For **Raynals**:

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

### 3. Open the tool

- Open any Browser and go to <http://0.0.0.0:3838/>

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



The screenshot shows the Raynals web application interface. The left sidebar contains navigation links: Raynals (selected), Load input, Analysis, Export, Simulation, User guide, and About. The main area has two main sections: Input and Preprocessing.

**Input Section:**

- 1. DLS files: A table with one row labeled "test".

Condition	Include	Read	S
carbonic anhydrase A1 12:02:17	<input checked="" type="checkbox"/>	1	
carbonic anhydrase A2 12:05:51	<input checked="" type="checkbox"/>	1	
- Set experiment parameters: A dropdown menu set to "test" and a "Remove" button.

**Experiment parameters:** A section with a "test" button and a "Remove" button.

**Preprocessing Section:**

- Buttons: "(Un)select all", "Update".
- Filter by initial value: A dropdown menu set to "1".
- BQ filter: Tolerance set to "1.2".
- Time limit (μs): Set to "100".
- Group by: A dropdown menu set to "None".