11falsenonelisttrue

Compute Resources

Have questions or need help with compute, including activation or issues? Follow this link.

User Agreement

Docker Usage

The information on this page assumes that you have a knowledge base of using Docker to create images and push them to a repository for use. If you need to review that information, please see the links below.

https://washu.atlassian.net/wiki/spaces/RUD/pages/1705115761/Docker+and+the+RIS+Compute1+Platform?atlOrigin=eyJpljoiNzc4YTZjNjlxYmQwNGI3OTk4M2Q0M\

https://washu.atlassian.net/wiki/spaces/RUD/pages/1864892726/Docker+Basics+Building+Tagging+Pushing+A+Custom+Docker+Image?atlOrigin=eyJpljoiMTVjMjNIM

storageN

The use of storageN within these documents indicates that any storage platform can be used.

Current available storage platforms:

storage1

storage2

Image Details

Includes RoseTTAFold All-Atom

Docker Image

]]>

Docker Tag

The <tag> will refer to the version of the Docker container. Please see below for the available versions.

Running RoseTTAFold All-Atom Non-interactively

Copy the script runscript.sh

Copy the script bsub-non-interactive.sh

Keep both scripts in the same directory.

Change the variables such as the COMPUTE_GROUP, OUTPUT_PATH, INFERENCES_PATH among others.

E.g.

Copy the base.yaml config file and put it in the config/inference directory.

Create a config inference yaml file.

The inference config file should inherit the base settings from the base.yaml file.

The defaults should be base and _self_.

Set the job name; otherwise, the default job name will be "structure_prediction."

All the input files should have be prefixed with inputs/.

For example, the K7N608.fasta file should be set as inputs/K7N608.fasta

Example config file named Vmn1r78_E1050.rtaa.yaml

Launch the non-interactive app

> # Do not include the yaml file extention. ./bsub-non-interactive.sh Vmn1r78_E1050.rtaa]]>

Go to the OUTPUT_PATH to find the results. A successful run should generate a pdb file.

The output log should look like the following

Available RoseTTAFold Versions

Current Version:

1.0.0