GUIdock

USER MANUAL

Latest version available at https://github.com/WebDataScience/GUIdock

GUIdock is a Docker Package containing the entire computational environment to run applications with a graphical user interface. As a proof of concept, we focus on supporting Cytoscape, a Java-based standalone program with a graphical user interface for the visualization and analyses of gene networks in biology. In addition to Cytoscape, our container includes R, Rserve, Bioconductor packages igraph, networkBMA and a Cytoscape app called CyNetworkBMA. GUIdock contains the entire pipeline and all the tools (including Cytoscape that connects to preloaded RServe, a Bioconductor package called "networkBMA" and all its dependencies) to generate gene regulatory networks.

This manual demonstrates the installation and instructions to run GUIdock.

Docker Image	: https://hub.docker.com/r/kristiyanto/guidock/
Dockerfile	: https://github.com/WebDataScience/GUIdock

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Linux

Running GUIdock (Script)

A bash script to run and install GUIdock is available in:
https://github.com/kristiyanto/GUIdock/tree/master/Install%20and%20Run%20/LINUX

Download a file from the link above and run the script with following command to start GUIdock.

```
#Locate to script file
#Use following command to start GUIdock

sh runGUIdockLinux.sh
```

Alternatively, a tarball file is also available.

The script and tarball will attempt to start Docker Engine or install it if it is not installed. Once started, it pulls the Docker Image and run it.

During the run, a folder .guidock/GUIdock-SHARED is created under user home directory. ~/.guidock/GUIdock-Shared in the Linux system is linked with /root/GUIdock-SHARED within the container.

OS X

Installation (Script)

As shortcut, a bash script to run installation commands below is available in: https://github.com/WebDataScience/GUIdock/tree/master/Install%20and%20Run%20/MAC

Once downloaded, unzip a file and run the script with following command to install all the required softwares.

```
# Install from script

sh install-mac.sh
```

The script, however does not install Docker Toolbox. Docker Toolbox will have to be downloaded from their website and installed separately. Docker Toolbox can be downloaded from: https://www.docker.com/toolbox.

Installation (Manual)

Alternatively, required packages can also be installed independently by running following instructions:

1) Docker Toolbox

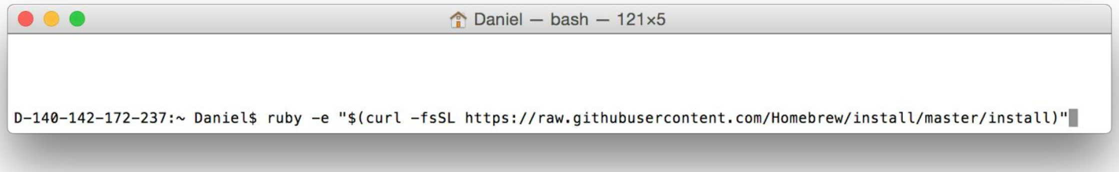
Docker Toolbox contains Docker Virtual Machine and Kitematic as a Docker Client for Macintosh and Windows User. Docker Toolbox can be downloaded from: https://www.docker.com/toolbox

2) Home Brew

Using only Docker Toolbox gives all that Docker Engine promises. However, to have GUI delivered in Mac from Docker containers, more software are needed. To make installation easier, software can be installed using home brew (http://brew.sh/).

To install Home Brew, enter this command in OS X terminal window:

```
# Install Home Brew

ruby -e "$(curl -fsSL
https://raw.githubusercontent.com/Homebrew/install/master/insta
ll)"
```

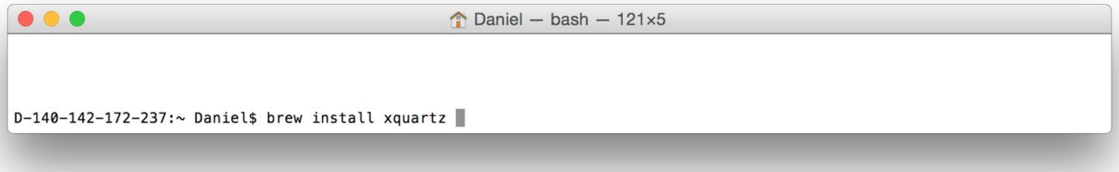


```
D-140-142-172-237:~ Daniel$ ruby -e "$(curl -fsSL https://raw.githubusercontent.com/Homebrew/install/master/install)"
```

3) XQuartz

XQuartz is an open source program to enable X Windows on OS X. With Home Brew installed, XQuartz can be installed entering this command in OS X terminal window:

```
# With home brew installed, install xquartz

brew install xquartz
```

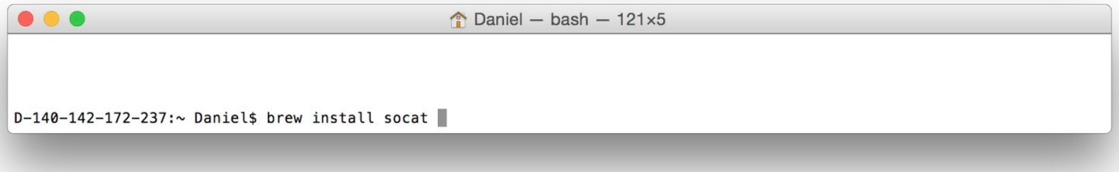


```
D-140-142-172-237:~ Daniel$ brew install xquartz
```

4) Socat

XQuartz is an open source program to enable X Windows on OS X. With Home Brew installed, enter the following command in terminal window:

```
# With home brew installed, install socat

brew install socat
```



```
D-140-142-172-237:~ Daniel$ brew install socat
```

Running GUIdock (SCRIPT)

A script to run GUIdock is available in:
https://github.com/WebDataScience/GUIdock/tree/master/Install%20and%20Run%20/MAC

Download a file from the link above and unzip a file.

To run GUIdock, run the script using the following command:

```
# Download and locate to installation file.
# Use following command to start GUIdock

sh mac-start.sh
```

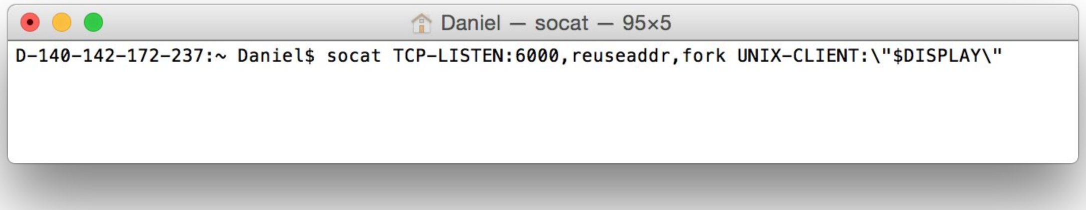
Running GUIdock (MANUAL)

Alternatively, GUIdock can also be launched manually by following instructions below:

