

A.

```
Dockerfile
FROM centos:centos7

# name of the maintainer of this image
MAINTAINER laetitia.guillot@univ-rennes1.fr
USER root
# install the latest upgrades
RUN yum -y update && yum clean all
RUN yum -y install csh
RUN yum -y install unzip
RUN yum -y install zip
# install dos2unix et git
RUN yum -y install git git-core git-daemon-run
RUN yum -y install dos2unix

RUN git clone https://github.com/laeticlo/Ectoline.git EctoLine
RUN dos2unix /EctoLine/thirdparty/pepnovo/pepnovo.3.1b/Models/**/*.*
RUN dos2unix /EctoLine/thirdparty/pepnovo/pepnovo.3.1b/Models/*/*.*

ENV PATH /EctoLine/ports/x386-linux/bin:$PATH
ENV PATH /EctoLine/scripts:$PATH
```

B.

The screenshot shows the Galaxy web interface for running a workflow named "peptimapper". The interface includes a top navigation bar with "Galaxy" and various menu items like "Analyze Data", "Workflow", "Shared Data", "Visualization", "Admin", "Help", and "User". A left sidebar contains a "Tools" section with a search bar and a list of tool categories such as "FASTA manipulation", "Protein characterization and function", "Protein and peptide sequences tools", "Get Data", "Send Data", "Convert Formats", "Fetch Sequences", "Proteogenomics tools", "Statistics", "Graph/Display Data", "Text Manipulation", "Peptimapper", "Filter and Sort", "Join, Subtract and Group", and "Workflows". The main content area is titled "Running workflow 'peptimapper'" and contains four steps:

- Step 1: PepNovoTag (version 3.1)**
  - Spectra file (MGF format): S25: cyto\_06.mgf
  - Tag length: 5
  - Number of tags per spectra: 10
- Step 2: PepMatch (version 2.0)**
  - PSTs file (Text): Output dataset 'pstsfile' from step 1
  - Chromosome file (Fasta): S26: Ectsi\_V2.fasta
  - Mass tolerance: 0.5
  - Min. hits: 2
  - Min. peptides: 3
  - Distance: 5000
- Step 3: ClustToGFF (version 2.0)**
  - Clusters file (Text): Output dataset 'clustersfile' from step 2
  - GFF files repository (Zip): 508: gff3\_juin20123\_plus.zip
- Step 4: ClustQualify (version 2.0)**
  - Clusters file (Text): Output dataset 'clustersfile' from step 2
  - GFF files repository (Zip): 508: gff3\_juin20123\_plus.zip

At the bottom, there is a checkbox for "Send results to a new history" and a "Run workflow" button.

Tools

search tools

Inputs

- FASTA manipulation
- Protein characterization and function
- Protein and peptide sequences tools
- Get Data
- Send Data
- Convert Formats
- Fetch Sequences
- Proteogenomics tools
- Statistics
- Graph/Display Data
- Text Manipulation
- Peptimapper
- Filter and Sort
- Join, Subtract and Group

Workflows

Workflow Canvas | peptimapper

