RubioSeq-GUI 1.0
Manual
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1. Preface
This document is meant to serve as a guide for the practical use of RUbioSeq-GUI, a graphical user interface (GUI) for RUbioSeq. It includes explanations of all functionalities to give an idea of basic usage.

2. License
RUbioSeq-GUI developed by the SING group is licensed under a GNU GPL 3.0 License (http://www.gnu.org/copyleft/gpl.html).

3. Prerequisites
All programs listed below and their corresponding dependencies must be correctly installed:
- Java version 1.7 (http://www.java.com/). Executable directory must be added to the PATH environment variable.
- RUbioSeq 3.7 (http://rubioseq.sourceforge.net/).

4. Installation
To install RUbioSeq-GUI user just have to:
1. Download the file RubioSeq-GUI-v1.0.tar.gz from the repository: http://sourceforge.net/projects/rubioseq/files/SourceVersions/.
2. Unpack the file into a folder and you will see three files:
   - rubioseq-gui-webapp.war
   - launch-rubioseq-gui.sh
   - stop-rubioseq-gui.sh

5. RUbioSeq-GUI
1. *Launching and stopping RUbioSeq-GUI*
To launch RUbioSeq-GUI user simply has to run the script launch-rubioseq-gui.sh provided with RUbioSeq-GUI. This command will deploy the RUbioSeq-GUI application in the user machine.

```
> ./launch-rubioseq-gui.sh
```
When the deployment of the application finishes, the default local browser is launched in order to show the welcome page of RUbioSeq-GUI (Figure 1). User can access to the welcome page from other browsers since the application is available at the URL http://localhost:8080/login.zul

An automatic and parallelized suite of pipelines to speed up your NGS data analysis

Welcome to RUbioSeq!

RUbioSeq is a software suite to perform NGS data analysis in an automatic, parallelized and reliable way which is crucial to eliminate manual steps and to speed up result generation. RUbioSeq provides pipelines using state-of-art tools for:

1. Single nucleotide variant (SNVs) calling
2. Copy number variation (CNVs) detection.
3. Bisulfite-seq (BS-seq) data analysis.
4. ChIP-Seq experiments.

More info at http://rubioseq.sourceforge.net/

Figure 1. RUbioSeq-GUI welcome screen.

If the default port used by the application (8080) is already in use in your computer the application cannot be deployed. In this case, you will see the following error in the console where you launched the script:

```
[launch-rubioseq-gui.sh] Port 8080 is already in use by other application. Please, use option -p <port> to specify a free port
```

To fix this problem you have to manually select an available port adding the option -p <port> to the launch script. For example, if you want to deploy the application in the port 10000, you should type:

```
> ./launch-rubioseq-gui.sh -p 10000
```

After the first launching RUbioSeq-GUI user should login as Administrator (section 3) in order to configure the application to be used by users.

To stop RUbioSeq-GUI user simply has to run the script stop-rubioseq-gui.sh provided with RUbioSeq-GUI. This command will stop the execution of the RUbioSeq-GUI application in the user machine.
2. **RUbioSeq-GUI profiles**

The first step for the user when using RUbioSeq-GUI is to select a profile to log in the application. There are two profiles:

- **Administrator.** This profile allows the user to manage and configure the RUbioSeq-GUI application (select a RUbioSeq installation and configure it, manage users and datastores, etc.).
- **User.** Allows the user to make use of RUbioSeq, that is, to create, launch, manage and monitor experiments.

User can select a profile in the welcome screen (Figure 1). There is a single Administrator account (called *admin*) so in order to login user only should introduce the password (default *admin* passord is *admin* and can be changed after first login). There is also a default user account (with username *rubiosequser* and password *rubioseqpass*) and new users can create their own accounts by clicking the 'New Account' button.

