Proline Zero User Guide

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Overview of Proline

Proline is a suite of software and components dedicated to mass spectrometry proteomics. Proline lets you extract data from raw files, import results from MS/MS identification engines, organize and store your data in a relational database, process and analyze this data to finally visualize and extract knowledge from MS based proteomics results.

More information on Proline Suite could be found on profiproteomics website: **http://www.profiproteomics.fr/proline**
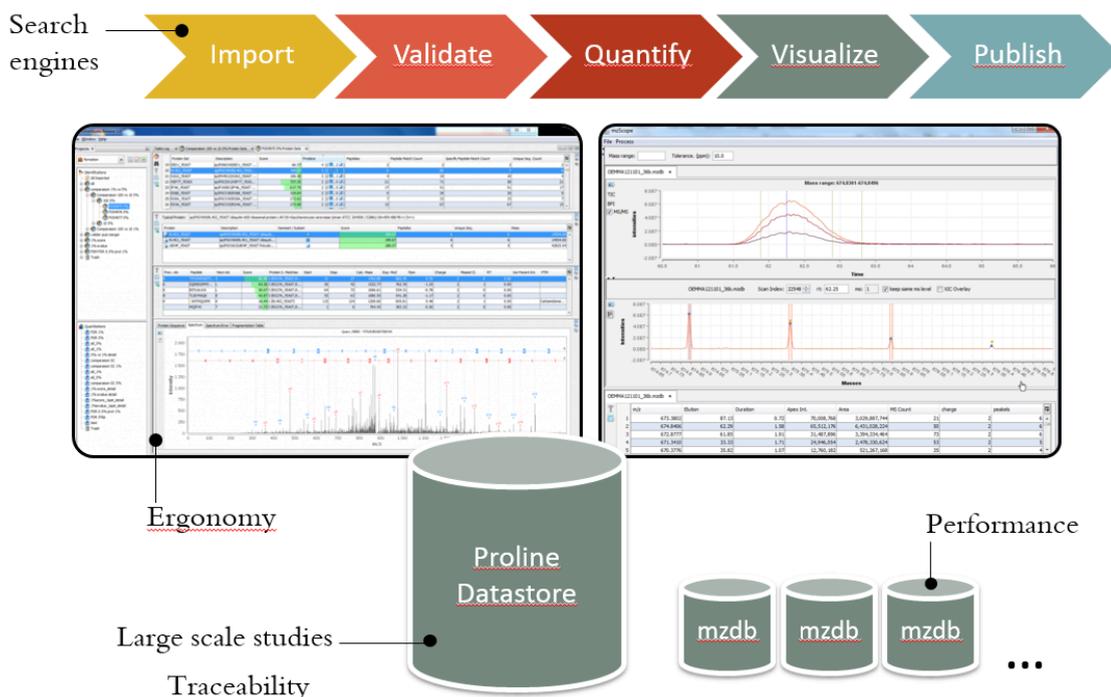
Proline Zero

Proline Zero is an all-in-one solution running on a workstation or a laptop for a single user. This distribution integrates Proline Server (the server Core component, Cortex), Proline Admin (for system administration purpose) and Sequence Repository (to gather protein sequence from fasta files). It also integrates the GUI, Proline Studio.

This documentation describes specifically the functionalities of the GUI of Proline-Zero launcher. All concepts, features and documentation of Proline Suite are accessible on profiproteomics support page. It is also possible to download Proline Zero and it's documentation from the download page.

Note that Proline is initially designed to be executed on powerful servers therefore your PC should have at least 8GB of ram memory.

