

KAEA Docker tutorial

This is a tutorial intended to explain to KAEA users how to create a docker container of the pipeline using docker and git.

1) Docker Installation

The first step is to install Docker on the host system. This will allow you to retrieve an image of the pipeline. The first step to do is to create a docker account: <https://id.docker.com/login/> Then download the docker installation file that corresponds to your OS and install it.

2) Git Installation

Git will be used to retrieve the needed files from the Github repository. To install git, please open your command line and type in:

```
## Installing on Linux
sudo apt install git-all
```

The easiest way to install Git on a Mac is to install the Xcode Command Line Tools which comes with Git among other things. On Mavericks (10.9) or above you can do this simply by trying to run the git command from the Terminal. To check if Git has been properly installed, type in:

```
## Installing on Mac
git --version
```

Or you can download Git here: <https://git-scm.com/download/mac> and go through the installation process.

3) Retrieve Dockerfile

Create a directory where you would like to work and head in that directory. Type in:

```
git clone https://github.com/Mahmoudhallal/Docker.git
```

4) Build and run Docker

Follow the following script to build the docker container:

```
cd /Docker/
docker build -t kaea .
docker run -v <local_data_path>:/home/user/KAEA/data -it docker_trial /bin/bash
```

<local_data_path> being the path to the MaxQuant data file on the local host.

This might take ~5 minutes.

5) Create conda environment

Create the conda environment and activate it:

```
cd /snakemake/  
#create the env  
conda env create --name snakemake-general --file environment.yaml  
  
#Activate the env  
source activate snakemake-general
```

This might take ~5 minutes.

You have set up a conda environment and activate it and it is ready to run. Go to the config file (config.yaml) and modify according to your samples.