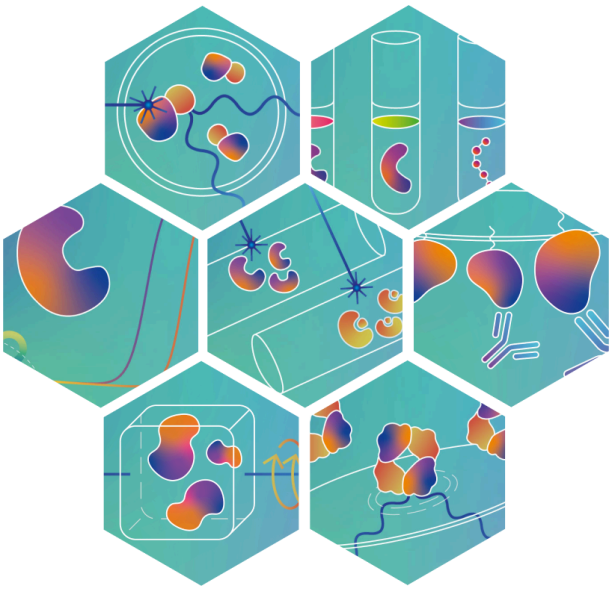
Running the eSPC tools on macOS

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 chip
   The .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_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**:

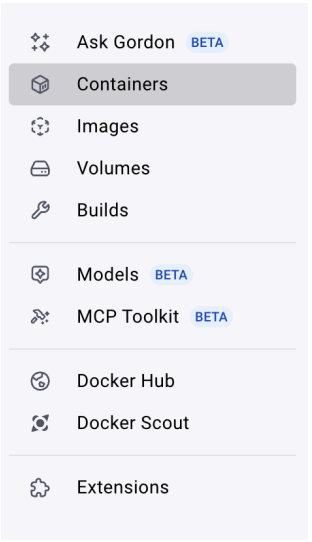
```
$ docker pull emblspc/kingenie_espc:1.0
$ docker run -p 3838:3838 emblspc/kingenie_espc:1.0
```

vii. For **Raynals**:

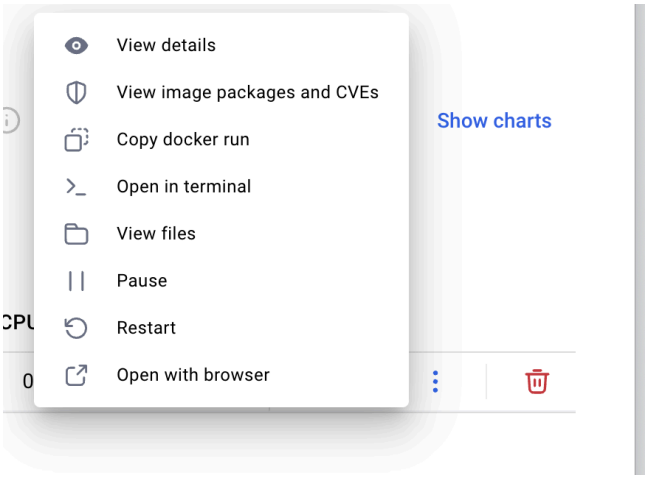
```
$ docker pull emblspc/raynals_espc:1.0
$ docker run -p 3838:3838 emblspc/raynals_espc:1.0
```

4. Open the tool

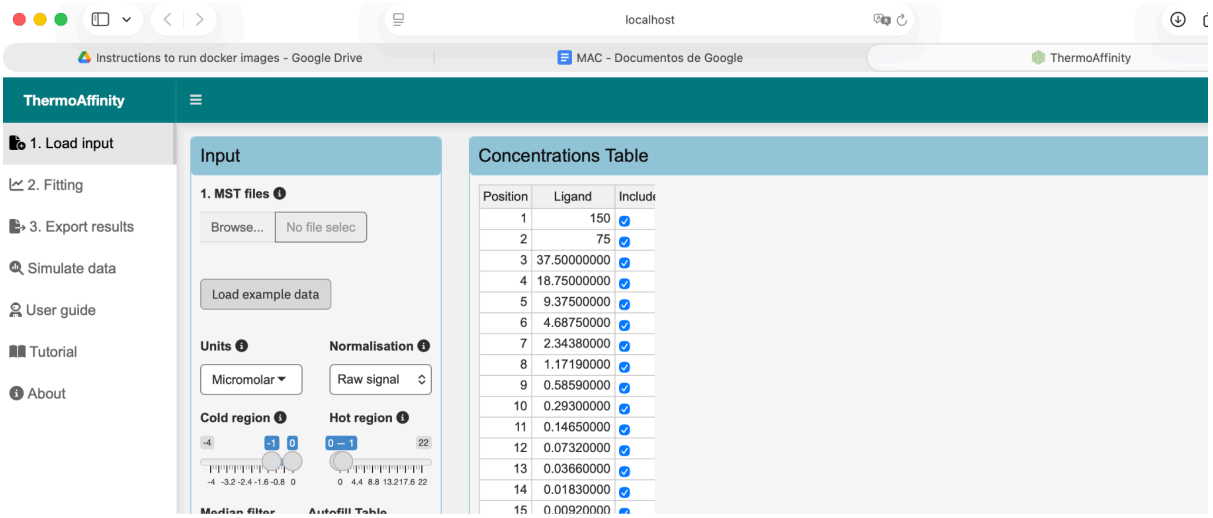
a. Open Docker Desktop and navigate to the *Containers* tab



