USER GUIDE

TIID SOFTWARE

TOOL IDENTIFYING ISLANDS OF DEFENSE

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List of dependencies

All tests were run on the Linux operating system Ubuntu version 22.10. To run the tool, the Java virtual machine version 17 or higher must be installed on the operating system, available at:

https://www.oracle.com/java/technologies/downloads/.

After installation, you can check that everything is correct by running the test below in your terminal:

```
(base) veras@veras:~$ java --version
java 19.0.2 2023-01-17
Java(TM) SE Runtime Environment (build 19.0.2+7-44)
Java HotSpot(TM) 64-Bit Server VM (build 19.0.2+7-44, mixed mode, sharing)
```

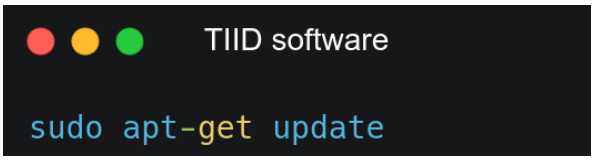
Figure 1. How to check the Java version.

1. Steps to install Mysql on Ubuntu

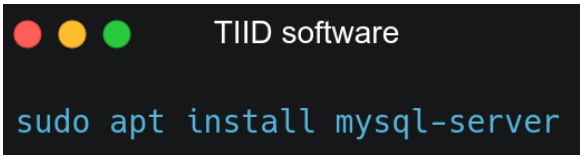
We will install the latest version of MySQL, as you know apt is the repository in Ubuntu 22.10. All the packages are installed via the apt repository.

Let's follow the installation steps on Ubuntu 22.10:

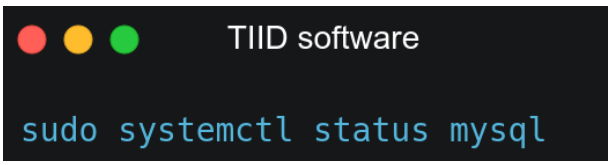
1. Update the Ubuntu Package manager.



2. As a next step let's install the MySQL server with the below command

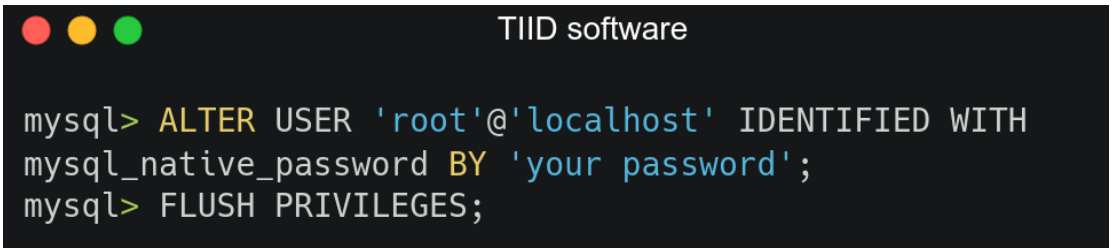


3. Now that we have MySQL installed, we need to check whether the MySQL service is running. You can verify this using the below command.




```
(base) veras@veras:~$ sudo systemctl status mysql
● mysql.service - MySQL Community Server
     Loaded: loaded (/lib/systemd/system/mysql.service; enabled; preset: enabled)
     Active: active (running) since Thu 2023-04-20 15:07:30 -03; 4 days ago
       Docs: man:mysqld(8)
             http://dev.mysql.com/doc/refman/en/using-systemd.html
    Process: 1305 ExecStartPre=/usr/share/mysql-8.0/mysql-systemd-start pre (code=e>
   Main PID: 1395 (mysqld)
     Status: "Server is operational"
      Tasks: 41 (limit: 18886)
     Memory: 310.2M
        CPU: 32min 26.940s
     CGroup: /system.slice/mysql.service
             └─1395 /usr/sbin/mysqld
```

4. Changing the default authentication mechanism of MySQL to "mysql_native_password" and assigning root password.



Note: In the first run of the tool the database will be created, this process will occur only once.