3. **Administrator**

When user logs in as *admin* he or she lands in the Administrator panel (Figure 2) where there are available the three main administrator functions:

- **RUbioseq-GUI Configuration.**
- **Users.**
- **Datastores.**

This section gives an in depth explanation of the administrator functions as well as of the concept of *datastore*, which is key in the use of this application.
1. Understanding the concept of Datastore

Since this application can be running in a server where there is a local installation of RUbioSeq and can be accessed via web in order to manage it, it is necessary to keep server security avoiding that users have access to the local file system. For this reason, RUbioSeq-GUI works with **datastores** instead of allowing users to use the server file system to select input files or saving experiment configuration files.

A **datastore** consists of a simple name pointing to a local path. For instance, one can think in a datastore called 'Public_datastore' pointing to the path '/home/data_repository'. When a user wants to access this datastore, user will see a list of the files in 'Public_datastore/' and he/she will not have idea about the real path of this files.

Moreover, a datastore has:

- A mode, which can be **Shared** or **Private**.
  - **Shared** means that the datastore will be shared by all the application users (useful for creating a common data repository).
  - **Private** means that the datastore will be associated to a specific user.
- A type, which can be **Input**, **Output** or **Input/Output**.
  - **Input** means that the datastore will be only used for selecting input files (for instance, the reference genome in a SNV experiment configuration).
  - **Output** means that the datastore will be only available for selecting output files (for instance, for saving an experiment configuration file).
  - **Input/Output** means that the datastore will be used both for input and output. Note: **Shared** datastores have always the type **Input**.

*Figure 2. Administrator panel.*
By default, there is a Private datastore of type Input/Output called 'admin_default' and pointing to '/' which is associated to the administrator profile. This datastore allows the administrator to configure the application and is also useful if RUbioSeq-GUI is used in a private computer so that the administrator is also a regular user and he/she can access to the whole server file system. It is responsibility of the administrator to manage user's datastores, which are necessary to make this application functional.

2. RUbioSeq-Configuration

The RUbioSeq-Configuration page (Figure 3) allows the administrator to:
- Configure the RUbioSeq path.
- Edit the configProgramPaths.xml files for the different RUbioSeq pipelines.
- Establish the datastore creation policy.

In the RUbioSeq Path field user has to select (by clicking the button) the directory of a local installation of RUbioSeq (i.e. the directory that contains the RUbioSeq.pl script).

If a valid RUbioSeq Path is introduced, the application will allow the user to edit the configProgramPath.xml files corresponding to the configuration of the different pipelines supported. By clicking in the different buttons (SNV [Variant Caller], CNV [CnvCaller], Methylation or ChipSeq) user will be brought to a new page where the corresponding configProgramPath.xml can be edited.

For instance, if user clicks the SNV button the screen showed in Figure 4 will appear.
Here the user can edit all the parameters required for this pipeline, which are showed in two different tabs: *Mandatory parameters*, for those that must be configured compulsorily, and *Optional parameters*, for those that are optional. The configuration can be saved by clicking in the *Save* button (placed in the right upper corner bellow the menu). For more information about these configuration files, please, read the RUbioSeq manual.

From this screen, user can come back to the Administrator panel or the RUbioSeq-GUI Configuration screens by using the navigation menu.

![Configuration Screen](image)

**Figure 4. Editing the SNV configProgramPaths.xml file.**

Finally, in the RUbioSeq-GUI Configuration screen user can establish the datastores policy. If the option *Create datastore on user registration* is checked, a private datastore will be created for each user just before its registration. This means two things: (i) that the application will create a folder with the username in the root directory path specified and (ii) a private datastore associated to the new user will be created in the application.

### 3. Manage users

The Users page (Figure 5) allows the administrator to manage the users of the
application. Administrator can edit their data (e-mail, password and set if they are administrators or not) or remove their accounts.

4. Manage datastores

The Datastores page (Figure 6) allows the administrator to manage the datastores of the application. Administrator can edit their data (e-mail, password and set if they are administrators or not) or remove their accounts.

Figure 5. Users management page.

Figure 6. Datastores management page.
4. User

When a user login with his/her personal account lands at the user home (Figure 7) where there are available the main functions:

- **Creating new experiments** (Create SNV/CNV/ChipSeq/Methylation Experiment).
- **Edit an existing XML configuration file** (Edit Experiment).
- **Execute an experiment with RUBioSeq** (Execute Experiment).
- **View user experiments** (My Experiments).