Architecture
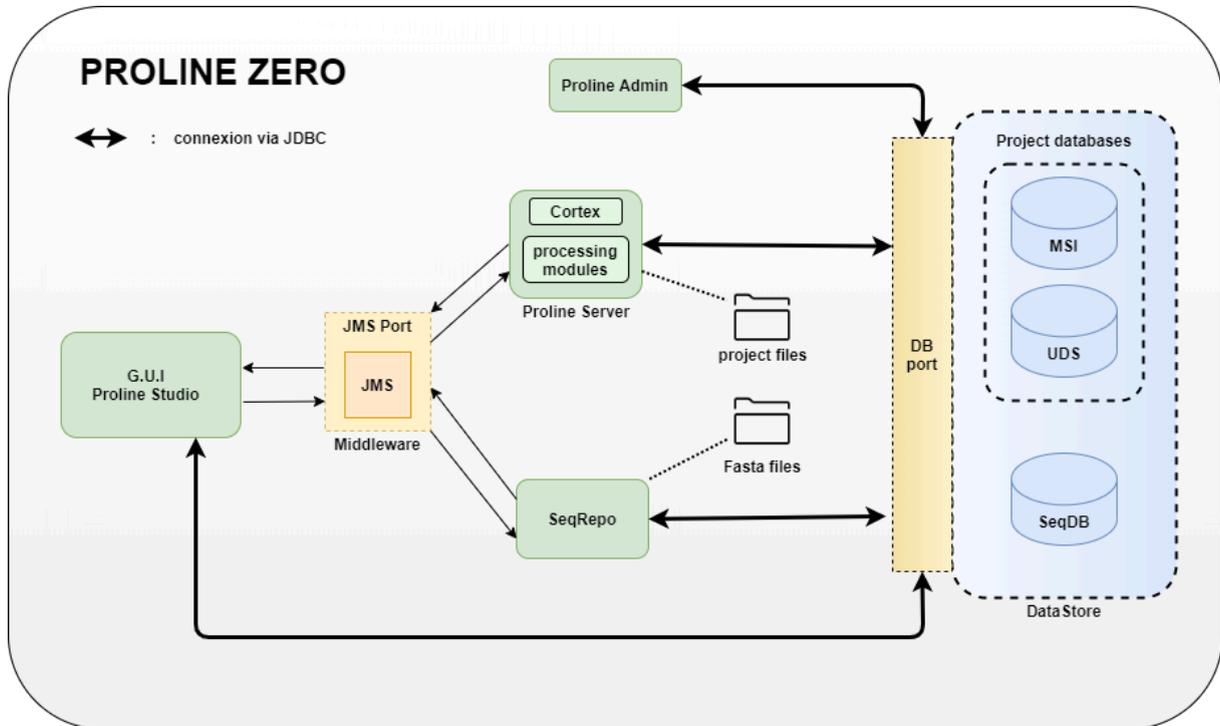
HOW TO

When Proline Zero is launched, a window is displayed, allowing users to configure settings for all proline modules before launching them.

Allocated memory, server, mounting points, sequence repository parsing rules and other options could be customized. Each of these elements has its own panel. This GUI will also help solving errors before launching the application.
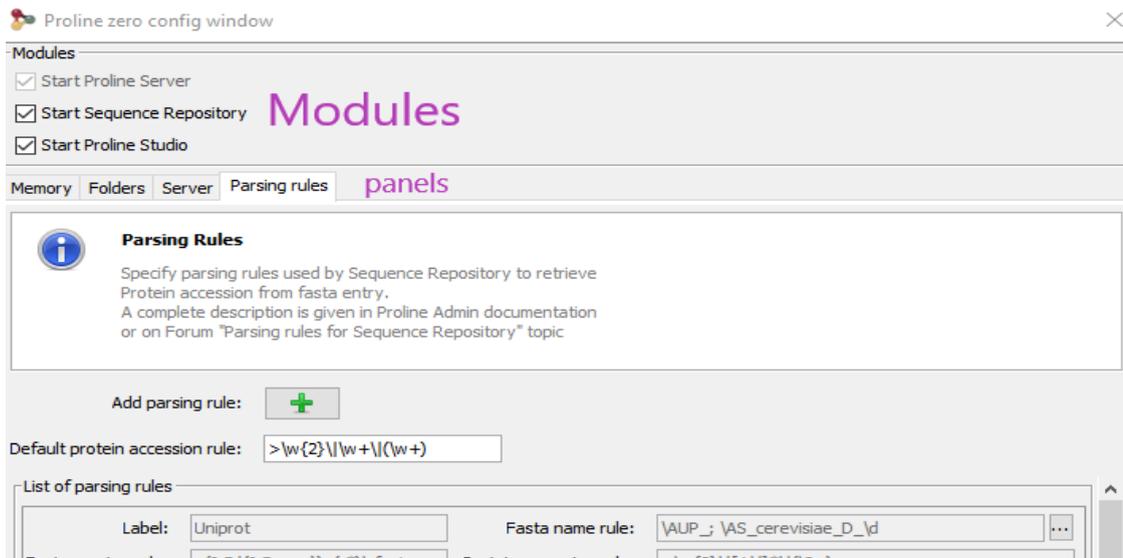
At the top of the panel you will find three checkboxes that allow you to decide which modules will be started:

You can choose to start or not Proline Studio or Sequence Repository, Proline Server is mandatory. Depending on whether or not these options are selected, some features may not be available.

At the bottom of the panel you will find three buttons and a check box :

 allows you to reset the parameters as they were when the application was launched, reading back these parameters from configuration files.

 will save the current configuration in configuration files and launch Proline Suite. A systematic check of possible errors is always done. Proline Suite won't start if there are "fatal" errors.

 will close the application without changing configuration.

 If this checkbox is selected, the configuration window will not be displayed at the next startup.

Memory Panel

This Panel allows you to configure memory allocation for all modules : Proline Studio client and server components: the datastore, the JMS server, Sequence Repository and Proline Server.