2. BLAST Installation

To proceed with the blast installation follow the steps below

```
allan@ubuntuMySQL:~$ sudo apt install ncbi-blast+
Lendo listas de pacotes... Pronto
Construindo árvore de dependências... Pronto
Lendo informação de estado... Pronto
Os pacotes adicionais seguintes serão instalados:
  libmbedcrypto7 libmbedtls14 libmbedx509-1 ncbi-data
Os NOVOS pacotes a seguir serão instalados:
  libmbedcrypto7 libmbedtls14 libmbedx509-1 ncbi-blast+ ncbi-data
0 pacotes atualizados, 5 pacotes novos instalados, 0 a serem removidos e 64 não
 atualizados.
É preciso baixar 16,1 MB de arquivos.
Depois desta operação, 72,7 MB adicionais de espaço em disco serão usados.
Você quer continuar? [S/n]
```

To check the installation

```
allan@ubuntuMySQL:~$ blastn -version
blastn: 2.12.0+
 Package: blast 2.12.0, build Mar  8 2022 16:19:08
```

3. PATRIC Command-line Interface Client installation

To install the BV-BRC command line interface 1.039 the user must download the package "*patric-cli-1.039.deb*" from the link: https://github.com/PATRIC3/PATRIC-distribution/releases/download/1.039/patric-cli-1.039.deb

The user can choose to install using dpkg, following the example below. Or you can double-click the package after downloading and use Ubuntu's smart installer.

`sudo dpkg -i` *`patric-cli-1.039.deb`*

At the end of the installation process it is necessary to replace Patric's login script with a custom one for TIID software, the version of the script is shared in this repository. Download it and replace it in the path /usr/share/patric-cli/deployment/plbin/p3-login.pl, see an example below.

sudo cp /home/veras/Download/p3-login.pl /usr/share/patric-cli/deployment/plbin/

After installing the dependencies and setting the password the user must configure the TIID properties file available in the folder called properties, the name of the file to be edited is t4ID.properties and it has the following structure.

```
1 linkDownload=https://ngdc.cncb.ac.cn/padsarsenal/download.php
2 downloadLocation=lib/data
3 userDB=root
4 password="your Password"
```

In line (1) we have the link to download the files from the padsarsenal database, it is set as default, so only change it if you are sure. Line (2) indicates the location where the files will be saved after the download, (3) is the database user, in this case, the superuser root, and finally line (4) the password for the database user.

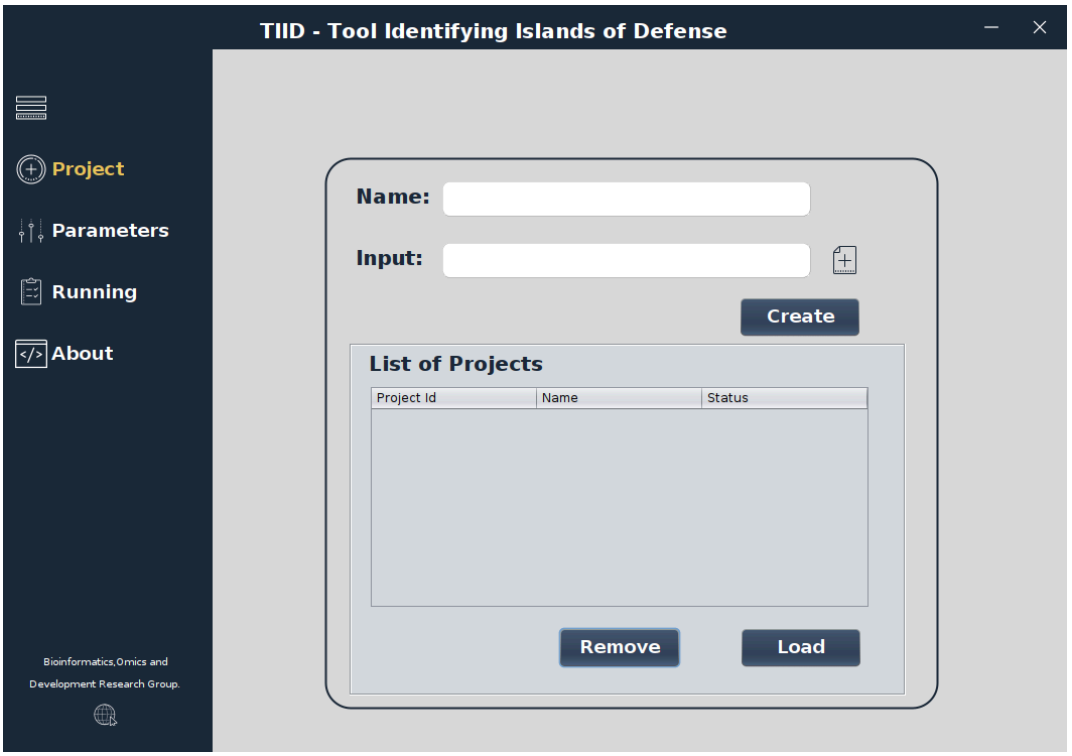
4. Screen Description

Below are all the screens that make up the TIID software. The user will have a side menu bar that will give access to the other windows.