1) Preparation

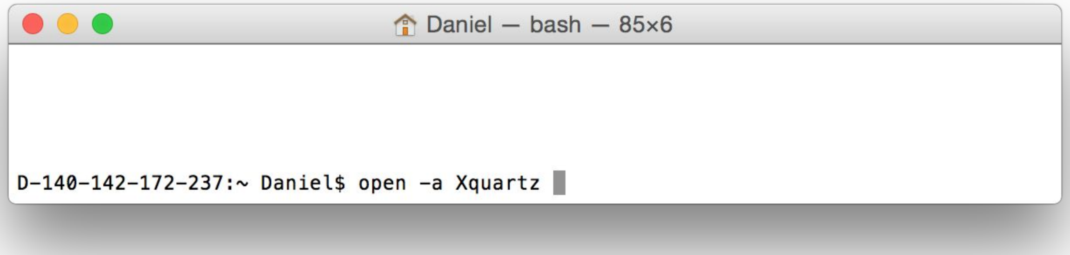
Docker engine runs in a virtual machine in OS X. To enable Display to be delivered to Mac OS, use socat to open incoming X11 Graphic interaction from Docker Machine and Xquartz to display the graphics.

```
# Run to socat bind

socat TCP-LISTEN:6000,reuseaddr,fork UNIX-CLIENT:\"$DISPLAY\"
```



```
D-140-142-172-237:~ Daniel$ socat TCP-LISTEN:6000,reuseaddr,fork UNIX-CLIENT:\"$DISPLAY\"
```

```
# Open xquartz to accept incoming graphic
open -a xquartz
```

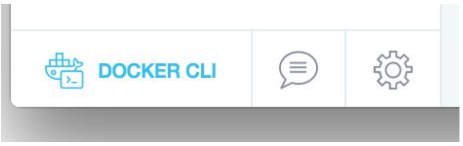


```
D-140-142-172-237:~ Daniel$ open -a Xquartz
```

It may also a good idea to check if the firewall is blocking the incoming connection from docker container.

2) Running GUIdock

Once Mac OS is ready to receive graphic streams from Docker container, ensure that Docker Engine (Kitematic) is up and running. Click on the Docker CLI in Kitematic to launch a new terminal

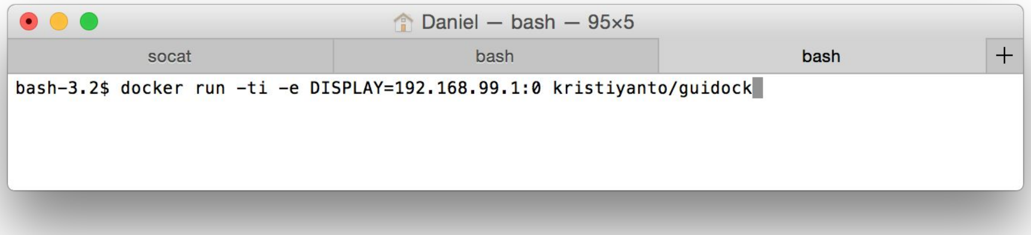


Within Docker CLI terminal windows, run GUIdock by running following commands:

```
# Pull latest image of GUIdock from repository.
docker pull kristiyanto/guidock

#  Find out the Mac’s IP address
ifconfig | grep "inet"
```

The MAC-IP-ADDRESS number you want to identify is immediately after the "inet" field.

```
# Run the GUIdock. Once loaded, a Cytoscape GUI Window pops up.

# Replace MAC-IP-ADDRESS with the IP number you identified from
ifconfig

docker run -ti -e DISPLAY=MAC-IP-ADDRESS:0 kristiyanto/guidock
```



```
bash-3.2$ docker run -ti -e DISPLAY=192.168.99.1:0 kristiyanto/guidock
```

-ti : To enable docker container in interactive mode.
-e : To set up the DISPLAY environment variable into the docker container so that the GUI can be sent to Mac OS machine.
IP address : MAC OS private address (VirtualBox's interface), this address should be reachable by Docker Machine.
Port Number : Port number of X11 is 0 (zero).

Next: Cytoscape Demo

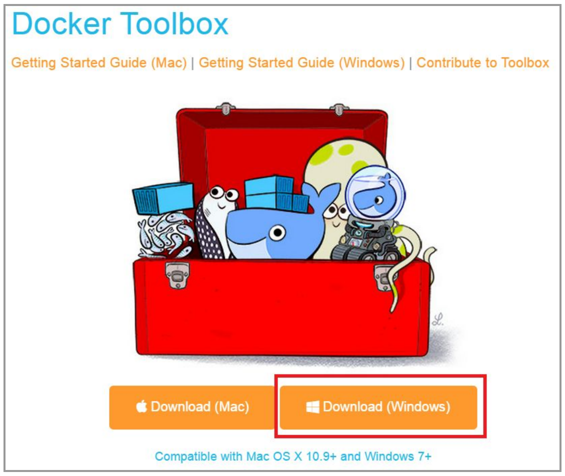
WINDOWS

Installation

1) Docker ToolBox

Install Docker ToolBox. Docker ToolBox can be downloaded from:
https://www.docker.com/toolbox

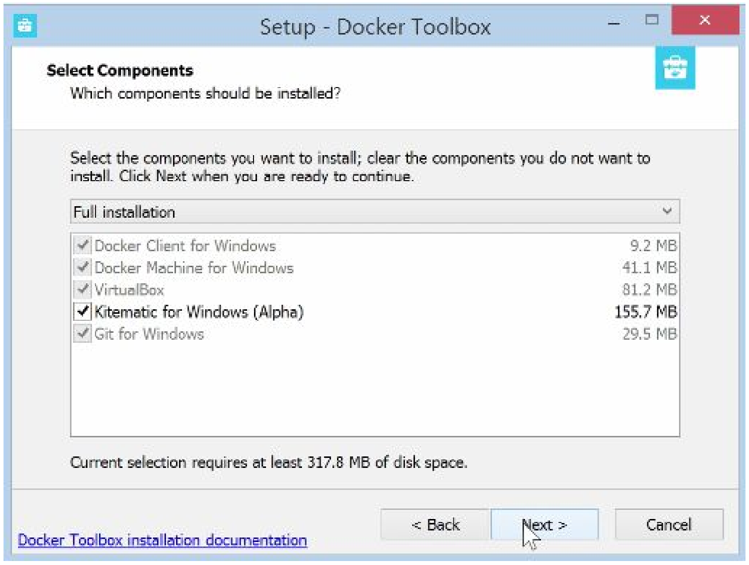
Click the link above and choose "Download (Windows)".


Docker Toolbox
Getting Started Guide (Mac) | Getting Started Guide (Windows) | Contribute to Toolbox
Download (Mac)
Download (Windows)

Compatible with Mac OS X 10.9+ and Windows 7+

Go to folder where the installation file is saved and run the installation file.

Click "Next" until you see "Selection Components" window. This will install Docker client, Docker machine, VirtualBox, Kitematic and Git for Windows.



Select Components

Which components should be installed?