You can choose three different types of Allocation Mode :

- If **automatic mode** is selected, you only have to specify the total amount of memory that will be allocated for the Proline Suite. The system will automatically dispatch memory between components.
- In **Semi-automatic** mode, the amount of memory is defined for Proline Studio as well as for all server components.
- In **manual** mode, the amount of memory for each component should be specified by the user.

Total memory :

Total memory corresponds to the total memory allocated to Proline Suite (Client+Server). This value is either specified by the user in automatic mode or calculated in other cases. An optimal setting depends on the amount of ram on your pc.

Error management

If the memory settings you specified are not valid (for example if memory is too small or too large for a component) the GUI will display pop-ups such as this one :
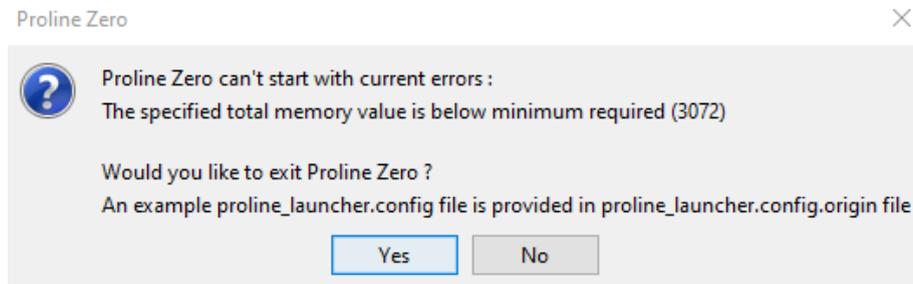
Mounting Points Panel

A first field allows you to specify the maximum size in MB of the temporary directory used by Proline for working files.

Once this size is reached you will be asked if you want to clear it.

Result identification files (Mascot, OMSSA or X!Tandem) as well as mzDB files (for the XIC Quantitation process) are only browsed from the Proline Server side. These folders should be specified in order to permit the server to access these files. In the same way, fasta folders path should be configured to allow Sequence Repository to browse and parse fasta files.

The *Folder* panel allows you to visualize, modify and repair mounting points and fasta folders. Mounting Points consist in a label and a path for result and mzDB folders, Fasta folder contains only paths without label.
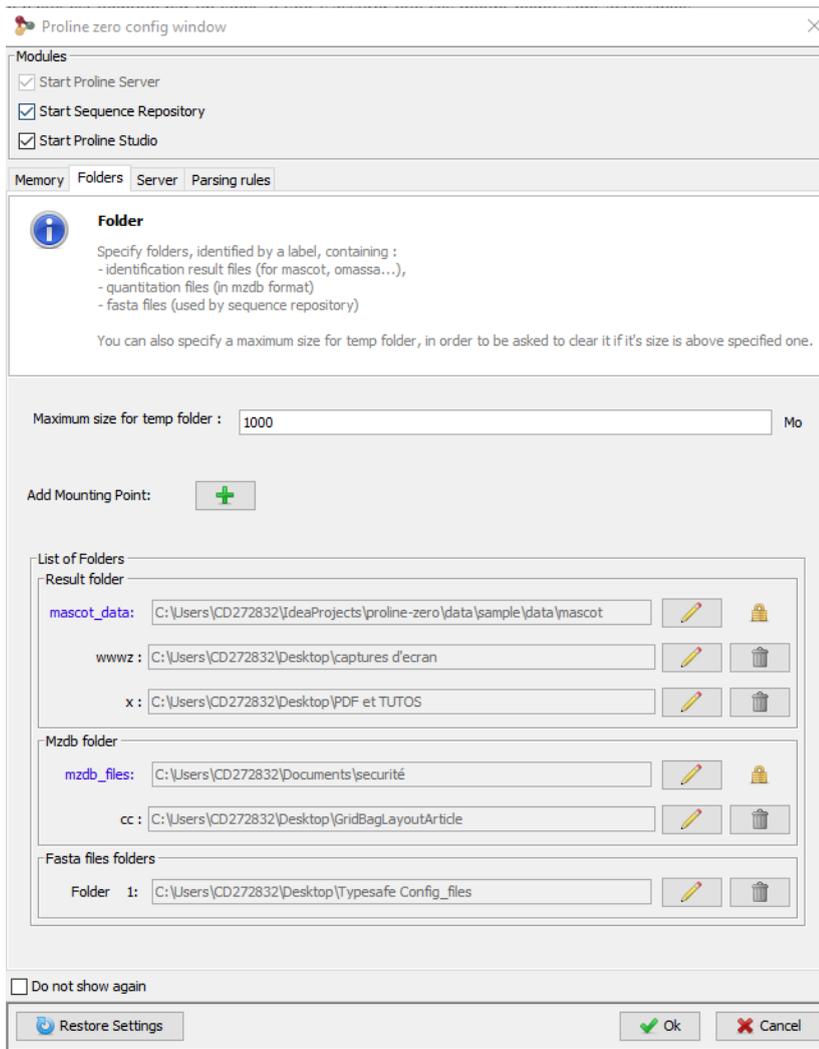
To add a mounting point, simply click on the Add button .