In the main window, the user can create the project and input the organisms to perform the analysis. In this window, it is possible to load previously created projects that for some reason have not finished their processing.

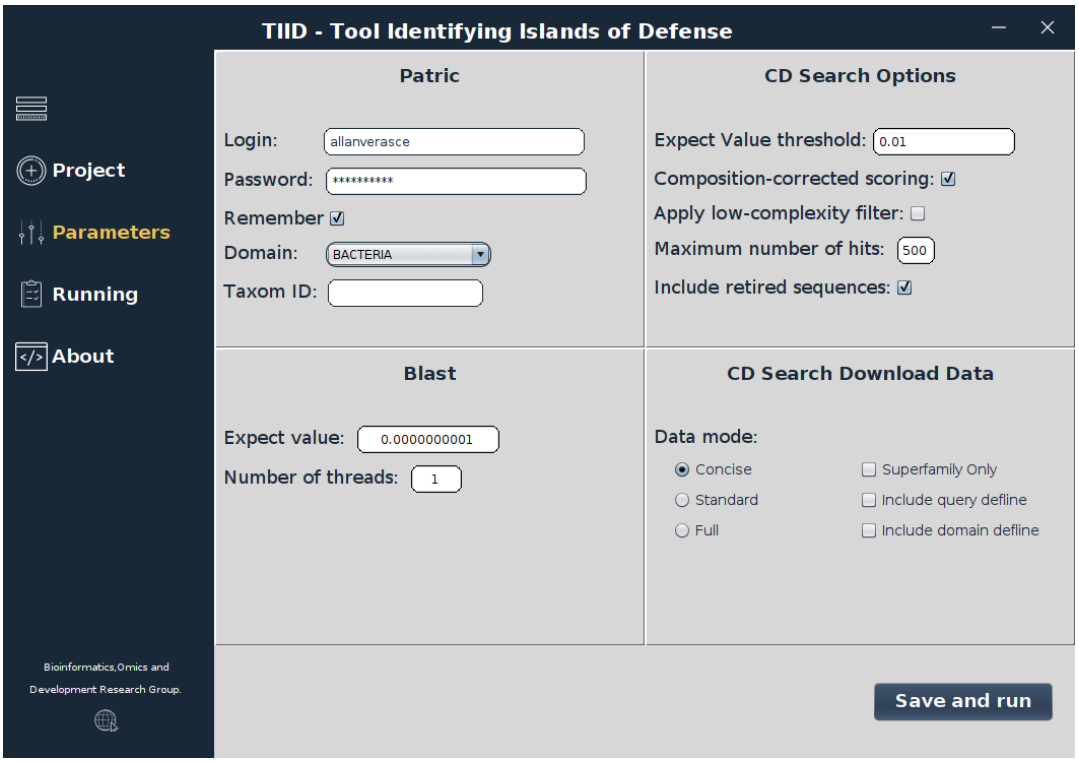
If the user wants to load a project, all he has to do is select it from the list, click on it, and then press the load button. Analogously, if you want to delete a project, after selecting it, click on the remove button.

So to create a new project, the user must inform the project name and add the input data, then it is necessary to press the "*Create*" button.