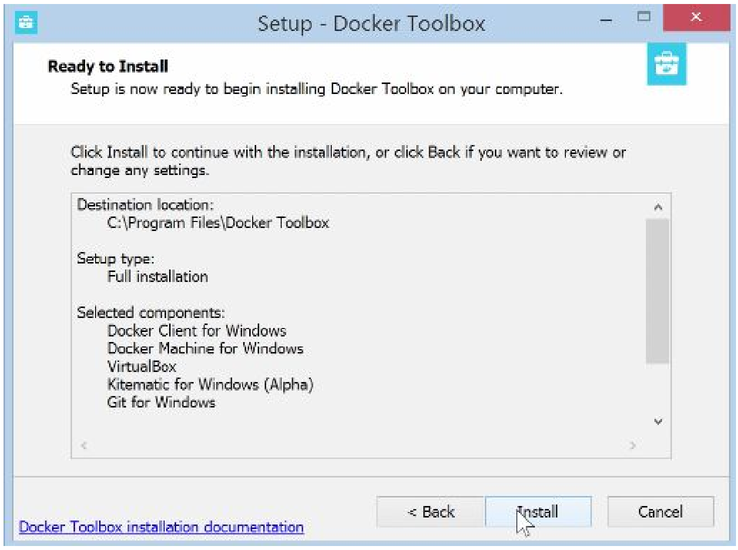
Select the components you want to install; clear the components you do not want to install. Click Next when you are ready to continue.

Full installation

☑ Docker Client for Windows	9.2 MB
☑ Docker Machine for Windows	41.1 MB
☑ VirtualBox	81.2 MB
☑ Kitematic for Windows (Alpha)	155.7 MB
☑ Git for Windows	29.5 MB

Current selection requires at least 317.8 MB of disk space.

Click "Next" until you see "Ready to Install" window and click "Install".



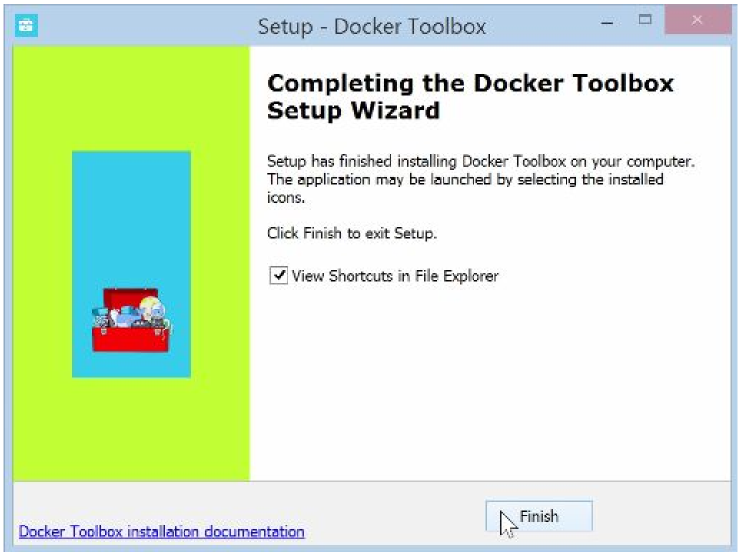
Ready to Install

Setup is now ready to begin installing Docker Toolbox on your computer.

Click Install to continue with the installation, or click Back if you want to review or change any settings.

```
Destination location:
      C:\Program Files\Docker Toolbox

Setup type:
      Full installation

Selected components:
      Docker Client for Windows
      Docker Machine for Windows
      VirtualBox
      Kitematic for Windows (Alpha)
      Git for Windows
```

Click "Finish" to complete the installation.



Setup - Docker Toolbox

Completing the Docker Toolbox Setup Wizard

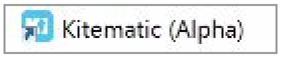
Setup has finished installing Docker Toolbox on your computer. The application may be launched by selecting the installed icons.

Click Finish to exit Setup.

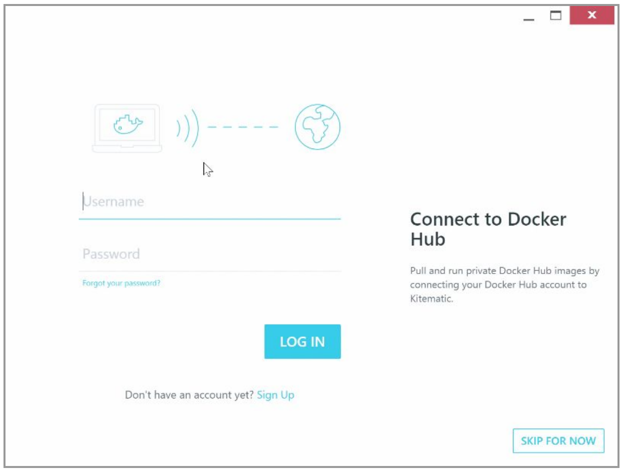
☑ View Shortcuts in File Explorer

Docker Toolbox installation documentation

To run the Docker Engine, double click on "Kitematic (Alpha)" shortcut.



On the first run, it will create the Docker VM and all the required environments. If you have a Docker account, enter your username and password. If you don't have an account, click "Skip for now".



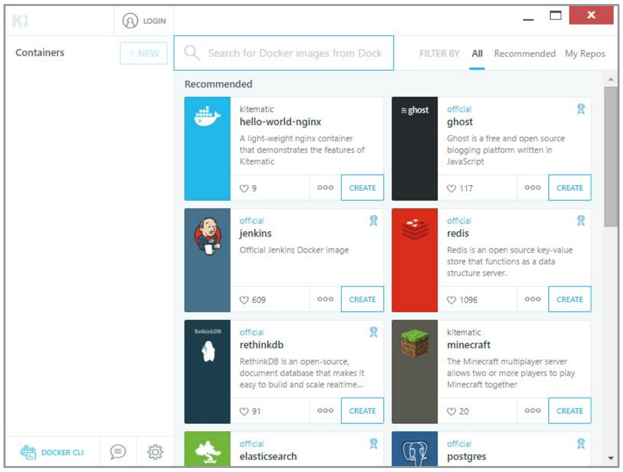
Username

Password

Connect to Docker Hub

Pull and run private Docker Hub images by connecting your Docker Hub account to Kitematic.