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

a. Open **Terminal** and run:

$ brew install docker

$ brew install colima

2. Pull the docker image and run it

a. Open **Terminal** and run:

$ colima start

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_espc:1.1

For **FoldAffinity**:
$ docker pull emblspc/foldaffinity_espc:1.0
$ docker run -p 3838:3838 emblspc/foldaffinity_espc:1.0

For **ChiraKit**:
$ docker pull emblspc/chirakit_espc:1.0
$ docker run -p 3838:3838 emblspc/chirakit_espc:1.0

For **PhotoMol**:
$ docker pull emblspc/photomol_espc:2.0
$ docker run -p 3838:3838 emblspc/photomol_espc:2.0

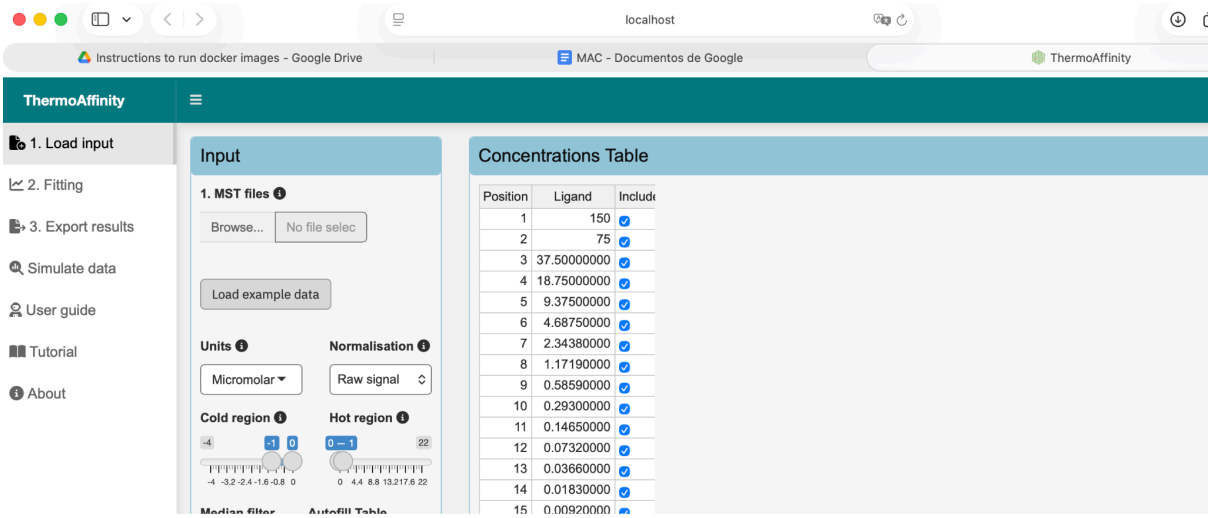
For **KinGenie**:
$ docker pull emblspc/kingenie_espc:1.0
$ docker run -p 3838:3838 emblspc/kingenie_espc:1.0

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.


localhost
Instructions to run docker images - Google Drive
MAC - Documentos de Google
ThermoAffinity
ThermoAffinity
1. Load input
2. Fitting
3. Export results
Simulate data
User guide
Tutorial
About
Input
1. MST files
Browse...
No file selec
Load example data
Units
Micromolar
Normalisation
Raw signal
Cold region
Hot region
Concentrations Table
Position
Ligand
Include
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