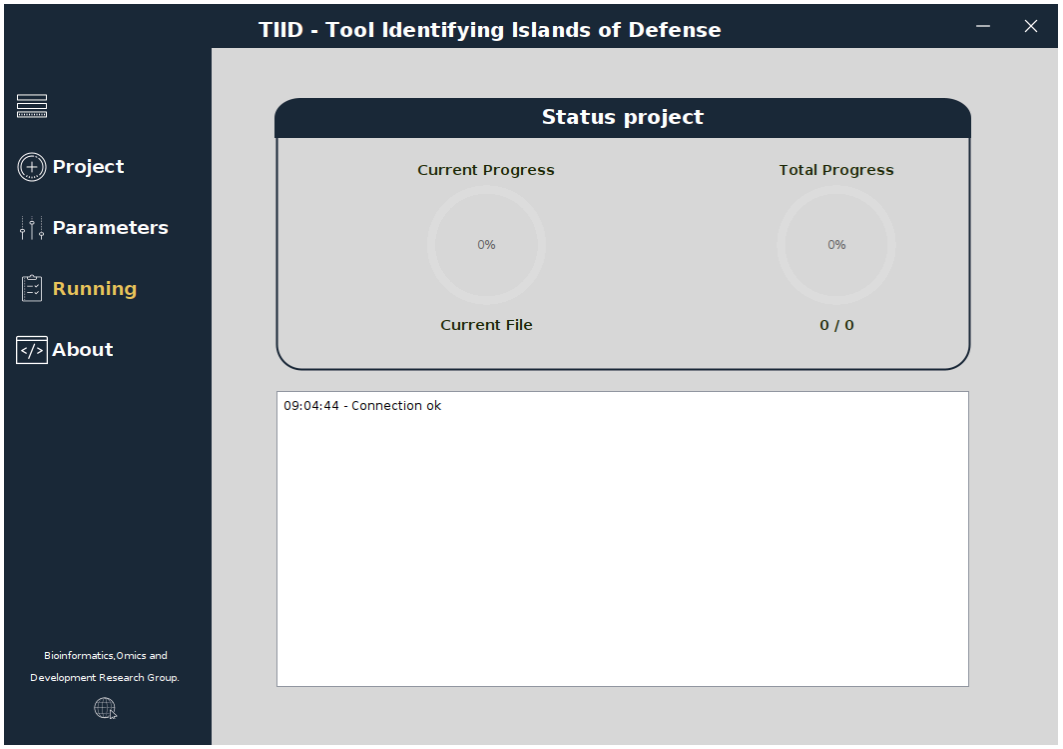
Main Window

After that, you will be directed to the parameters window to enter their values, then press the "*Save and Run*" button.



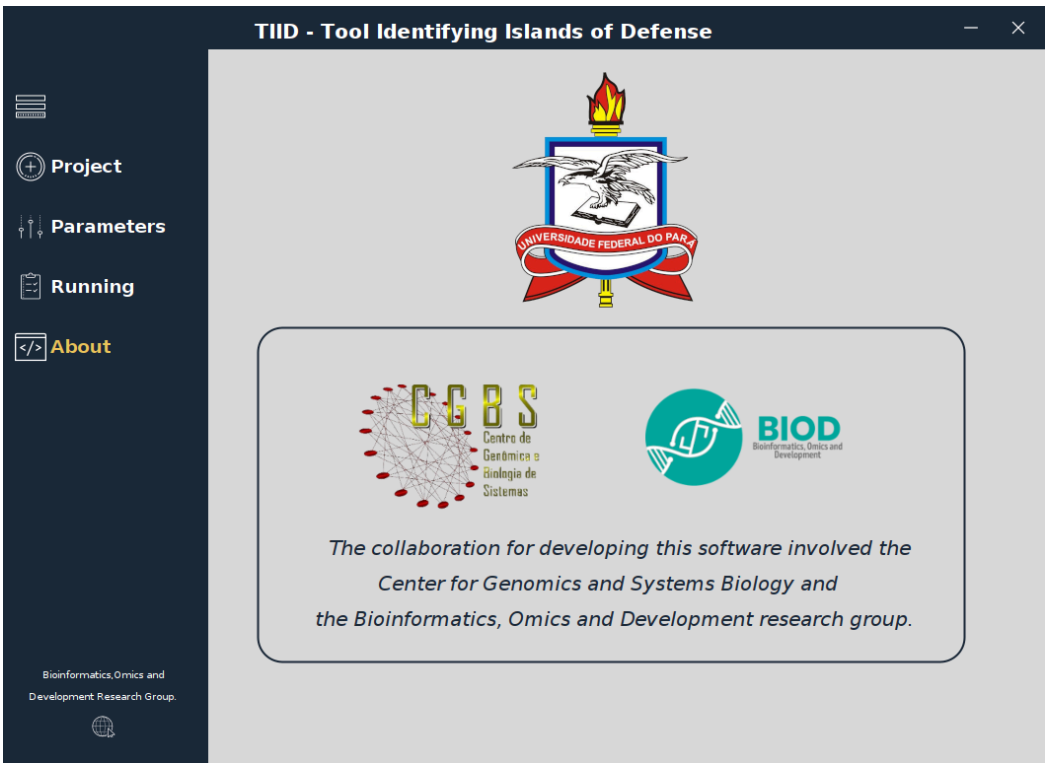
Parameter window

Then the execution window will be displayed, where the user can follow the processing by means of the taskbar and the logs directly in the interface, if more than one input file is added the quantity of them will be displayed in the total progress bar, while the individual progress can be followed in the current progress.