Don't have an account yet? Sign Up



Containers

Search for Docker images from Dock

FILTER BY All Recommended My Repos

Recommended

kitematic
hello-world-nginx
A light-weight nginx container that demonstrates the features of Kitematic
9

official
ghost
Ghost is a free and open source blogging platform written in JavaScript
117

official
jenkins
Official Jenkins Docker image
609

official
redis
Redis is an open source key-value store that functions as a data structure server.
1096

official
rethinkdb
RethinkDB is an open-source, document database that makes it easy to build and scale realtime...
91

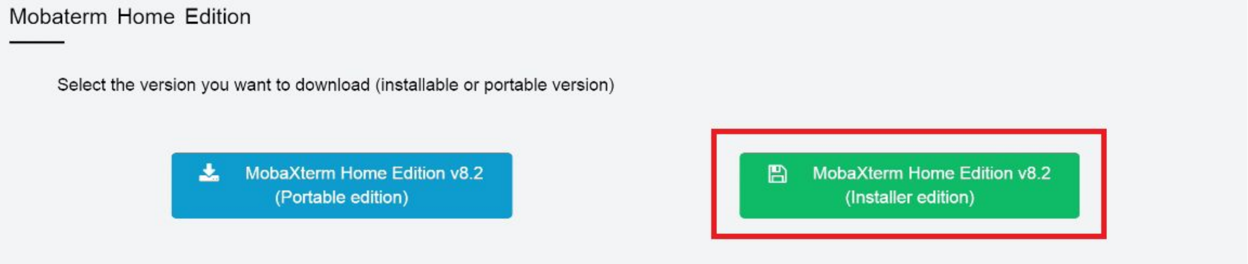
kitematic
minecraft
The Minecraft multiplayer server allows two or more players to play Minecraft together
20

official
elasticsearch

official
postgres

2) MobaXterm

To have GUI delivered in Windows, install MobaXterm to set up X11 forwarding. MobaXterm is an open source X11 emulator for Windows which allows remote GUI access to the application. MobaXterm can be downloaded from:
http://mobaxterm.mobatek.net/download-home-edition.html
Click the link above and choose version you want to download. We chose “MobaXterm Home Edition (Installer edition)” in this tutorial.



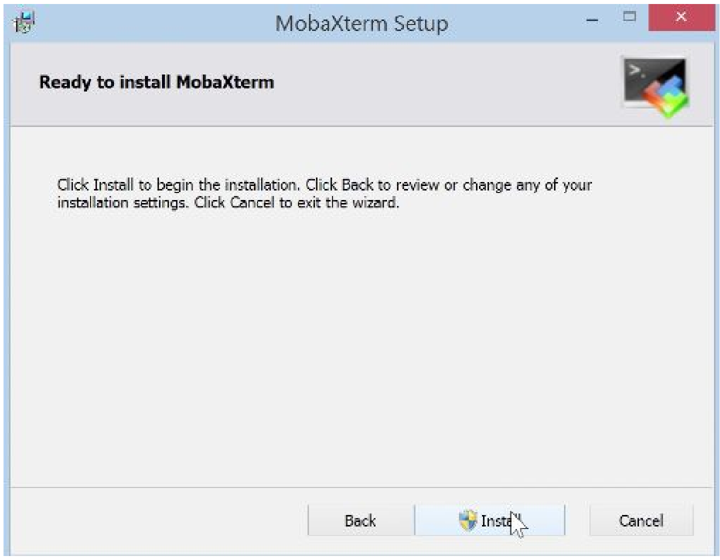
Mobaterm Home Edition

Select the version you want to download (installable or portable version)

MobaXterm Home Edition v8.2 (Portable edition)
MobaXterm Home Edition v8.2 (Installer edition)

Go to folder where the installation file is saved and run the installation file.

Click “Next” until you see “Ready to install MobaXterm” and click “Install” to install MobaXterm.



MobaXterm Setup

Ready to install MobaXterm

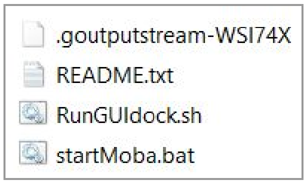
Click Install to begin the installation. Click Back to review or change any of your installation settings. Click Cancel to exit the wizard.

Running GUIdock (SCRIPT)

A shell script to run GUIdock is avilable in:

https://github.com/WebDataScience/GUIdock/tree/master/Install%20and%20Run%20/WINDOWS

Download a file from the link above and unzip a file. Double click on “RunGUIdock.sh” shell script file to run GUIdock. The script, however does not install Docker Toolbox and MobaXterm. Docker Toolbox and MobaXterm will have to be downloaded from their websites and installed separately.



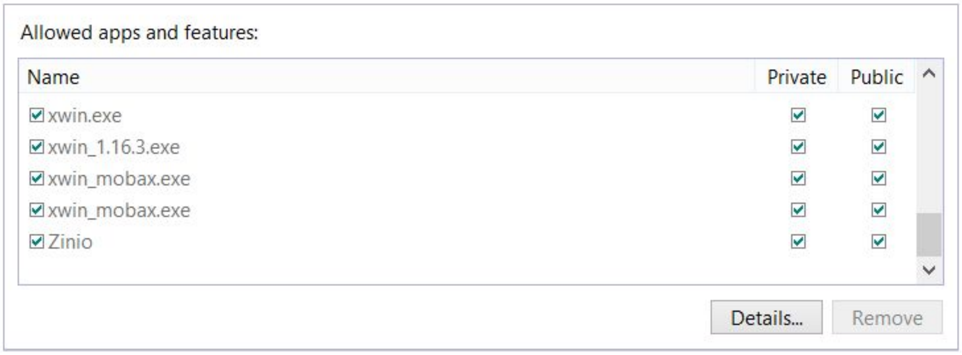
.goutputstream-WSI74X
README.txt
RunGUIdock.sh
startMoba.bat

Running GUIdock (MANUAL)

1) Preparation

Firewall
Make sure Firewall allows Docker Machine to access MobaXterm X11 service. This can be done either by disabling the firewall for Private Networks, or by manually list MobaXterm in Firewall as follow:

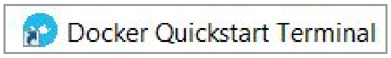
Control Panel -> System and Security -> Windows Firewall -> Allow an app or feature through Windows Firewall; check boxes for MobaXterm



Allowed apps and features:

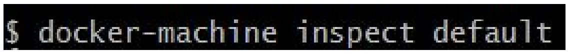
Name	Private	Public
☑ xwin.exe	☑	☑
☑ xwin_1.16.3.exe	☑	☑
☑ xwin_mobax.exe	☑	☑
☑ xwin_mobax.exe	☑	☑
☑ Zinio	☑	☑

IP Addresses
Open “Docker QuickStart Terminal”.



