Introduction

Spectre is available as a Docker container, thanks to the efforts of Givanna Putri. Docker is a cloud service that allows anyone to deliver software packages as a "complete unit" in a form of container. What this means is that the software package is released as a standalone computing environment, pre-installed with necessary pre-requisite libraries required by the software, and pre-configured for user convenience.

Spectre's Docker image will match the most recent versions of Spectre (denoted as 'master', referring to the master branch in Github). To download this version, simply follow the instructions below. If you wish to load a specific version of Spectre, you can specify a version (e.g. v0.5.3, v0.5.4. etc) instead of using 'master'. You can see a list of versions available via docker on this page.

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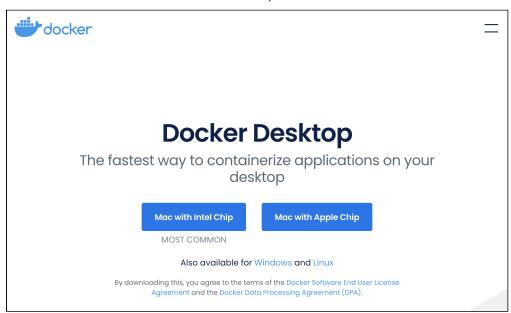
First time using Docker? Download and set up 'Docker Desktop'

Download Docker desktop app

Go to the following address:

i https://www.docker.com/products/docker-desktop

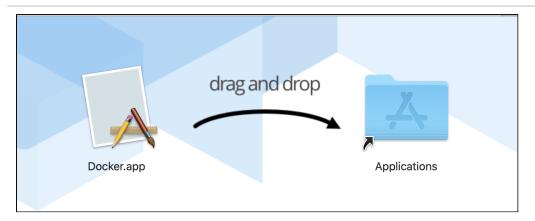
Download the correct version of Docker Desktop.



Go to your downloads folder and open the '.dmg' file.



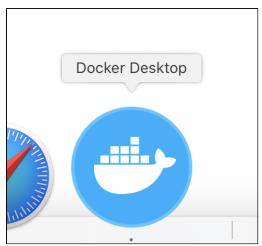
When the following window opens, drag and drop the 'Docker.app' icon into the 'Applications' shortcut.



You should now be able to find 'Docker' in your applications folder.

Set some preferences (optional)

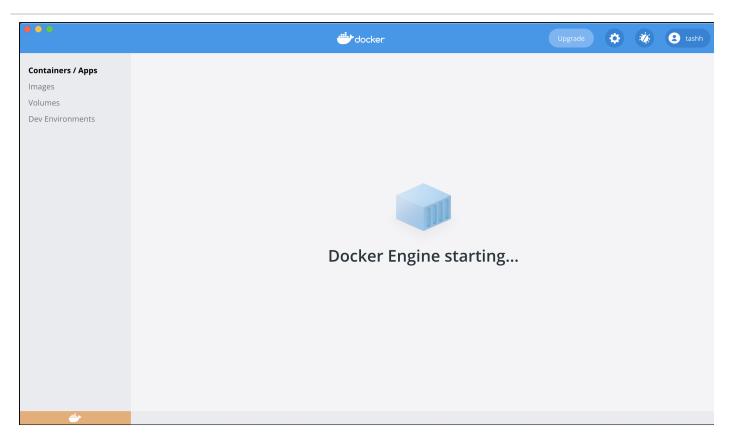
Open Docker app from the applications folder or bar at the bottom of the screen.



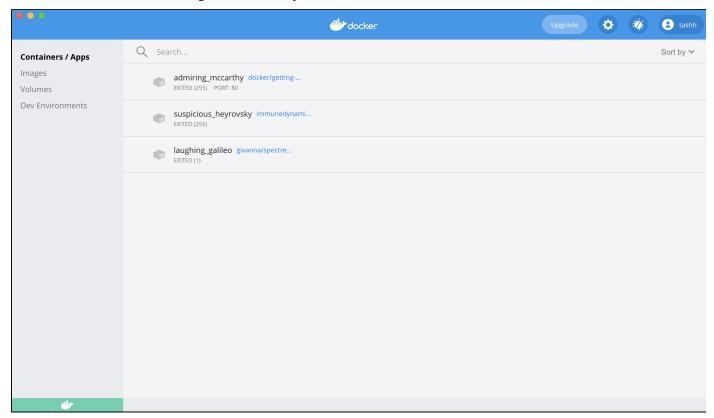
Once you turn it on, you should see the following icon in the bar at the top of the screen.