Run Window and Log

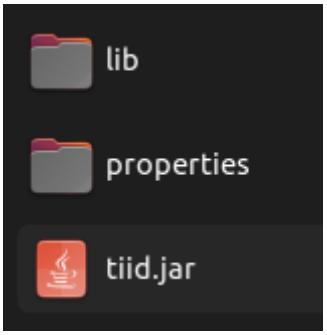
The About window brings up information about the BIOD research group.



About Screen

5. Download and set permissions

When unpacking the software file you will get the structure shown in the image below:

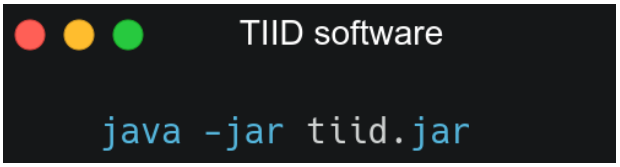


You then need to configure the permissions of the operating system, for example, open the Linux terminal and run the command below in the root folder of the software.

chmod -R 777 tiid

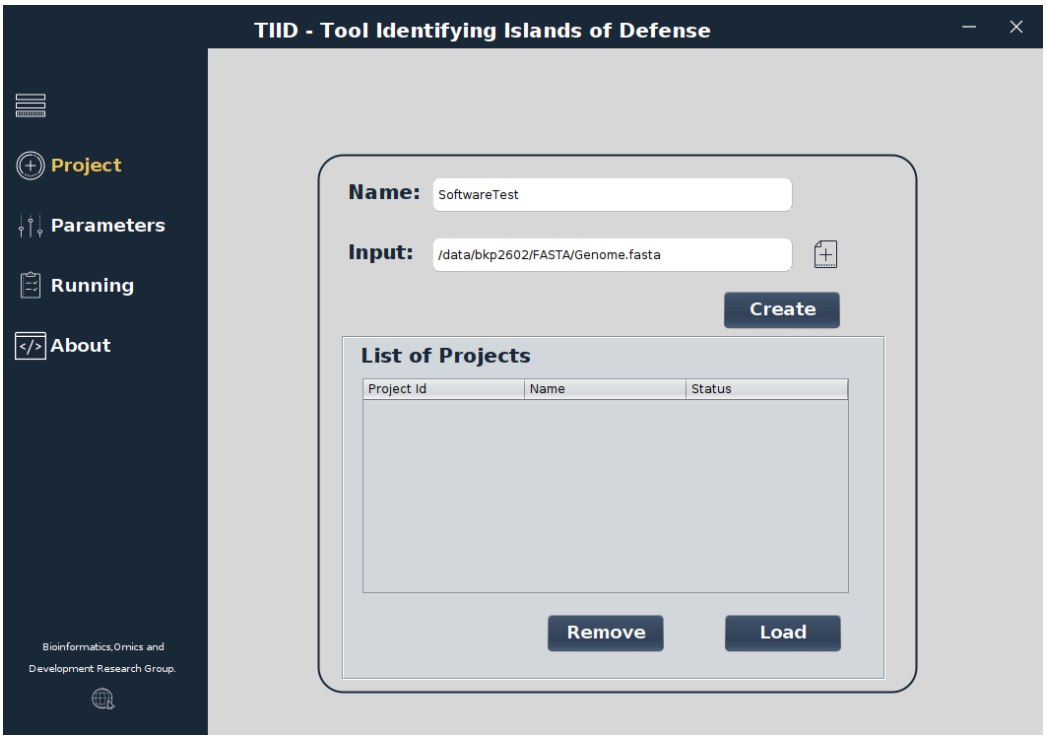
6. How to run TIID?

To run the TIID software you must enter the software folder where you downloaded it and run the following command line.