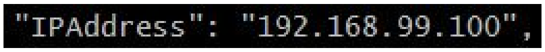
To obtain IP Addresses, type the following command in “Docker QuickStart Terminal”:

```
docker-machine inspect default
```



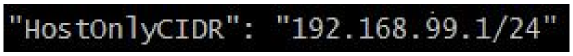
```
$ docker-machine inspect default
```

Locate to the IP Address of Docker Machine.



```
"IPAddress": "192.168.99.100",
```

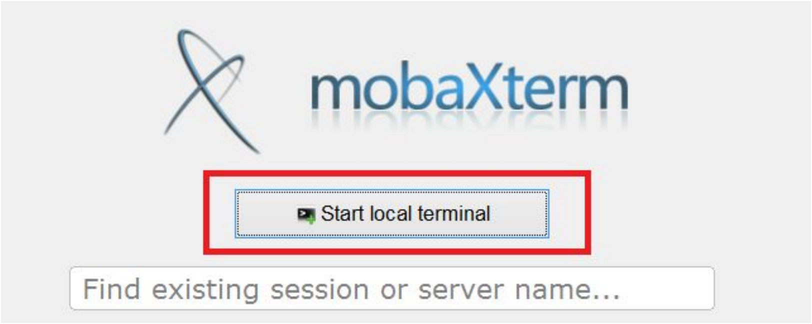
Locate to IP Address of Docker Client.



```
"HostOnlyCIDR": "192.168.99.1/24"
```

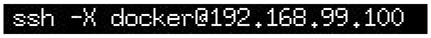
2) Running GUIdock

Open MobaXterm, click "Start local terminal".



Type the following command to use SSH to connect Docker host in terminal.

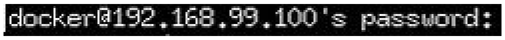
```
# 1. SSH with X11 forwarding to Docker host.
ssh -X docker@DockerMachineIPAdress
```



```
ssh -X docker@192.168.99.100
```

Docker default username is "docker" and password is "tcuser". Enter "tcuser" when a password is asked. Password can be saved after the first login.

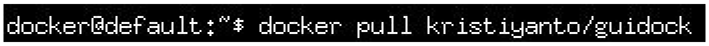
```
#2. Login with password "tcuser"
tcuser
```



```
docker@192.168.99.100's password:
```

Pull the latest GUIdock image from the repository by typing the following command in terminal:

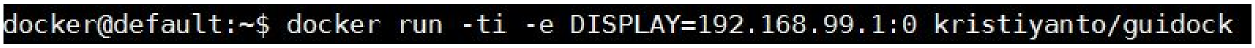
```
# 3. Pull latest image of GUIdock from repository.

docker pull kristiyanto/guidock
```



```
docker@default:~$ docker pull kristiyanto/guidock
```

Run GUIdock image by typing the following command in terminal

```
#4. Run the GUIdock. Once loaded, a Cytoscape GUI Window pops
up.

docker run -ti -e DISPLAY=WindowsIPAddress:0
kristiyanto/guidock
```



```
docker@default:~$ docker run -ti -e DISPLAY=192.168.99.1:0 kristiyanto/guidock
```

-ti : To enable docker container in interactive mode.

-e : To set up the DISPLAY environment variable into the docker container so that the GUI can be sent to Windows machine.

IP address : Windows private address (VirtualBox's interface), see Preparation Section to check IP Address. This address should be reachable by Docker Machine.

Port Number : Port number of X11 is 0 (zero).

Next: Cytoscape Demo

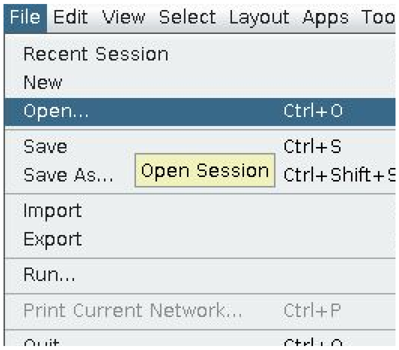
Cytoscape Demo

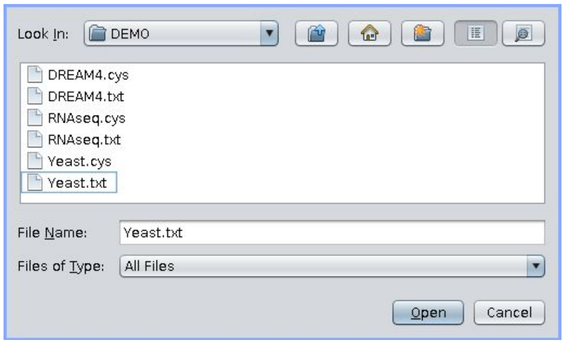
Demo files and saved-sessions are included in the GUIdock container, located in /root/DEMO folder.
The files and the demo including:

1. Dream4.cys : A 210 by 101 table in which the first column identifies time and the remaining columns are the expression levels for 100 genes in a simulated network after an application (at t=0) and removal (at t=500) of a perturbation (21 time points in each time series). Based on the time series file for the first network in the 100-gene in silico network sub-challenge from DREAM 4, Challenge 2 (Marbach *et al.* 2009, Marbach *et al*. 2010, Prill *et al.* 2010). A key column was added to the original file to facilitate import into Cytoscape.
2. RNAseq.cys : 84-gene subset of the RNAseq Cancer cell line data. Klijn *et al.* generated an extensive RNAseq gene expression data across 675 frequently used human cancer cell lines. We downloaded the the variance stabilized version of the normalized RNAseq data produced by the DESeq Bioconductor package from http://research-pub.gene.com/KlijnEtAl2014/. We then extracted a subset of 84 genes that belong to 21 cancer-related pathways that are known to be functionally altered in cancer (see Supplementary Table 12 in Klijn *et al*. Note that this is a steady-state (non-time series) dataset.
3. Yeast.cys : A 582 by 102 table in which the first two columns identify the replicate and time (in minutes) after drug perturbation, and the remaining 100 columns are the expression measurements for a subset of 100 genes from the yeast-rapamycin experiment described in Yeung et al. (2011). There are 582/6 = 97 replicates (the 95 segregants plus two parental strains of the segregants), each with measurements at 6 time points. The complete time series data is available from Array Express (Parkinson et al. 2007) with accession number E-MTAB-412. When using this file, please remember to adjust source format in the inference dialog. Also, exclude replicate and time columns from input to the algorithm.

Open Demo Session

Once Cytoscape application is started, click "File" and "Open" to open one of the session files from "/root/DEMO" folder.



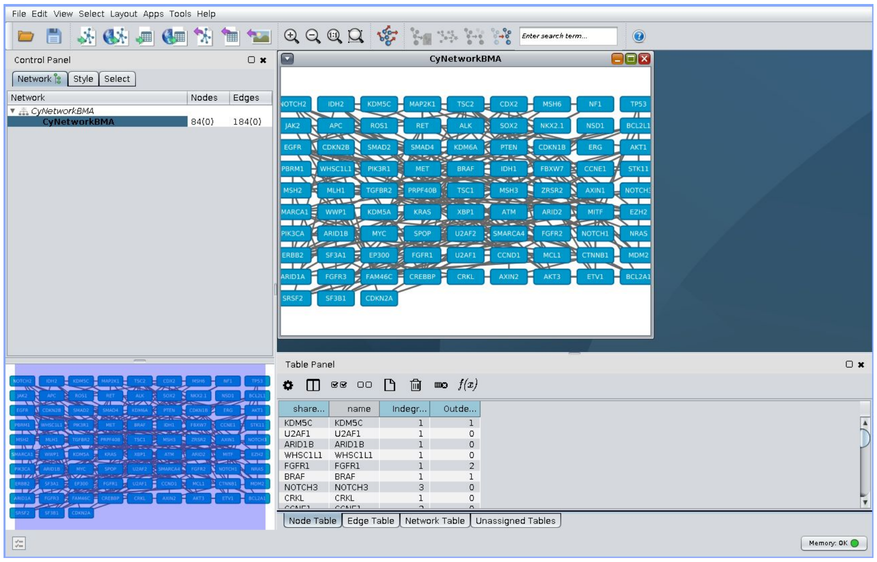

Look In: DEMO

DREAM4.cys
DREAM4.txt
RNAseq.cys
RNAseq.txt
Yeast.cys
Yeast.txt

File Name: Yeast.txt

Files of Type: All Files

Select any of the .cys file to open saved cytoscape session. The following image is gene networks of RNAseq.cys file.