Additionally the program itself should open. Wait a few moments while the 'Docker Engine' starts.

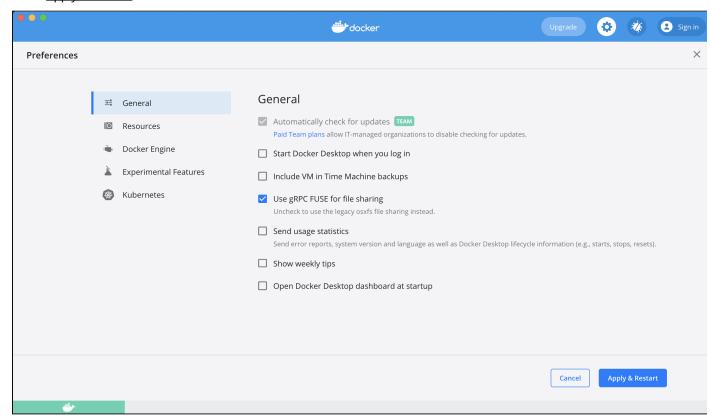


The icon in the lower left will turn green when ready.



Click the gears icon to open 'preferences'. Make sure you untick the options in General to mimic the screenshot below. This is to ensure Docker doesn't start when you boot your computer, and it doesn't share your usage data to Docker by default. Leave the automatic update checked if you prefer it to check for updates regularly.

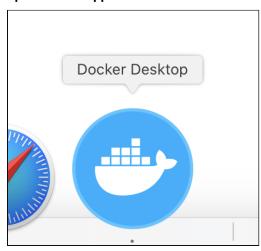
Press 'Apply & Restart' when done.



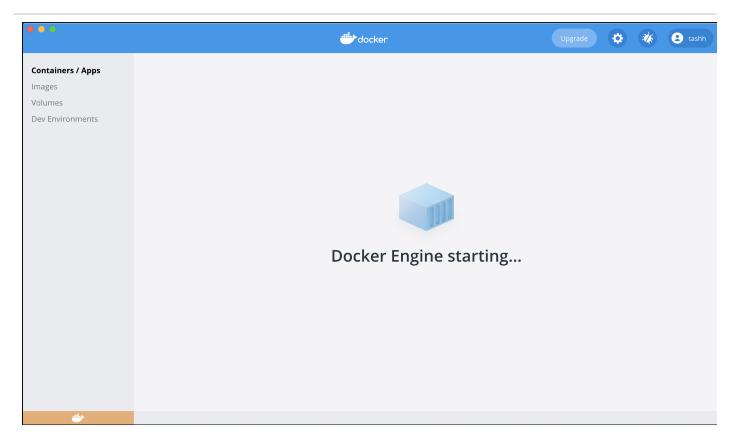
Close app until you would like to use it.

Running Spectre using Docker

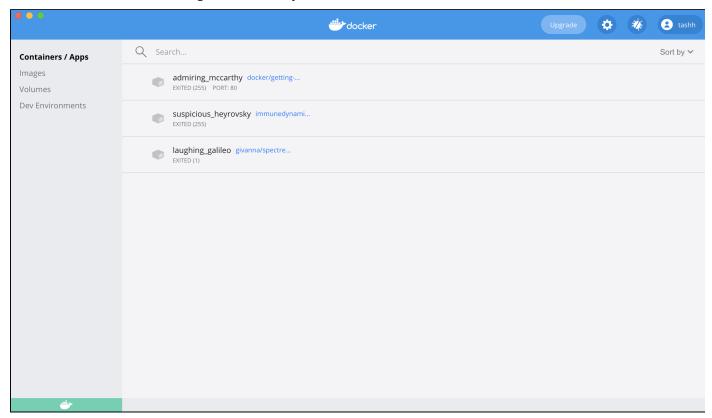
Open Docker app



Wait a few moments while the 'Docker Engine' starts.



The icon in the lower left will turn green when ready.



