LAPKB
Laboratory of Applied Pharmacokinetics & Bioinformatics

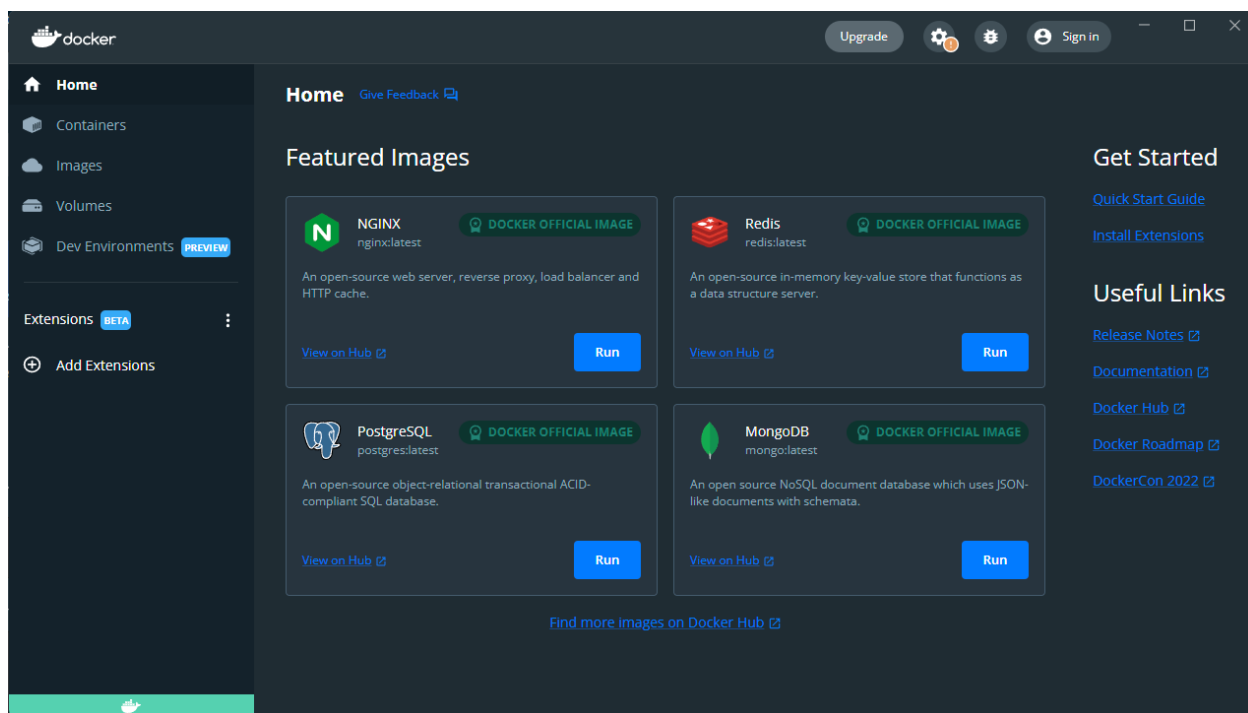Optimizing drug therapy for populations and individuals

Pmetrics via Docker

Pmetrics is now available as a self-contained installation using Docker, a free disk image maker. Users install Docker, and then obtain the Pmetrics image, which contains all the software needed to run models locally on the user's computer. There is no longer any need to obtain R, Rstudio, Pmetrics, and gfortran separately.

Step 1: Install and Launch Docker

- Windows users: https://docs.docker.com/desktop/windows/install/
- Mac users: https://docs.docker.com/desktop/mac/install/. *Remember to select the right installation based on the processing chip in your computer (M1 vs. Intel).*
- Linux users (or servers): https://docs.docker.com/desktop/linux/install/