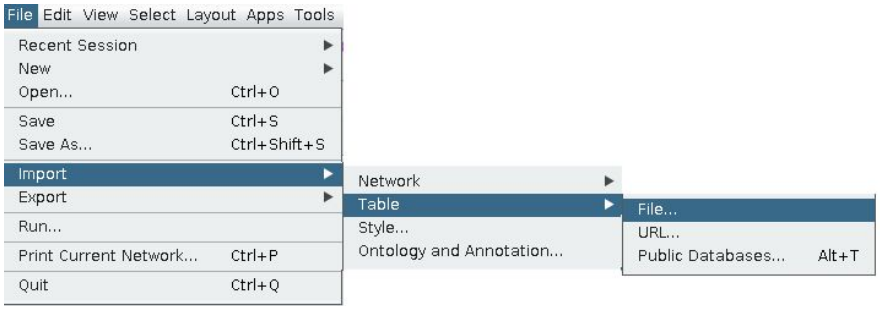


Network	Nodes	Edges
CyNetworkBMA		
CyNetworkBMA	84(0)	184(0)

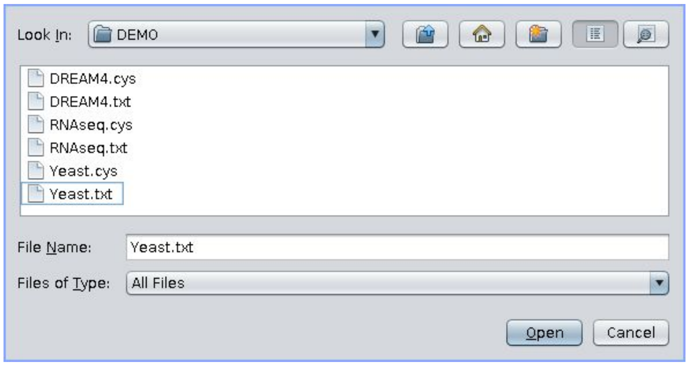
share...	name	Indegr...	Outde...
KDM5C	KDM5C	1	1
U2AF1	U2AF1	1	0
ARID1B	ARID1B	1	0
WHSC1L1	WHSC1L1	1	0
FGFR1	FGFR1	1	2
BRAF	BRAF	1	1
NOTCH3	NOTCH3	3	0
CRKL	CRKL	1	0
CCNE1	CCNE1	2	0

Inferring Gene Networks

Demo files can also be imported into Cytoscape by using the Import menu. On Cytoscape, open test data by going to File -> Import -> Table -> File



And select any of the .txt files to load demo files into Cytoscape. The files are located in "/root/DEMO"

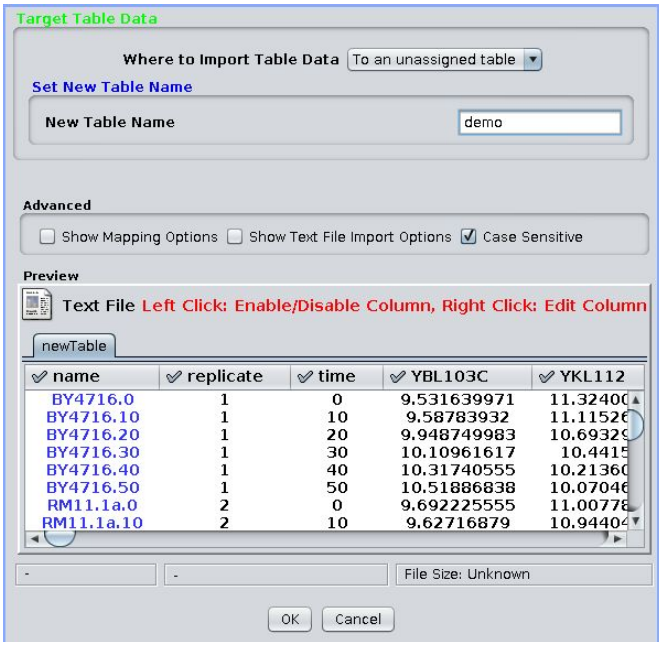

Look In: DEMO

DREAM4.cys
DREAM4.txt
RNAseq.cys
RNAseq.txt
Yeast.cys
Yeast.txt

File Name: Yeast.txt

Files of Type: All Files

In the following dialog window, choose the option to import data into an unassigned table and enter new table name.



Where to Import Table Data: To an unassigned table

New Table Name: demo

Advanced

□ Show Mapping Options □ Show Text File Import Options ☑ Case Sensitive

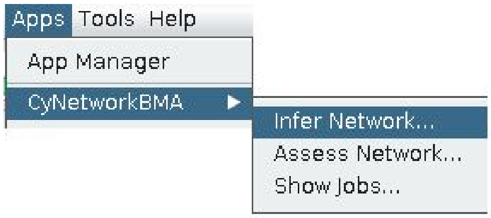
Preview

Text File Left Click: Enable/Disable Column, Right Click: Edit Column

✓ name	✓ replicate	✓ time	✓ YBL103C	✓ YKL112
BY4716.0	1	0	9.531639971	11.32400
BY4716.10	1	10	9.58783932	11.1152
BY4716.20	1	20	9.948749983	10.6932
BY4716.30	1	30	10.10961617	10.4415
BY4716.40	1	40	10.31740555	10.2136
BY4716.50	1	50	10.51886838	10.0704
RM11.1a.0	2	0	9.692225555	11.0077
RM11.1a.10	2	10	9.62716879	10.9440

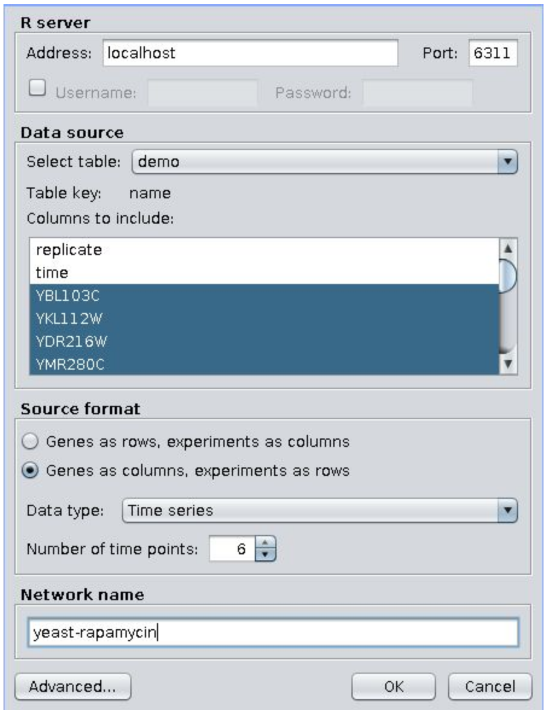
- | - | File Size: Unknown

Run the network inference algorithm by going to Apps -> CyNetworkBMA -> Inter Network



In the following dialog window, specify the columns to include and source format.