Open 'Terminal' (on Mac) and run the following code

Can be found in the applications folder, or the bar at the bottom of your screen.





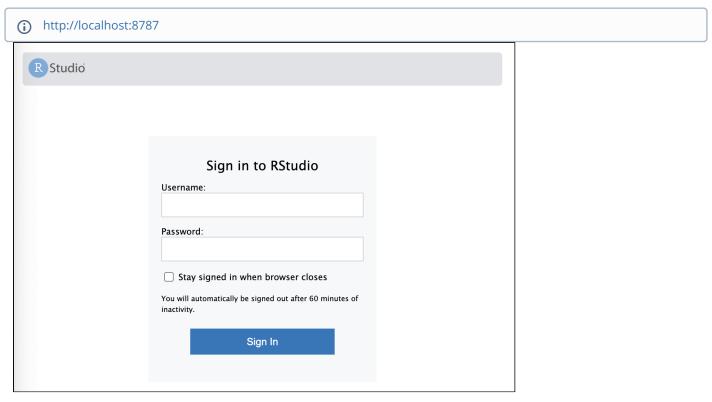
Copy the following code into the terminal and press ENTER.

```
docker run --rm -e PASSWORD=spectre -p 8787:8787 -v ~:/home/rstudio/spectre_dir --name=spectre
immunedynamics/spectre:master
(base) vlan-2682-10-17-83-40:~ thomasa$ docker run --rm -e PASSWORD=spectre -p 8787:8787 -v ~:/home/
rstudio/spectre_dir --name=spectre immunedynamics/spectre:master
[s6-init] making user provided files available at /var/run/s6/etc...exited 0.
[s6-init] ensuring user provided files have correct perms...exited 0.
[fix-attrs.d] applying ownership & permissions fixes...
[fix-attrs.d] done.
[cont-init.d] executing container initialization scripts...
[cont-init.d] userconf: executing...
[cont-init.d] userconf: exited 0.
[cont-init.d] done.
[services.d] starting services
[services.d] done.
```

By default, the RStudio session that Docker will launch will be able to see everything in your <u>Home</u> directory and below. This is achieved in the code above using the '~' symbol. If you have data elsewhere (on a server etc) you can navigate to that location using Finger and drag + drop the target directory/folder into terminal: In terminal, add the following segments, and then hit ENTER:

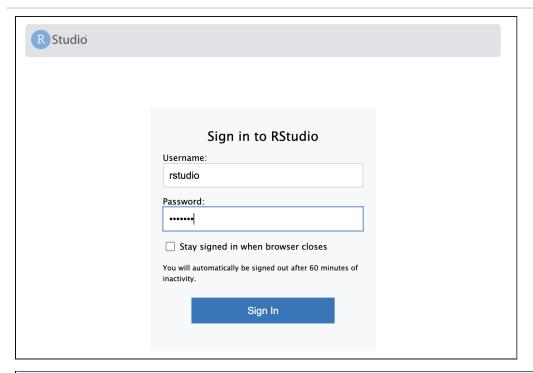
- docker run --rm -e PASSWORD=spectre -p 8787:8787 -v
- DRAG+DROP the target folder from finder
- :/home/rstudio/spectre_dir --name=spectre immunedynamics/spectre:master

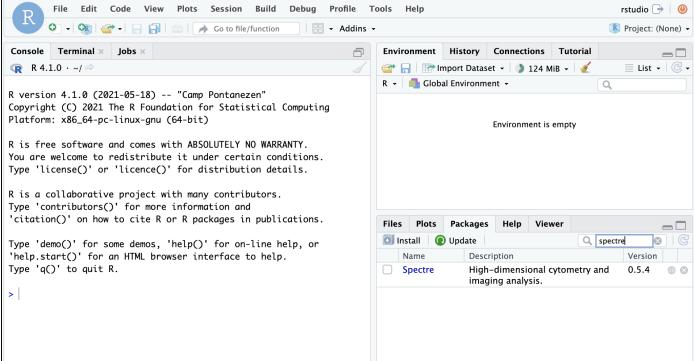
Open your preferred web browser (chrome, safari, etc) and go to the following address