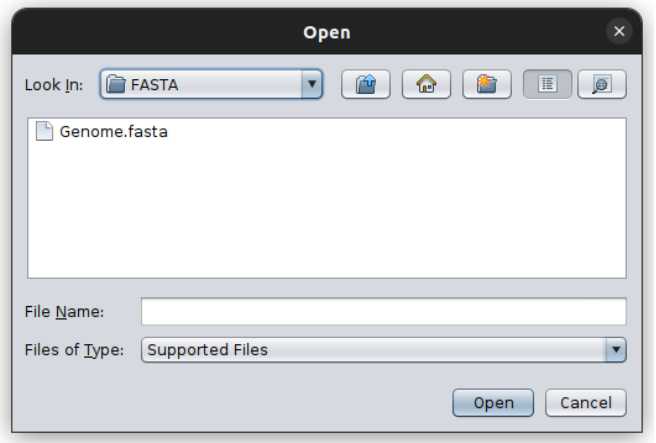


7. Creating a project

Enter the name of the project and then press the button with the plus symbol; this will open the navigation window for adding files in fasta format.

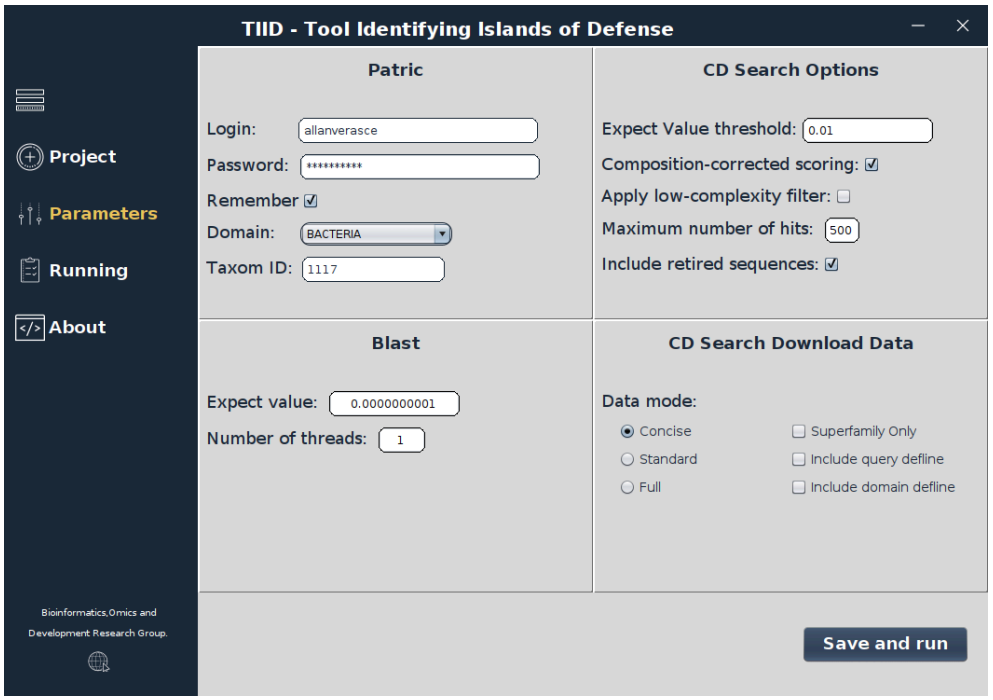


Select the file or files in FASTA format and press open.