<u>Data file</u>	<u>Columns to include</u>	<u>Source format</u>
Dream4.txt	Select all columns except “Time”	● Genes as columns ● Data Type: Time series ● Number of time points: 21
RNAseq.txt	Select all	● Genes as rows ● Data Type: Steady state
Yeast.txt	Select all columns except “replicate” and “time”	● Genes as columns ● Data Type: Time series ● Number of time points: 6



R server

Address: localhost Port: 6311

□ Username: Password:

Data source

Select table: demo

Table key: name

Columns to include:

replicate
time
YBL103C
YKL112W
YDR216W
YMR280C

Source format

○ Genes as rows, experiments as columns

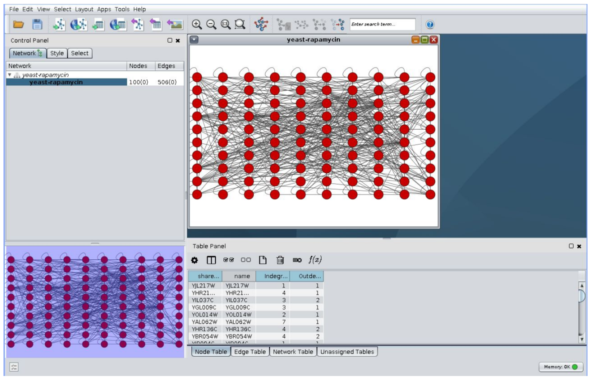
● Genes as columns, experiments as rows

Data type: Time series

Number of time points: 6

Network name

yeast-rapamycin



Network	Nodes	Edges
yeast-rapamycin		
yeast-rapamycin	100(0)	506(0)

yeast-rapamycin

share...	name	Indegr...	Outde...
YJL217W	YJL217W	1	1
YHR21...	YHR21...	4	1
YIL037C	YIL037C	3	2
YGL009C	YGL009C	3	1
YOL014W	YOL014W	2	1
YAL062W	YAL062W	7	1
YHR136C	YHR136C	4	2
YBR054W	YBR054W	4	2

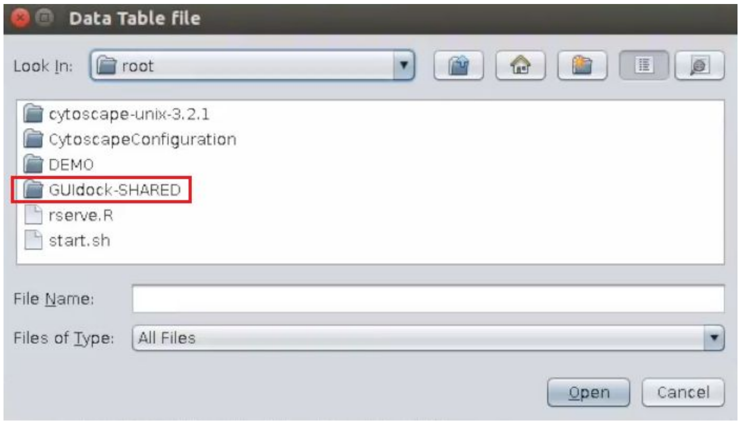
Transferring files between a container and the local filesystem

Transferring files (Linux)

To transfer files in Linux, run the script using the following command to start GUIdock.

```
#Locate to script file
#Use following command to start GUIdock

sh runGUIdockLinux.sh
```

The script creates a shared folder ".guidock/GUIdock-SHARED" under user home directory. ~/.guidock/GUIdock-Shared in the Linux system is linked with /root/GUIdock-SHARED within the container.



To open shared folder in Linux system, type the following commands in terminal:

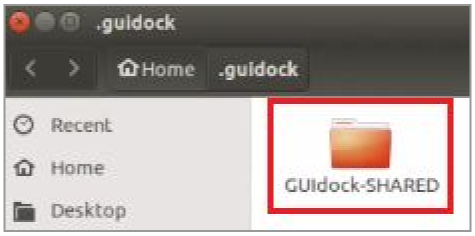
```
#Locate to .guidock directory
cd .guidock/
```

```
cd .guidock/
```

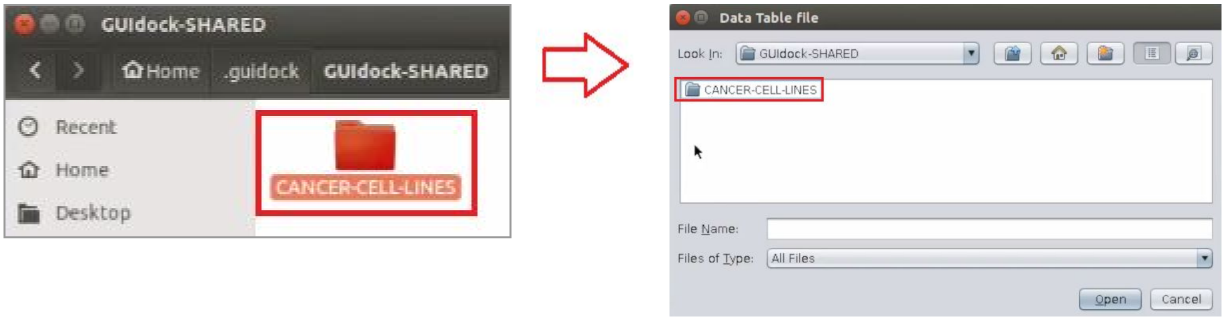
```
#Open shared folder
xdg-open .
```

```
xdg-open .
```

Double click on the shared folder “GUIdock-SHARED”.



In shared folder, copy and paste a file or folder you want to share. The folder is added to the “/root/GUIdock-SHARED” directory in the container.



To share files or folders between a container and Linux system, add them in "GUIdock-SHARED" folder.

Transferring files (OS X)

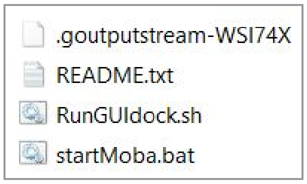
To transfer files between a container and the local filesystem in OS X, run the script using the following command to start GUIdock.

```
# Download and locate to installation file.
# Use following command to start GUIdock

sh mac-start.sh
```

Open terminal and follow the steps for "**Transferring a file from the local machine to running container"** and **"Transferring a file from running container to the local filesystem**
" below.