Launch Docker. It should look like this:
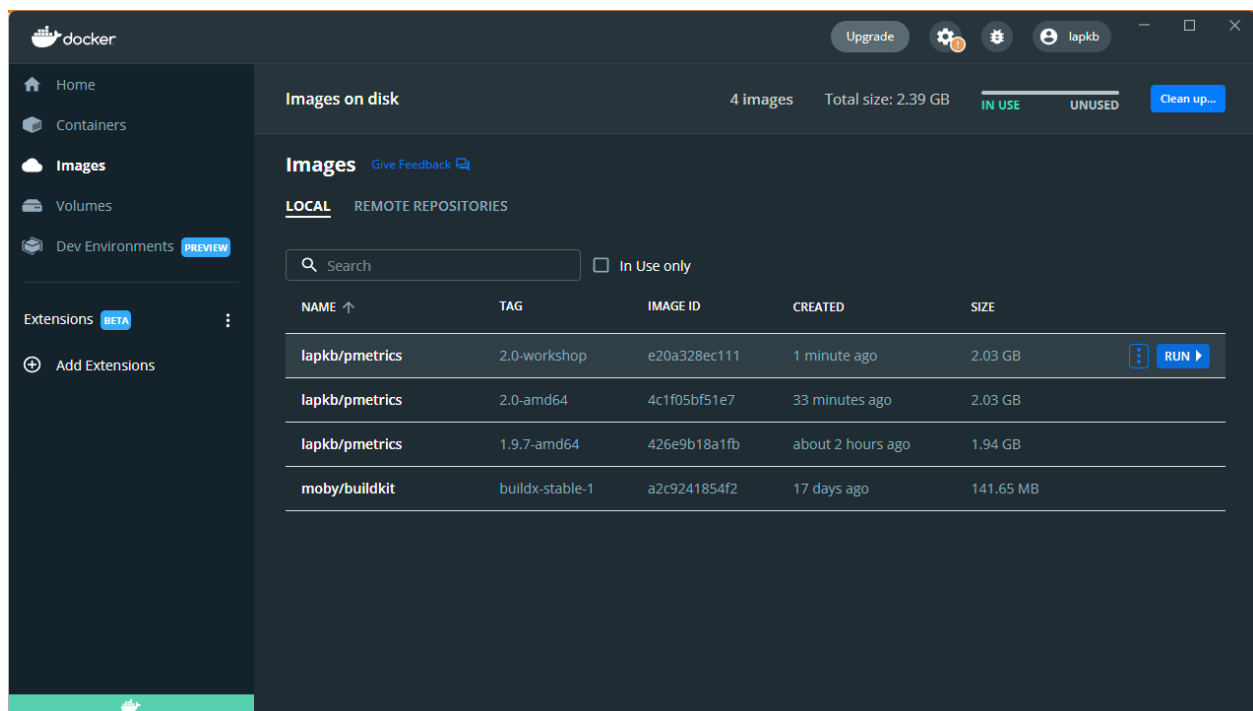
Step 2: Obtain the Pmetrics Image

- Open a [terminal](#) window, also known as Command Prompt in Windows.
- In your terminal window paste the following command to download the Pmetrics image into Docker: docker pull lapkb/pmetrics:2.0-workshop. Wait for the process to complete. All lines will say "Pull complete" when done.
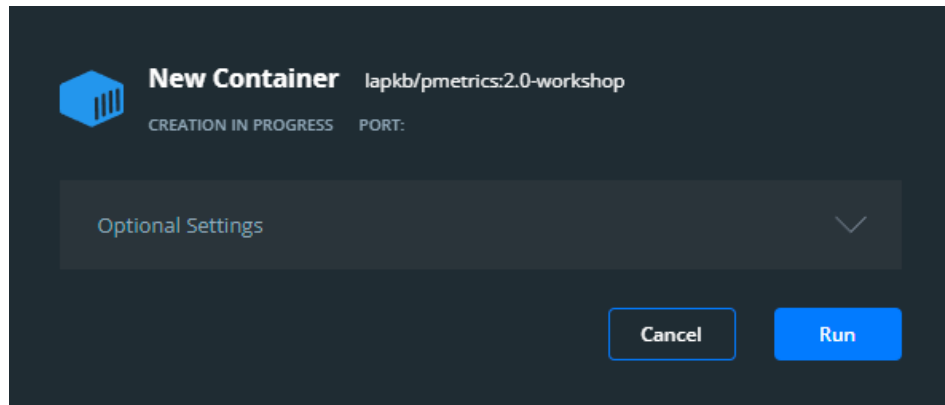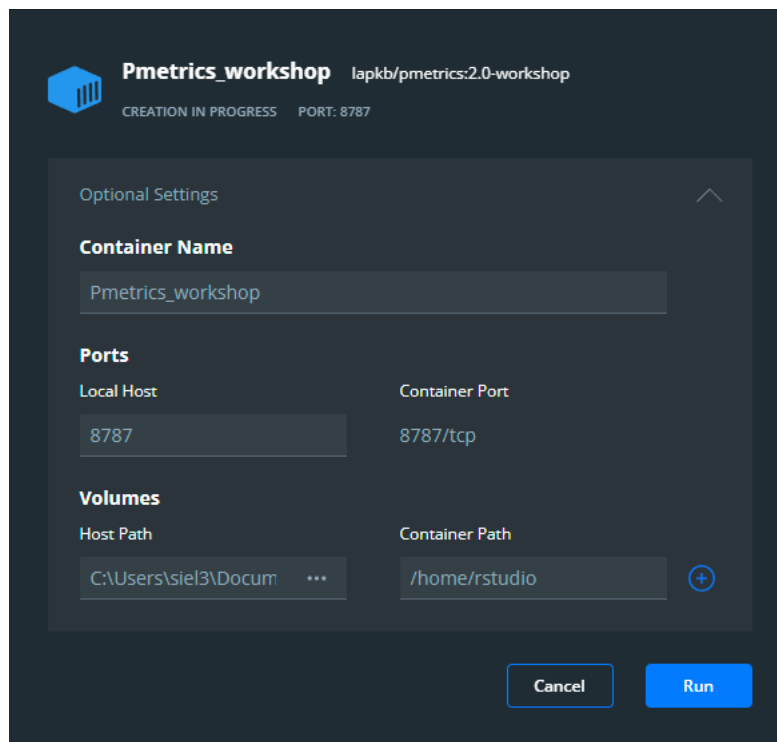

