

PARGT User's Guide for macOS

(Version 1.0)

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PARGT is a standalone software package developed to predict antimicrobial resistance proteins in bacteria. It is written mainly in python3 though some modules are implemented in R and called from the main python script.

1. To install and use PARGT on a Mac:

- Download “PARGT_Mac.zip” from Github link- <https://github.com/abu034004/PARGT> . Unzip it and save it in a directory.
- Download “Materials_PARGT_Mac.zip” from <https://drive.google.com/file/d/1TqT9G4M70GjuPnV4UCCpTluRaFTcOdxO/view?usp=sharing> . Unzip it and save the unzipped files in the “PARGT_Mac” folder. Please note that this zip file contains PSIBLAST, legacy BLAST and PSIPRED that can also be downloaded from <ftp://ftp.ncbi.nlm.nih.gov/blast/executables/blast+/LATEST/> , <ftp://ftp.ncbi.nlm.nih.gov/blast/executables/legacy.NOTSUPPORTED/2.2.26/> and https://drive.google.com/file/d/14WY4aoR3TZz2p4_Xb6vGBcjcZmvGnfYX/view?usp=sharing , respectively, if different versions of BLAST and PSIPRED need to be installed on your machine.
- You will need to install “Jupyter Notebooks” if you want to use the notebook version of this program. For installation, visit the link: <https://www.anaconda.com/download/> and install anaconda for python 3. To install it from a terminal window, please visit the link: <https://jupyter.org/install> .
- You may get an error indicating permission has been denied while running legacy BLAST and PSIPRED files. If this occurs, please follow the steps below:
Step 1: Run the command “sudo chmod 755 psipred”.
Step 2: Use the ‘cd’ command to go the directory where the “PARGT_Mac/blast/bin” folder has been saved and run the commands “sudo chmod 755 blastpgp” and “sudo chmod 755 makemat”.
Note that you need administrative permissions to perform these two steps.
- Edit the fasta file “input_seq.fasta” to include sequences you want to test. Note that there are some default example test sequences in this file, and you can also use example test sequences available in the folder “test examples”.
- Next, use the ‘cd’ command to go to the directory where the “PARGT_Mac” folder has been saved and then type the command “jupyter notebook”.

After a couple of seconds, a new page for Jupyter Notebook will appear in your default browser. A screenshot is shown below.

localhost:8888/tree

jupyter

Files Running Clusters

Select items to perform actions on them.

Upload New

Name	Last Modified	File size
blast	17 hours ago	
test examples	15 minutes ago	
PARGT.ipynb	Running 11 hours ago	32 kB
AAC.R	11 hours ago	828 B
CTDC.R	11 hours ago	2.99 kB
CTDD.R	11 hours ago	5.67 kB
CTDT.R	11 hours ago	3.39 kB
error.log	17 days ago	0 B
file_with_pkgTest.R	19 days ago	217 B
GL_updated.R	a month ago	4.24 kB
input_seq.csv	33 minutes ago	6.61 kB
input_seq.fasta	an hour ago	11.6 kB
out.ckp	34 minutes ago	193 kB
out.ss	34 minutes ago	37.7 kB
out.txt	a month ago	12 kB
PARGT.py	seconds ago	23.2 kB

Click on PARGT.ipynb (marked by the red circle in the figure above). PARGT will open up in a new browser window or tab. A screenshot is shown below. Please note that the PARGT.py script is included if a user wants to use it rather than the notebook (.ipynb) version.

localhost:8888/notebooks/PARGT.ipynb

jupyter PARGT Last Checkpoint: 15 hours ago (autosaved)

File Edit View Insert Cell Kernel Widgets Help

Trusted Python 3

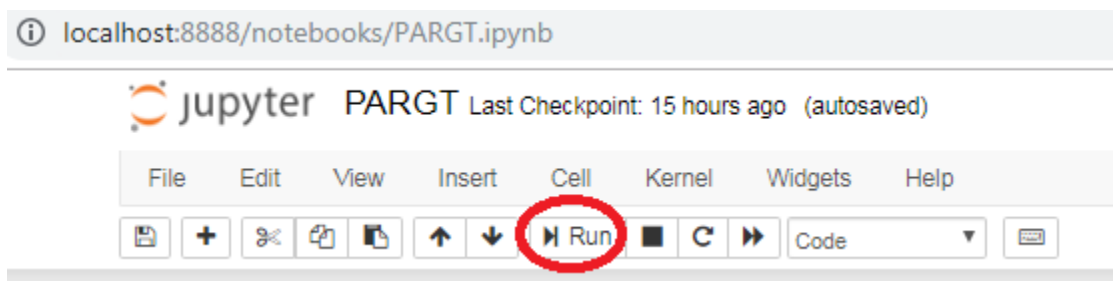
```

In [ ]: 1 import numpy as np
        2 import pandas as pd
        3 import os
        4 import sys
        5 import subprocess
        6 import rpy2
        7 from rpy2 import *
        8 import rpy2.robjects as ro
        9 from rpy2.robjects.packages import importr
       10 import rpy2.robjects.packages as rpackages
       11 from rpy2.robjects.vectors import StrVector
       12 #from rpy2.robjects import globalenv
       13 from rpy2.robjects.numpy2ri import numpy2ri
       14 from rpy2.robjects.packages import import STAP
       15 #numpy2ri.activate()
       16 from rpy2.robjects import pandas2ri
       17 import shutil
       18 from shutil import copyfile
       19 import math
       20 import re
       21 import fileinput
       22 import tkinter
       23 from tkinter import *
       24 #import tkFont
       25 #from PIL import Image
       26 #from PIL import ImageTk
       27 from IPython.display import display
       28 from IPython.display import HTML
       29 import IPython.core.display as di
       30
       31 di.display_html('<script>jQuery(function() {if (jQuery("body.notebook_app").length == 0) { jQuery(".input_area").toggle(); ;
       32
       33 di.display_html('<<button onclick="jQuery('.input_area').toggle(); jQuery('.prompt').toggle();">Toggle code</button>''', r

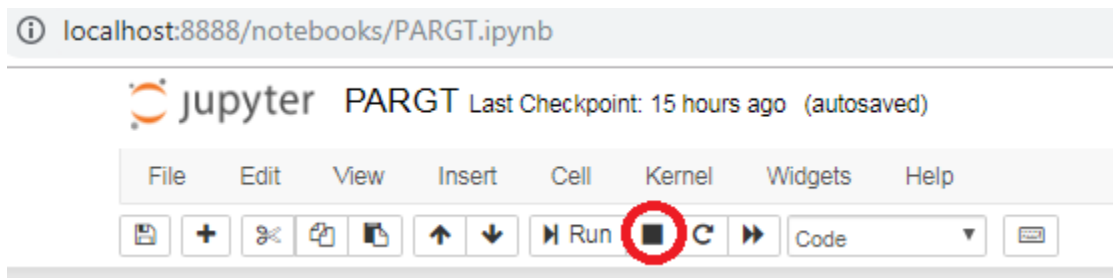
```

