If rstudio crashes frequently => restart the container maplet

**Create docker with different versions of rstudio**

docker run -e PASSWORD=pwd --rm -p 8787:8787 -v /Users/nis2034/Desktop/nis2034/Desktop/Nish/RProjects/maplet-test:/home/rstudio/home --detach --name maplet rocker/verse

if it didn't work

docker run -e PASSWORD=pwd --rm -p 8787:8787 -v /Users/nis2034/Desktop/nis2034/Desktop/Nish/RProjects/maplet-test:/home/rstudio/home --detach --name maplet rocker/verse:4.0.4

if it didn't work

docker run -e PASSWORD=pwd --rm -p 8787:8787 -v /Users/nis2034/Desktop/nis2034/Desktop/Nish/RProjects/maplet-test:/home/rstudio/home --detach --name maplet rocker/rstudio:latest

**For autonomics**

https://www.bioconductor.org/help/docker/

docker run -e PASSWORD=pwd --rm -p 8787:8787 -v /Users/nis2034/Desktop/nis2034/Desktop/Nish/RProjects/autonomics:/home/rstudio/home --detach --name maplet\_auto bioconductor/bioconductor\_docker:devel

http://localhost:8787/

uname : rstudio

password : pwd

**Install maplet**

devtools::install\_github(repo="krumsieklab/maplet", subdir="maplet")

installation options : 3

if any package installation failed - try to install them seperately.

library(maplet)

**Install autonomics**

if (!requireNamespace("BiocManager", quietly = TRUE))

install.packages("BiocManager")

# The following initializes usage of Bioc devel

BiocManager::install(version = '3.12')

BiocManager::install("autonomics")

https://bioconductor.org/packages/devel/bioc/vignettes/autonomics/inst/doc/using\_autonomics.html

https://github.com/Bioconductor/bioconductor\_docker/issues/27#issuecomment-852911932

https://bioconductor.org/packages/devel/bioc/vignettes/autonomics/inst/doc/using\_autonomics.html

**Create image**

docker commit -m "maplet setup 27April2021" -a "nis2034" maplet maplet:2.0

docker commit -m "docker hub push" -a "nis2034" maplet2 nis2034/auto-maplet

docker rmi 9f3753ef6df6

docker run -m=6g --cpu-shares=3 -e PASSWORD=pwd --rm -p 8786:8787 -v /Users/nis2034/Desktop/nis2034/Desktop/Nish/RProjects/autonomics:/home/rstudio/home --detach --name maplet2 maplet:2.0

**Git Fork**

https://docs.github.com/en/github/getting-started-with-github/fork-a-repo

1. Fork
2. Clone to local
3. git remote -v
4. git remote add upstream https://github.com/krumsieklab/maplet.git
5. git remote -v

origin https://github.com/nis2034/maplet.git (fetch)

origin https://github.com/nis2034/maplet.git (push)

upstream https://github.com/krumsieklab/maplet.git (fetch)

upstream https://github.com/krumsieklab/maplet.git (push)

1. git fetch upstream - to synch with krumsiek
2. git push - to update the fork

**To push to docker hub**

https://hub.docker.com/

docker login

uname: nis2034

pwd: Aiden123$

docker push nis2034/auto-maplet:latest

docker pull nis2034/auto-maplet:latest

https://docs.docker.com/docker-hub/

docker save -o docker\_images\_all.tar auto-maplet:latest, maplet:2.0, my-mysql-test:1.1.0, code.qatar-med.cornell.edu/bioinformatics/cancer\_metabolism/cancermeta-docker:1.1.1

docker save -o auto-maplet.tar nis2034/auto-maplet:latest

https://blog.ssdnodes.com/blog/docker-backup-volumes/

**Latest bioconductor docker installation**

docker pull bioconductor/bioconductor\_docker

docker run -e PASSWORD=pwd --rm -p 8787:8787 -v /Users/nis2034/Desktop/nis2034/Desktop/Nish/RProjects/autonomics:/home/rstudio/home --detach --name maplet\_auto\_june bioconductor/bioconductor\_docker:latest

Above didn't work

**Try with latest rstudio docker**

docker run -e PASSWORD=pwd --rm -p 8787:8787 -v /Users/nis2034/Desktop/nis2034/Desktop/Nish/RProjects/autonomics:/home/rstudio/home --detach --name maplet\_auto\_8June rocker/rstudio

devtools:: install\_github('bhagwataditya/autonomics',

repos = BiocManager::repositories(),

dependencies = TRUE, upgrade = FALSE)

Above didn't work

**Try with base rstudio docker (r 4.0.5) - current working one**

docker run -e PASSWORD=pwd --rm -p 8787:8787 -v /Users/nis2034/Desktop/nis2034/Desktop/Nish/RProjects/autonomics:/home/rstudio/home --detach --name maplet\_auto\_8June rocker/verse:4.0.5

devtools::install\_github('bhagwataditya/autonomics',

repos = BiocManager::repositories(),

dependencies = TRUE, upgrade = FALSE)

devtools::install\_github(repo="krumsieklab/maplet", subdir="maplet")

Create image

docker commit -m "maplet setup 27April2021" -a "nis2034" maplet maplet:2.0

docker commit -m "maplet setup as suggested by KS" -a "nis2034" maplet\_auto\_8June nis2034/auto-maplet\_r4.0.5