Step 3: Configure Docker

- Return to Docker and you should see an image like the first one in the screenshot below.

- Click on the blue RUN button for the line with the "2.0-workshop" tag.
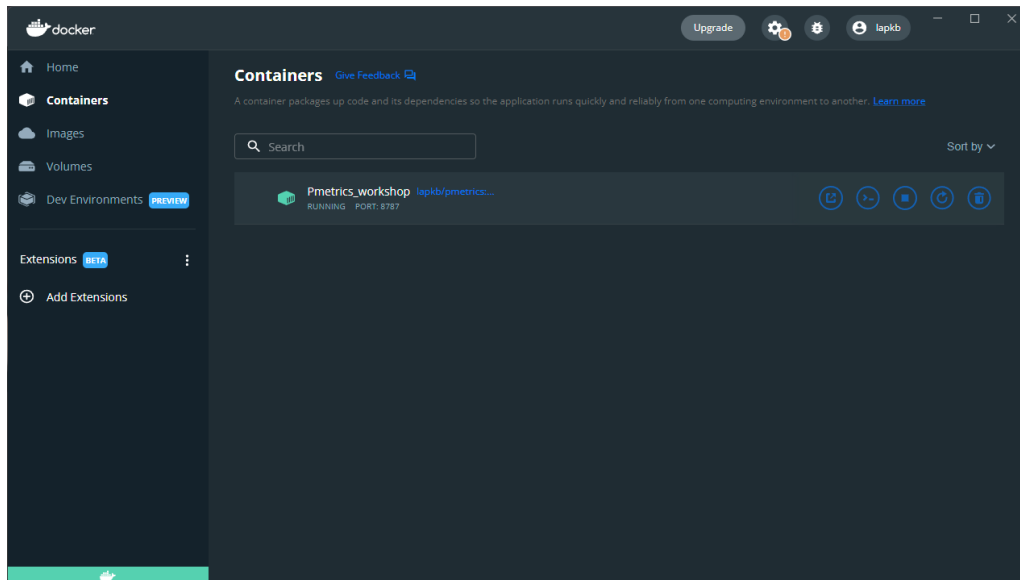- A new container wizard will appear.

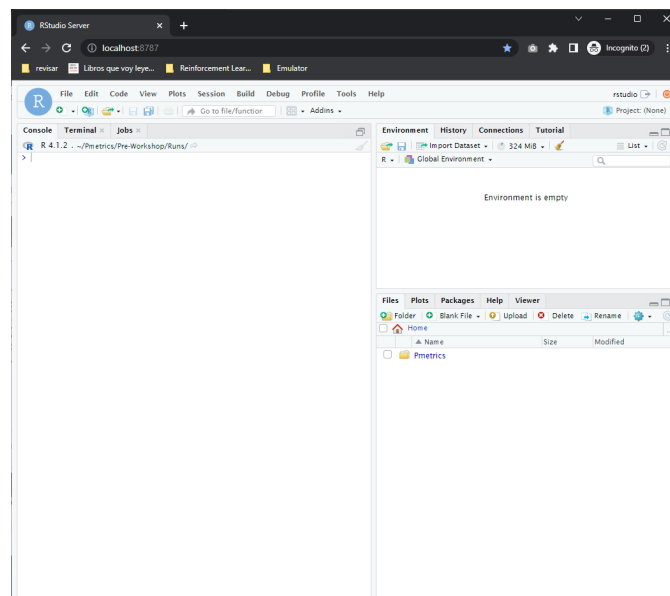- Click on Optional Settings to expand the settings menu:

- For container name, pick any name you want
- For port, our recommendation is to keep 8787.
- Finally, volumes are useful to synchronize one local folder on your hard drive with a folder inside the docker. ff paste the path of a local folder on your computer (The workshop image is programmed to create a Pmetrics folder with some files on this directory) and on the docker side always put /home/rstudio.
- The container name and volumes options are optional, but we recommend configuring both.