User can also edit his/her personal data by clicking in the text “Logged as <username>” which is placed in the right upper corner. This section explains the details of each function.

Moreover, when user moves to a any page different to the user home, a navigation bar (Figure 8) is presented in order to facilitate navigation. From this menu, user can go back to the user home (Home button) or directly access to the different functionalities.
1. Creating new experiments

RUBioSeq-GUI aims to facilitate the use of RUBioSeq to users and for this reason it includes the functionality of graphically creating the XML experiment configuration files needed to run RUBioSeq experiments. From the user home, users can access to the creation of XML configuration files for the SNV/CNV/ChipSeq/Methylation pipelines by clicking in the corresponding buttons. Apart from saving the XML files, user can also run the experiment.

1. Creating a new SNV Experiment

In this screen (Figure 9) user can edit all the parameters required for the XML configuration file of the SNV pipeline, which are showed in two different tabs: Mandatory parameters, for those that must be configured compulsorily, and Optional parameters, for those that are optional. For more information about these experiment parameters, please, read the RUBioSeq manual.

![Figure 9. Creation of a SNV experiment.](image)

The XML configuration file can be saved by clicking in the Export button (placed in
the right upper corner bellow the menu) which will be enabled if and only if the mandatory parameters have been introduced properly. Also, if the configuration is right, the Execute button will be enabled to allow the user to directly run an experiment using this configuration. Note that before executing an experiment the application will ask the user for saving the XML configuration file.

2. Edit an existing XML configuration file

RUbioSeq-GUI allows users to load and edit existing XML configuration files (Figure 10). To do that, user can click in the Edit Experiment button of the user home or the navigation menu.

![Figure 10. Editing an existing XML configuration file.](image)

In this page user just have to select an existing XML configuration file (by clicking the browse button) and the Experiment type is automatically detected by the application based on the type specified in the XML. After that, the Edit Experiment button will be enabled, allowing the user to load the file and edit it with the configuration editor (the one showed in the previous section).

3. Execute an experiment with RUbioSeq

RUbioSeq-GUI allows users to launch the different RUbioSeq pipelines using existing XML configuration files (Figure 11). To do that, user can click in the Execute Experiment button of the user home or the navigation menu.
In this page user have to: (i) select an XML configuration file (by clicking the browse button); (ii) select the execution mode: complete, to run the complete pipeline, or level, to run a specific level which should be selected. The Experiment type is automatically detected by the application based on the type specified in the XML. After that, the Run Experiment button will be enabled. Clicking this button will cause the execution of the experiment and user will be redirected to a new page where he/she can monitor the experiment progress (Figure 12).

In this view, user will see:

- A progress bar indicating the percentage of experiment executed.
- A text area with the content of the execution log.

When the experiment finishes (because it has been executed or because it has been aborted by an error) the user is notified by a popup message.

Note that the execution time of an experiment may exceed the session timeout (30 min.) so that after this period of time without user action this page will not be updated and the user may have to login and start monitoring this experiment again.
4. View User Experiments

RUbioSeq-GUI keeps track of the experiments launched by user and *My Experiments* section allows user to manage them (Figure 13).

For every experiment, user will see:

- **Working directory:**
- **Creation date:**
- **Type:** SNV, CNV, ChipSeq or Methylation.
- **Status:** Running (for those experiments that have been launched and are being executed), Finished (for those experiments that have finished) or Aborted (for those experiments that have been aborted by RUbioSeq).
- **Exec. Level:** the level of the pipeline executed (0 means all levels).
- **Actions:** different actions that can be performed with the experiment.
  - Remove experiment from the list.
  - Monitor experiment (if status is Running).
  - Refresh experiment status (if status is Running).
5. Edit user profile.

User can also edit his/her personal data by clicking in the text “Logged as <username>” (placed in the right upper corner) which redirects user to My profile section (Figure 14). In this section user can change her/his e-mail and update the password.

Figure 13. My Experiments section.

Figure 14. My profile section.