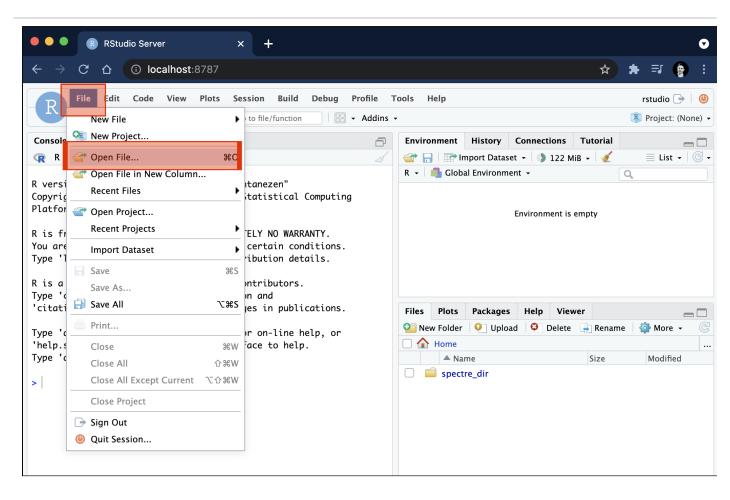
Sign in

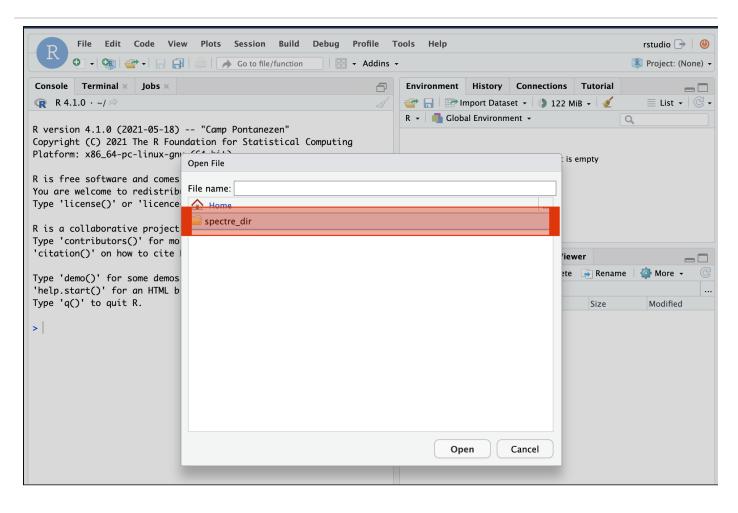
Name: rstudioPassword: spectre

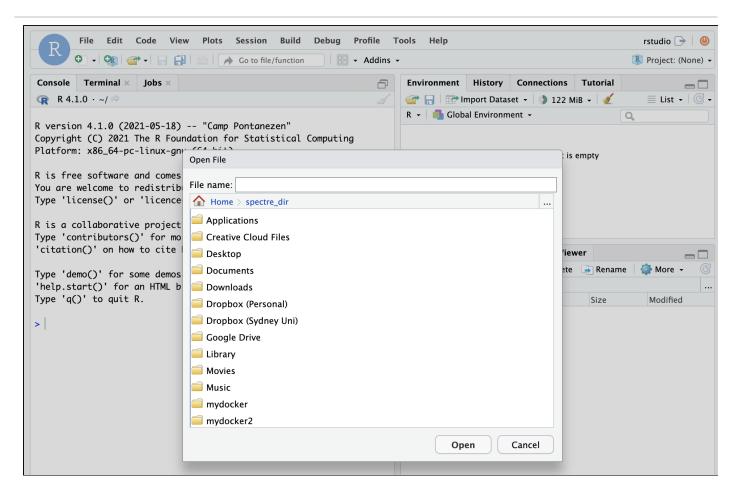


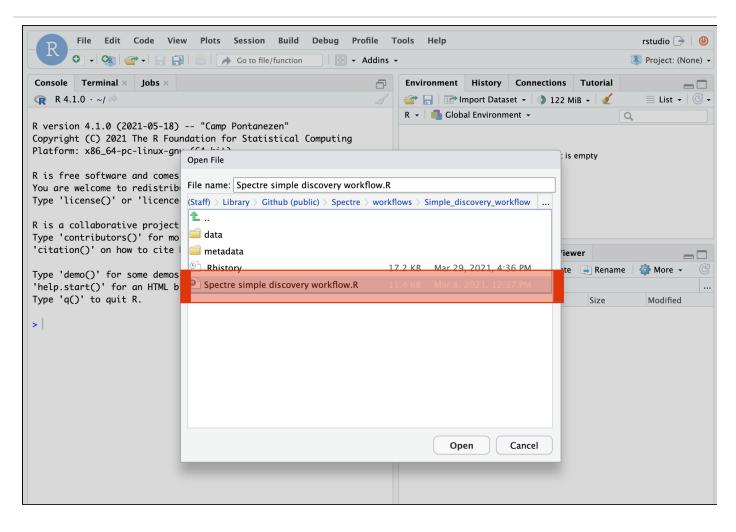


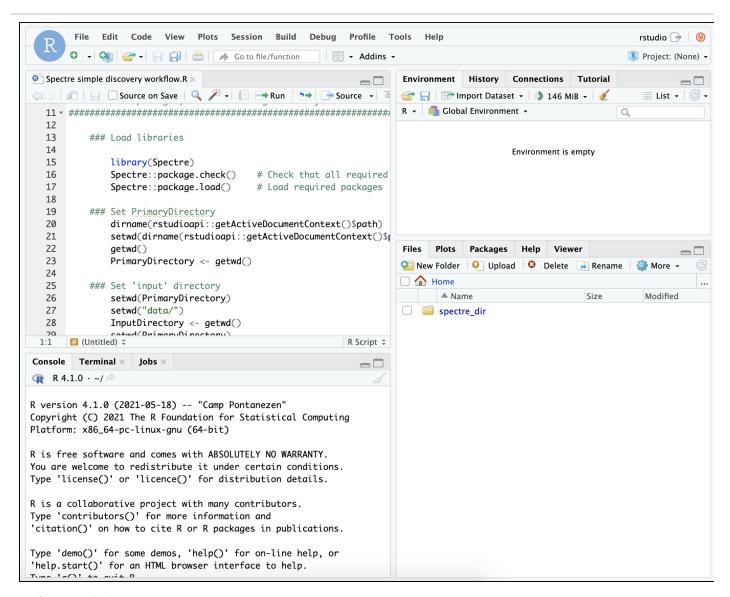
Open desired analysis script



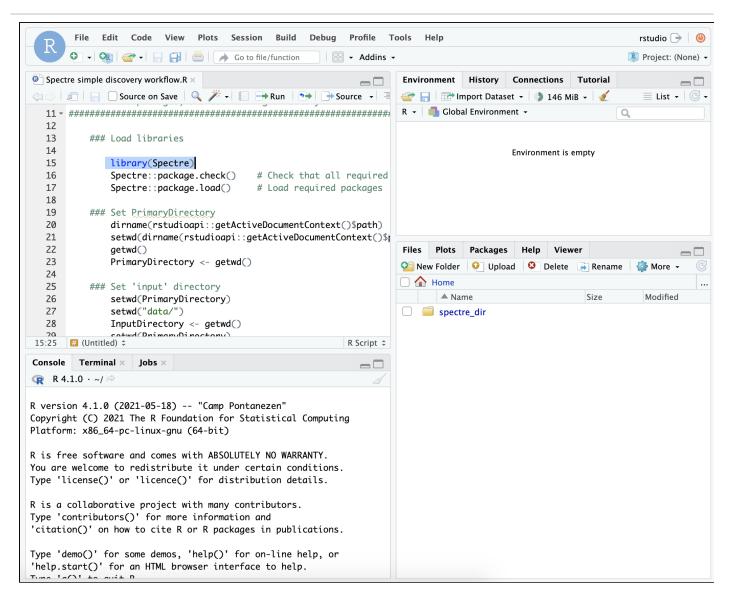








Perform analysis



Close when finished

```
^C[cont-finish.d] executing container finish scripts...
[cont-finish.d] done.
[s6-finish] waiting for services.
[s6-finish] sending all processes the TERM signal.
[s6-finish] sending all processes the KILL signal and exiting.
(base) TomA-MBP13t:~ thomasa$
```