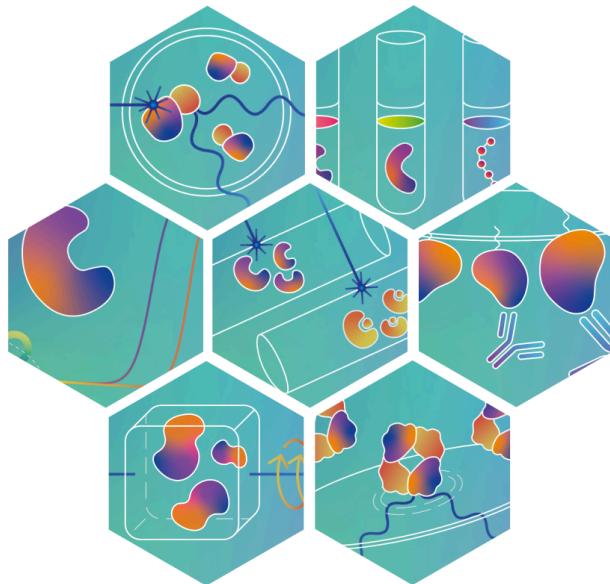


Running the eSPC tools on macOS

February 2026



To run the eSPC tools on macOS there are two alternatives:

- a) To use Docker Desktop
- b) To use Colima and the Docker Engine

The best option depends on the required license. As of Feb. 2026, Docker Desktop is free for: Small businesses (fewer than 250 employees AND less than \$10 million in annual revenue); Personal use; Education; Non-commercial open source projects. On the other hand, the Docker Engine is open-source software licensed under the Apache License, Version 2.0, making it free to use, modify, and distribute for any purpose, including commercial use.

Option A

1. Download Docker Desktop

- a. Go to the official Docker website:
<https://www.docker.com/products/docker-desktop/>
- b. Click **Download for Mac**
- c. Choose the correct version:
 - i. Mac with Apple chip (M1/M2/M3)
 - ii. Mac with Intel chipThe .dmg file will download to your computer.

2. Install Docker Desktop

- a. Open the downloaded .dmg file
- b. Drag the **Docker** icon into the **Applications** folder
- c. Open **Applications** → Double-click **Docker**
- d. Click **Open** if macOS asks for confirmation
- e. Enter your Mac password if prompted (Docker needs privileged access)
- f. Docker will start and the whale icon  will appear in the menu bar.

3. Pull the docker image and run it

- a. Open **Terminal** and run:
 - i. For **ThermoAffinity**:
\$ docker pull emblspc/thermoaffinity_esp:1.0
\$ docker run -p 3838:3838 emblspc/thermoaffinity_esp:1.0
 - ii. For **MoltenProt**:

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

iii. For **FoldAffinity**:

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

iv. For **ChiraKit**:

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

v. For **PhotoMol**:

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

vi. For **KinGenie**:

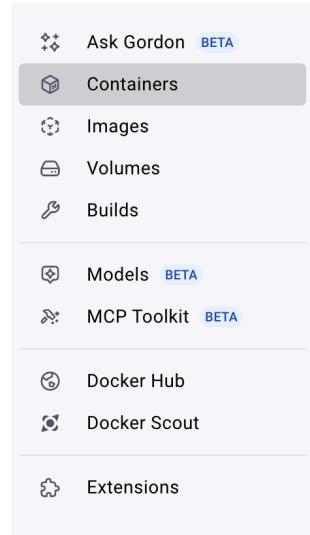
```
$ docker pull emblspc/kingenie_esp:1.0  
$ docker run -p 3838:3838 emblspc/kingenie_esp:1.0
```

vii. For **Raynals**:

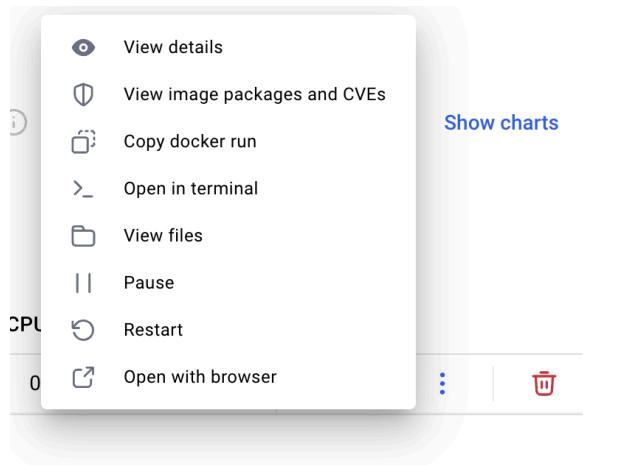
```
$ docker pull emblspc/raynals_esp:1.0  
$ docker run -p 3838:3838 emblspc/raynals_esp:1.0
```