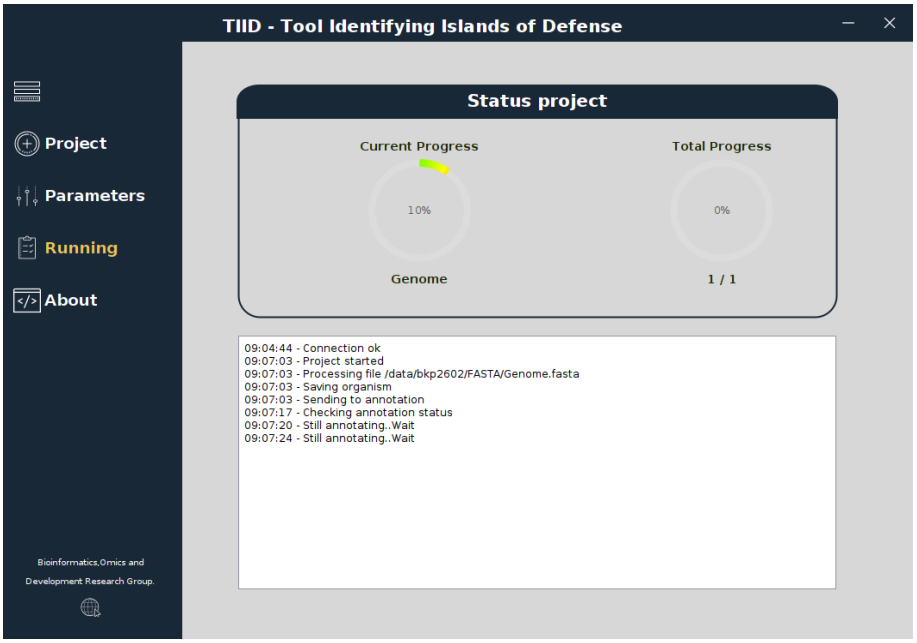


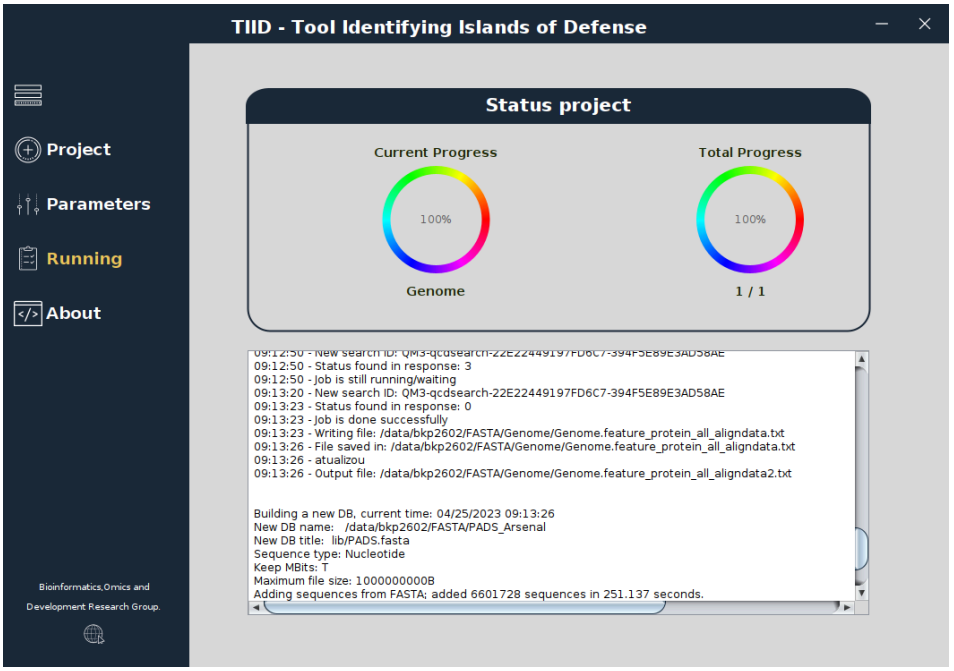
The parameters are grouped into: (i) Patric parameters (annotation system, the account must be previously created by the user) login, password, domain, and Taxom ID of the organism to be analyzed. if the user leaves the remember option checked, the user information and password will be saved in the interface. (ii) BLAST parameters: e-value and number of processors (Threads).

Cd-Search parameters are divided into options for submitting to the tool and for downloading the result, all of which are the same as in the process performed by the Web version of the tool.



In the following two windows, you can see the start and end of the processing of an analysis. You can see that as the steps are completed the user can follow the LOG of each and allied to this has an overview of the processing of the organism in question and others that are in the queue.





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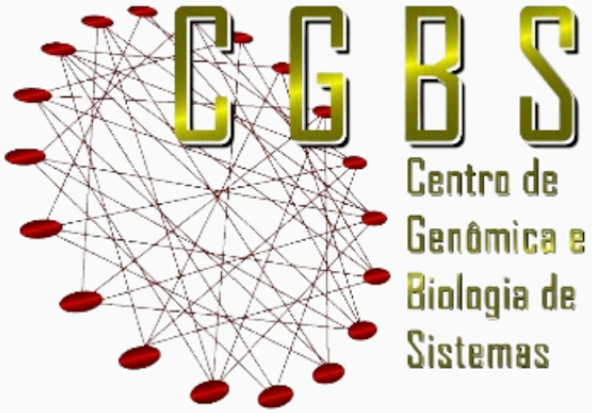
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BIOD
Bioinformatics, Omics and
Development