Before running the notebook, please install the rpy2 package using the command “conda install -c r rpy2” from the command prompt. Also, please install the tzlocal package using command “conda install -c conda-forge tzlocal” if needed. For details, please visit <https://anaconda.org/r/rpy2> and <https://anaconda.org/conda-forge/tzlocal> for the rpy2 and tzlocal packages, respectively. If your system cannot find the ‘psipred’ executable file, please install the psipred package using the command “conda install -c biocore psipred”. Also, if your system cannot locate the e1071 package, please install the e1071 package using the command “conda install -c r r-e1071”. For details, please visit <https://anaconda.org/biocore/psipred> and <https://anaconda.org/r/r-e1071> for the psipred and e1071 packages, respectively. All of the remaining packages should come with Jupyter Notebook by default. In the worst case, if any package is missing, please use the ‘conda install’ command to install the required packages. Alternatively, users can use the ‘pip install’ command to install the necessary packages rather than using the ‘conda install’ command.

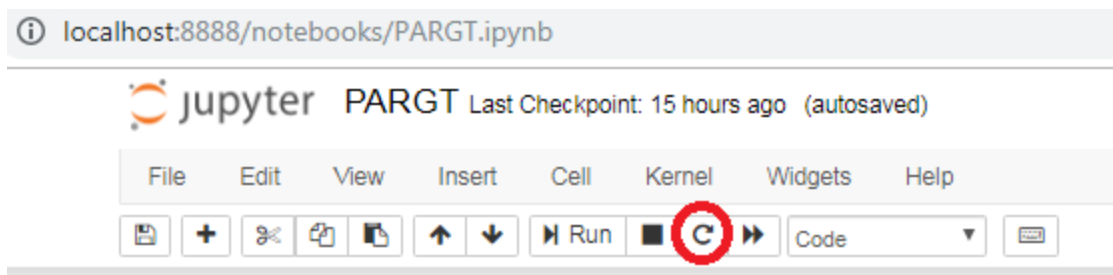
Next, click inside a code cell and then click on the “Run” button (circled in red in the following screenshot).



If you want to stop running the notebook, please click on “Interrupt the kernel” (i.e., the stop button) (circled in red in the following screenshot).



If an error occurs, you can restart the kernel. Click on the “restart the kernel” button (circled in red in the following screenshot).



After starting the notebook or script, a GUI should appear as in the following screenshot.



Please click on the option menu to see all options available in the tool as shown in the following screenshot.



A brief description of the options is given below.

- (a) **Predict aac/bla/dfr/bac/van resistance sequences:** This option is for predicting acetyltransferase (*aac*), beta-lactamase (*bla*), dihydrofolate reductase (*dfr*), bacitracin (*bac*) and vancomycin (*van*) antimicrobial resistance (AMR) proteins from the input fasta sequences in the default "input_seq.fasta" file.
- (b) **Include new aac/bla/dfr/bac/van resistance sequences:** These options are given for a user who wants to include new known AMR sequences to the original training data that comes with this tool. Again the sequences that a user wants to add need to be placed in the "input_seq.fasta" file.
- (c) **Include new aac/bla/dfr/bac/van non-resistance sequences:** These options are given for a user who wants to include new known non-AMR sequences to the training data that comes with this tool. Again the sequences that a user wants to add need to be placed in the "input_seq.fasta" file.

(d) **Restore training sets:** This option allows a user to reset all training datasets back to the original versions that came with this tool.

After successful execution, the tool will show a message- “The operation is successful!” and the predicted output will be available in the “predicted_resistance_sequences.fasta” file located in the “PARGT_Mac” folder.

If you find our tool useful, please cite the following papers.

Citations:

1. Chowdhury, A.S., Call, D.R. and Broschat, S.L., Submitted. PARGT: A Software Tool for Predicting Antimicrobial Resistance in Bacteria. Scientific Reports.
2. Chowdhury, A.S., Call, D.R. and Broschat, S.L., 2019. Antimicrobial Resistance Prediction for Gram-Negative Bacteria via Game Theory-Based Feature Evaluation. Scientific Reports.