4. Open the tool

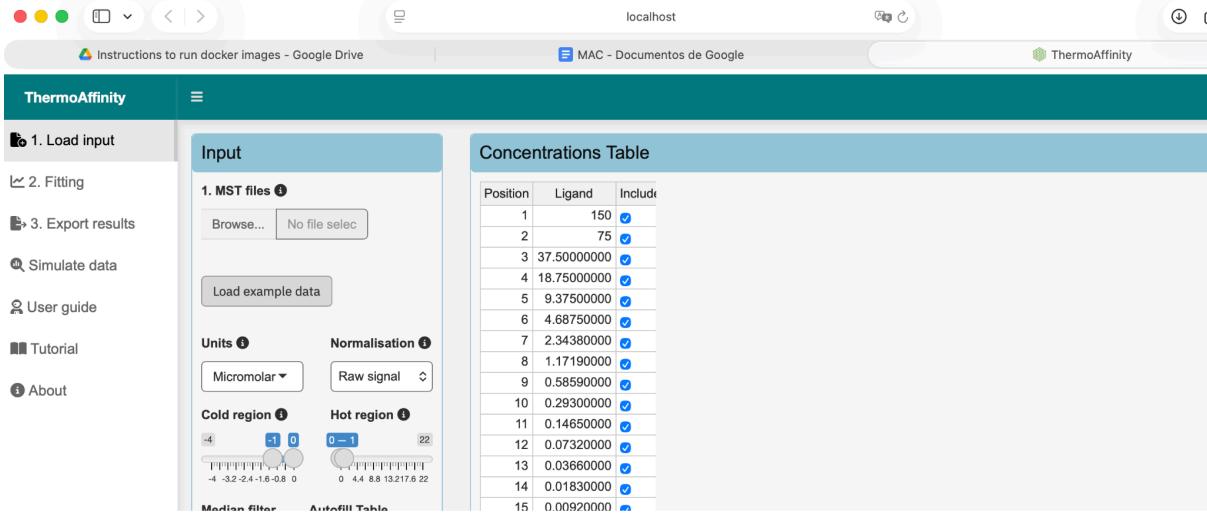
- Open Docker Desktop and navigate to the *Containers* tab



- b. Press on the three dots, right to the square and click on *Open with browser*



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



Option B

1. Install Docker CLI and Colima

- Open **Terminal** and run:


```
$ brew install docker
$ brew install colima
$ colima start
```

2. Pull the docker image and run it

- Open **Terminal** and run:

For **ThermoAffinity**:

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

For **MoltenProt**:

```
$ docker pull emblspc/moltenprot_espc:1.1
```

```
$ docker run -p 3838:3838 emblspc/moltenprot_esp:1.1
```

For FoldAffinity:

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

For ChiraKit:

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

For PhotoMol:

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

For KinGenie:

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

For Raynals:

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

Screenshot of the ThermoAffinity software interface running in a web browser (localhost). The interface is divided into two main sections: 'Input' and 'Concentrations Table'.

Input Section:

- 1. MST files:** A file selection input field showing "No file selected".
- Load example data:** A button to load sample data.
- Units:** Set to "Micromolar".
- Normalisation:** Set to "Raw signal".
- Cold region:** A slider scale from -4 to 22, with a central value of 0 highlighted.
- Hot region:** A slider scale from 0 to 22, with a central value of 13 highlighted.
- Median filter:** A button to apply a median filter to the data.
- Autofill Table:** A button to automatically fill the concentrations table.

Concentrations Table:

Position	Ligand	Includ
1	150	✓
2	75	✓
3	37.50000000	✓
4	18.75000000	✓
5	9.37500000	✓
6	4.68750000	✓
7	2.34380000	✓
8	1.17190000	✓
9	0.58590000	✓
10	0.29300000	✓
11	0.14650000	✓
12	0.07320000	✓
13	0.03660000	✓
14	0.01830000	✓
15	0.00920000	✗