

PARGT User's Guide for Mac

(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 main python script.

1. To install and use PARGT on Windows:

- 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/1f1WWxAkPvaX9ikXkhziU4FQv39JPwSW8/view?usp=sharing> . Unzip it and save it in the “PARGT_Mac” folder. Please note that this zip file contains legacy BLAST and PSIPRED that also can be downloaded from <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 needed to install in your machine.
- To install “Jupyter Notebook”, visit the link- <https://www.anaconda.com/download/> and install anaconda for python 3. To install it from terminal, please visit the link- <https://jupyter.org/install> .
- It may happen that you may get an error noticing permission denied while running legacy BLAST and PSIPRED executive files. In this situation, please consider the following steps.
Step-1: Run the command “sudo chmod 755 psipred”.
Step-2: use ‘cd’ command to go the directory where “PARGT_Mac/blast/bin” folder is saved and run the command “sudo chmod 755 blastpgp_universal-macosx” and “sudo chmod 755 makemat”.
- Provide the test fasta sequences in the file “input_seq.fasta”. Please note that there are some example test sequences available in the folder- “test examples”.
- Now, use ‘cd’ command to go the directory where “PARGT_Mac” folder is saved and then type command- “Jupyter notebook”.

Then after couple of seconds, a new page for Jupyter Notebook will appear in your default browser. A screenshot is given 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

Now, click on PARGT.ipynb (marked by red circle in the above figure). Then it will be open up in a new browser. A screenshot is given below. Please note that PARGT.py script is given if a user wants to use it instead of 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

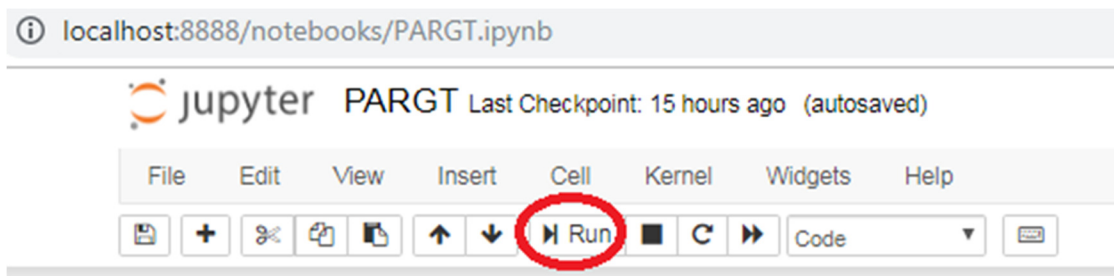
```

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 from rpy2.robjects import 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></script>')

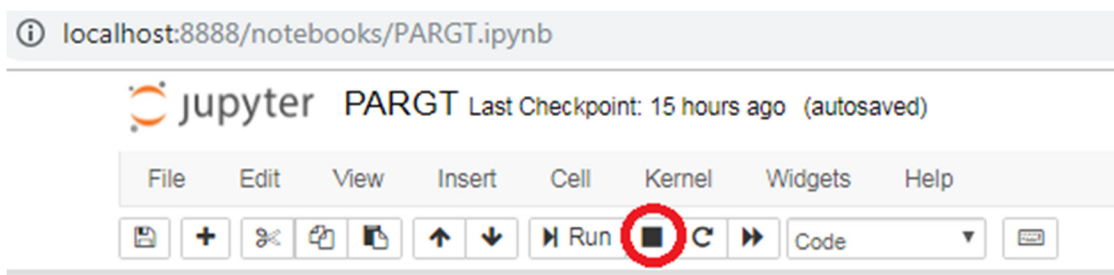
```

Before running the script, please install rpy2 package using command “conda install -c r rpy2” from Anaconda command prompt. Also, please install 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 rpy2 and tzlocal packages, respectively. It may happen that your system cannot find ‘psipred’ executable file. In that case, please install psipred package using command “conda install -c biocore psipred”. Also, if your system cannot locate e1071 package, please install psipred package using command “conda install -c r r-e1071”. For details, please visit <https://anaconda.org/biocore/psipred> and <https://anaconda.org/r/r-e1071> for 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 ‘conda install’ command to install the required packages. Also, users can consider ‘pip install’ command to install necessary packages as an alternative option.

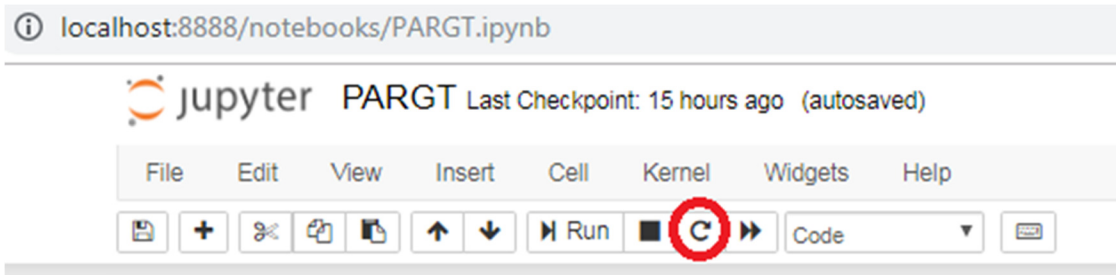
Now, click inside a code cell and then click on “Run” button (red marked in the following screenshot).



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



If you want to restart the kernel after facing an error, please click on “restart the kernel” button (red marked in the following figure).



After running the script, a GUI should appear as below.



Please click on the option menu to see all options available in the tool (please see below the figure).



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 “input_seq.fasta” file.
- (b) **Include new aac/bla/dfr/bac/van resistance sequences:** These options are for a user who wants to include new known AMR sequences to the original training data comes with this tool. Again the sequences that a user wants to add need to be given in the “input_seq.fasta” file.
- (c) **Include new aac/bla/dfr/bac/van non-resistance sequences:** These options are 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 given in the “input_seq.fasta” file.

(d) **Restore training sets:** This option is to reset all training datasets back to the original version came with this tool.

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

Citations:

1. Chowdhury, A.S., Call, D.R and Broschat, S.L., To be submitted. PARGT: A Standalone Software Tool for Predicting Antimicrobial Resistance in Bacteria. Nature Microbiology.
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.
3. Chowdhury, A.S., Khaledian, E. and Broschat, S.L., 2019. Capreomycin resistance prediction in two species of Mycobacterium using a stacked ensemble method. Journal of applied microbiology.