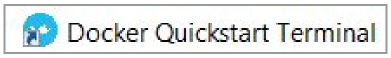
Transferring files (Windows)

To transfer files between a container and the local filesystem in Windows, double click on the shell script file to start GUIdock.



.goutputstream-WSI74X
README.txt
RunGUIdock.sh
startMoba.bat

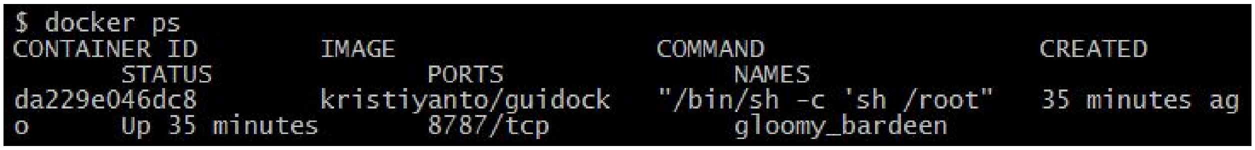
Open "Docker QuickStart Terminal" and follow the steps for "**Transferring a file from the local machine to running container"** and **"Transferring a file from running container to the local filesystem**" below.



Transferring a file from the local filesystem to running container

Check running container by typing the following command in terminal :

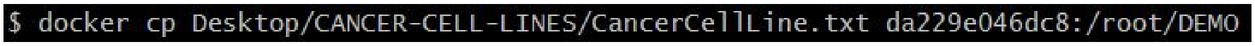
```
#List running containers

docker ps
```



```
$ docker ps
CONTAINER ID        IMAGE                         COMMAND                    CREATED
        STATUS              PORTS                         NAMES
da229e046dc8        kristiyanto/guidock           "/bin/sh -c 'sh /root"     35 minutes ag
o       Up 35 minutes       8787/tcp                      gloomy_bardeen
```

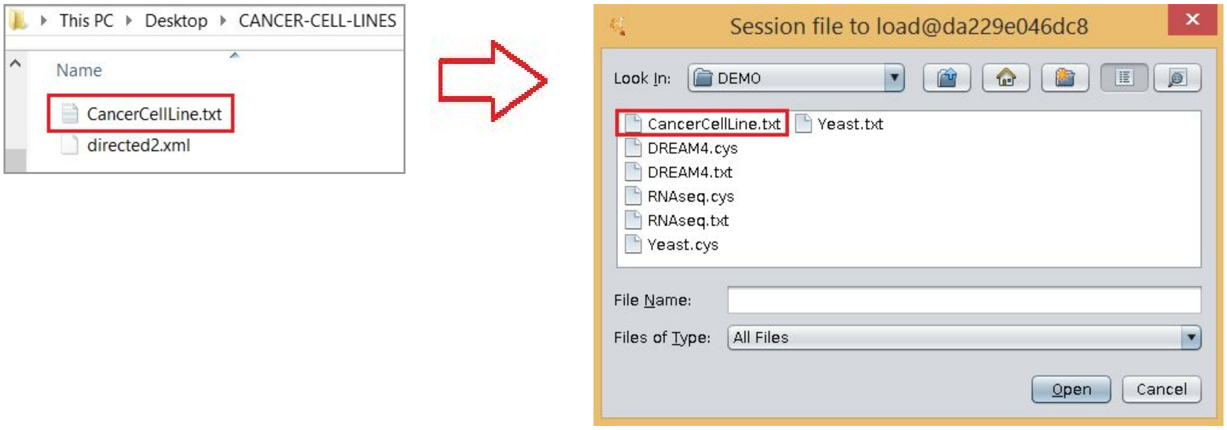
Transfer a file from the local filesystem to running container by typing the following command in terminal:

```
#Transfer file from the local filesystem to a container.

docker cp localPath containerID:path
```



```
$ docker cp Desktop/CANCER-CELL-LINES/CancerCellLine.txt da229e046dc8:/root/DEMO
```

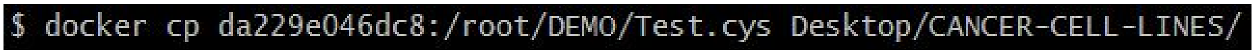
Data file is added to "/root/DEMO" directory.



Transferring a file from running container to the local filesystem

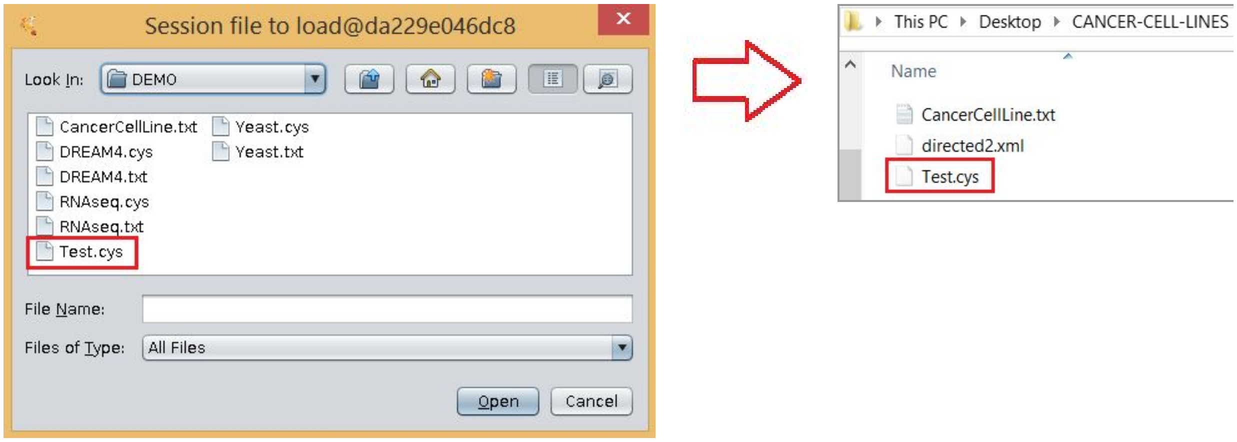
To transfer a file from running container to the local filesystem, type the following command in terminal:

```
#Transfer file from a container to the local filesystem.
docker cp containerID:path localPath
```



```
$ docker cp da229e046dc8:/root/DEMO/Test.cys Desktop/CANCER-CELL-LINES/
```

Data file is saved in "Desktop/CANCER-CELL-LINES" directory from running container.



Session file to load@da229e046dc8

Look In: DEMO

CancerCellLine.txt
DREAM4.cys
DREAM4.txt
RNAseq.cys
RNAseq.txt
Test.cys
Yeast.cys
Yeast.txt

File Name:

Files of Type: All Files

This PC ▸ Desktop ▸ CANCER-CELL-LINES

Name

CancerCellLine.txt
directed2.xml
Test.cys