If container is stopped

docker run -e PASSWORD=pwd --rm -p 8787:8787 -v /Users/nis2034/Desktop/nis2034/Desktop/Nish/RProjects/autonomics:/home/rstudio/home --detach --name maplet\_auto\_r4.0.5 nis2034/auto-maplet\_r4.0.5

install ggplot

install DT ---> install.packages("DT")

BiocManager::install("hmdbQuery")

Github version control

git init

git add --all

git commit -m "first commit"

git branch -M main

git remote add origin https://github.com/nis2034/Beef-Metabolomics.git

git push -u origin main

Pushing container to github

export CR\_PAT=ghp\_P3GJ58j1i0HPAzW7yR90IF5OiROLC42n4u7n

echo $CR\_PAT | docker login ghcr.io -u USERNAME --password-stdin

docker tag nis2034/auto-maplet\_r4.0.5:latest ghcr.io/nis2034/auto-maplet\_r4.0.5:latest

docker push ghcr.io/nis2034/auto-maplet\_r4.0.5:latest

docker inspect ghcr.io/nis2034/auto-maplet\_r4.0.5:latest

latest: digest: sha256:137f2e04607f9187e0aa87d6814da51fe8e7860d505ec04c1849e16be5d44207 size: 2426

docker pull ghcr.io/nis2034/auto-maplet\_r4.0.5:latest

if not working above, try the below

docker pull ghcr.io/nis2034/auto-maplet\_r4.0.5:latest @ sha256:137f2e04607f9187e0aa87d6814da51fe8e7860d505ec04c1849e16be5d44207

Read more about docker file

docker build -t ghcr.io/nis2034/auto-maplet\_r4.0.5:latest .

https://docs.github.com/en/packages/working-with-a-github-packages-registry/working-with-the-container-registry

To locally connect your container image to a repository, you must add this line to your Dockerfile:

LABEL org.opencontainers.image.source <https://github.com/OWNER/REPO>

**Windows**

echo ghp\_P3GJ58j1i0HPAzW7yR90IF5OiROLC42n4u7n> token.txt

type token.txt

type token.txt| docker login ghcr.io -u USERNAME --password-stdin

docker pull ghcr.io/nis2034/auto-maplet\_r4.0.5:latest

docker.exe run -e PASSWORD=pwd --rm -p 8787:8787 -v D:\\nis2034:/home/rstudio/home --detach --name

maplet\_auto\_r4.0.5 ghcr.io/nis2034/auto-maplet\_r4.0.5:latest

http://localhost:8787/

uname : rstudio

pwd : pwd

When using linux terminal always use docker.exe instead of docker command.

# Docker from [karstensuhre](https://github.com/karstensuhre)/[tensordocker](https://github.com/karstensuhre/tensordocker)

Cd /mnt/d/nis2034/metabolomics/beef\_data

To install the image from the command line:

Docker.exe pull ghcr.io/karstensuhre/tensordocker:1.0

Docker.exe stop "6b8eb2386254822f6c3dd0ef77ec63937dda1ea34ac34179e56e85898a9c61b8"

Docker.exe rm "6b8eb2386254822f6c3dd0ef77ec63937dda1ea34ac34179e56e85898a9c61b8"

To run the docker image (adapt the -v option to mount the required local directory):

Docker.exe run -v `pwd`:/home/rstudio/host -it --detach --name tensor -p8888:8888 -p8786:8787 ghcr.io/karstensuhre/tensordocker:1.0

Docker.exe run -v D:\\nis2034\\metabolomics:/home/rstudio/host -it --detach --name tensor -p8888:8888 -p8786:8787 ghcr.io/karstensuhre/tensordocker:1.0

Rstudio is not automatically started in the image. To start the server:

docker.exe exec -it tensor rstudio-server start

To access the rstudio server:

* <http://localhost:8786>  (rstudio interface, user: rstudio, password: pwd)

To obtain a shell in the container:

docker exec -it tensor /bin/bash

To update/install [maplet](https://github.com/krumsieklab/maplet) from the latest commit:

devtools::install\_github(repo="krumsieklab/maplet", subdir="maplet")

To update/install [autonomics](https://github.com/bhagwataditya/autonomics) from the latest commit:

remotes::install\_github('bhagwataditya/autonomics', repos = BiocManager::repositories(), dependencies = TRUE, upgrade = FALSE)

docker commit -m "Docker setup KS" -a "nis2034" tensor ghcr.io/nis2034/tensordocker\_nis2034:1.0

Github version control

Sudo git init

git add –all

sudo git commit -m "initial commit"

sudo git branch -M main

sudo git remote add origin https://github.com/nis2034/Beef-Metabolomics.git

git push -u origin main

uname : nis2034

password : ghp\_P3GJ58j1i0HPAzW7yR90IF5OiROLC42n4u7n

now onwards personal access token is the password.

Pushing container to github

cat token.txt| docker.exe login ghcr.io -u USERNAME --password-stdin

docker tag nis2034/auto-maplet\_r4.0.5:latest ghcr.io/nis2034/auto-maplet\_r4.0.5:latest

docker push ghcr.io/nis2034/auto-maplet\_r4.0.5:latest