Step 4: Launch Rstudio in Docker

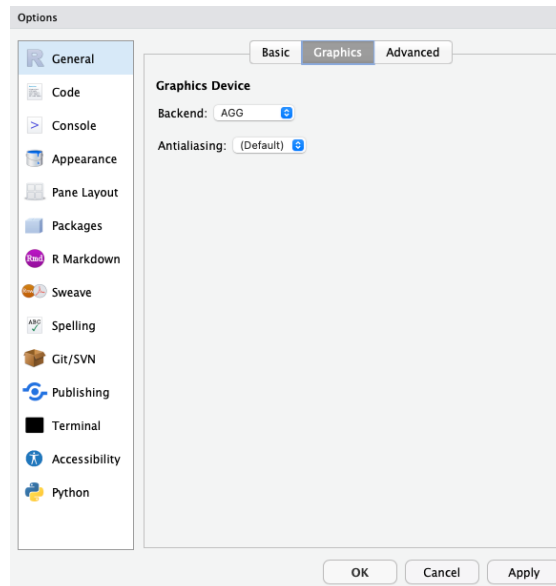- Now, if you go to the Containers tab on the docker client you will see our new docker up and running:

- The five circular blue buttons appear when you move your mouse over the Container. From right to left, the buttons are: Open in browser, CLI, Stop, Restart and Delete. Click on Open in browser, docker will open a website on your predefined browser:
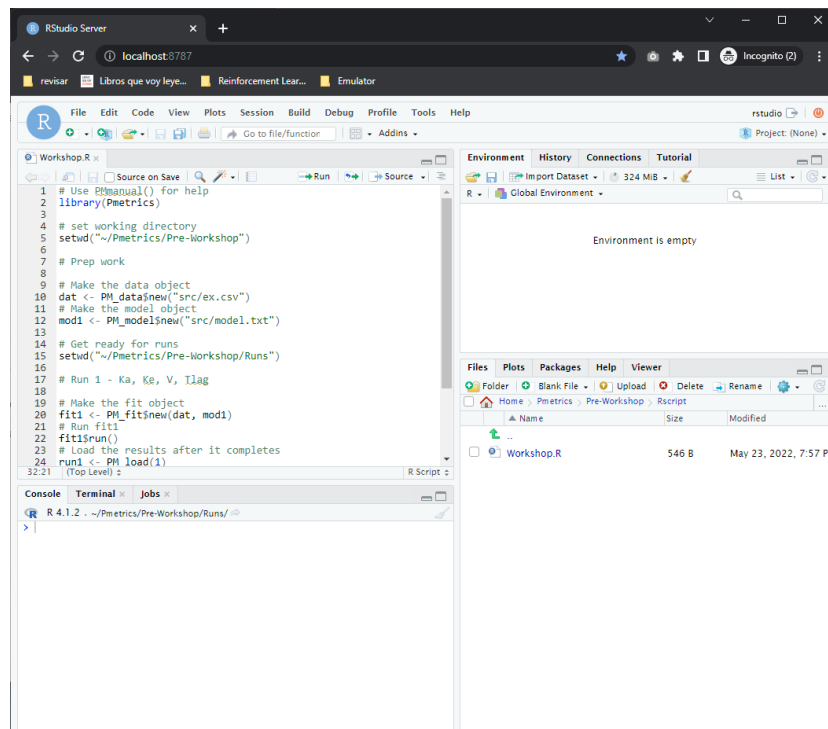
- **For Mac M1 chips only**, there is one last configuration. Rstudio will soon release an update that works better with M1. For now, you may see warning messages and to get plots working you

need to select Tools from the menu, then Global Options. Set the Graphics backend device to "AGG" as shown below.

Step 5: Pre-workshop script

- In Rstudio server, navigate over the folders shown at the lower right corner (Files tab) Pmetrics > Pre-Workshop > Rscript > Workshop.R. When you click Workshop.R the script should open.

- Execute the steps in the script!
  - You can place your cursor on a line and click the Run button at the top right of the window, or you can select the Code menu to see the keyboard shortcut on your system for "Run Selected Line(s)".
  - Clicking the Run button or pressing the keyboard shortcut will execute the line currently containing the cursor.
  - The cursor can be anywhere in the line.
  - If you select multiple lines, Run or keyboard shortcut will execute all of them.
- All the files you see here will be synchronized with the folder on your hard drive that you specified at the end of Step 3 above.
- Although the local folder is synchronized with the folder inside the docker, some malfunction may happen if we add/remove files to that folder when the docker container is turned on. Please make a backup of all your local files before launching or exiting Docker Rstudio.