A dialog box will show up :
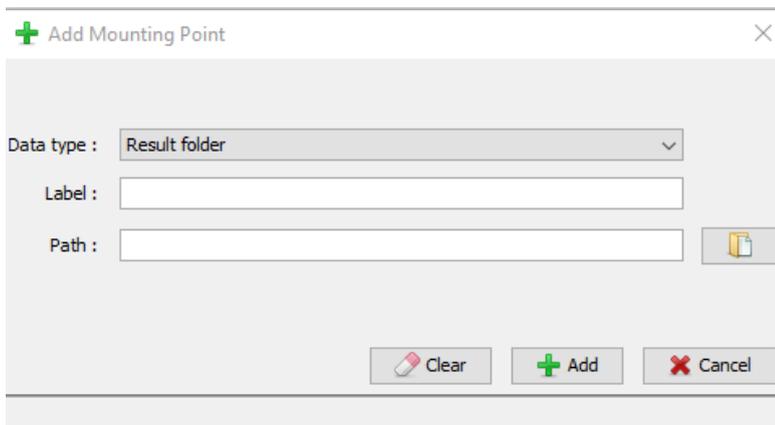
It is possible to add three different types of mounting points :

mzDB files, Mascot Files and Fastas Files.

At first select the type of the mount point you want to add in the menu bar :

You must then enter the label and the path.

Once you are done click on the add button :

The validity and uniqueness of the path is systematically checked. The uniqueness of the label is also required. If the entry is valid the mounting point you entered is saved and displayed inside the list. If not, pop-ups will help you to solve the problem

You can cancel the operation by clicking the cancel button

The clear button erases the entries in the form.

All mounting points are displayed in the list :

It is possible to modify a mounting point by clicking on the Edit button to the right of the mount point.

By clicking on the edit button a dialog box opens :
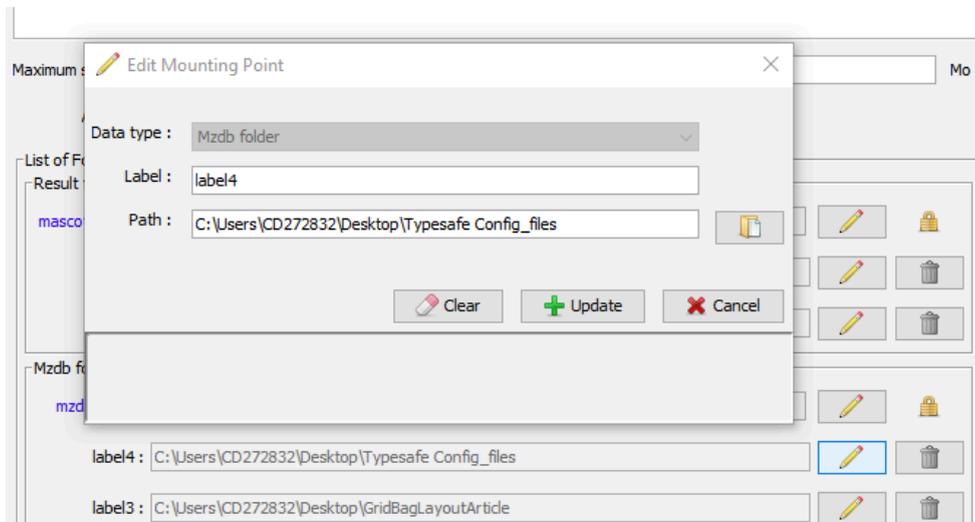
After modifying the values, the user finalizes the edition by clicking on the "update" button
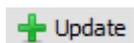
If the fields are correctly filled in, i.e. if the label and the path are not already used, the update is done and the dialog is closed.

Update can be canceled at anytime with cancel button

The mounting points can be deleted by clicking on the button .

The default mounting points (with a blue label) cannot be deleted hence there is no button and a small icon is displayed instead . Although these elements are not erasable It is possible to change their paths.

Error management

At startup Proline checks the validity of all mount point paths. If a path is not valid it will be displayed in red.
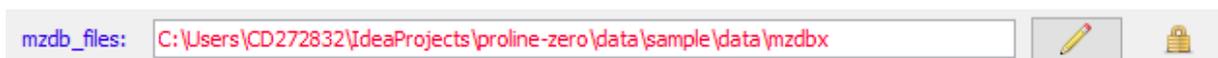
A warning is also displayed before the window is visible:
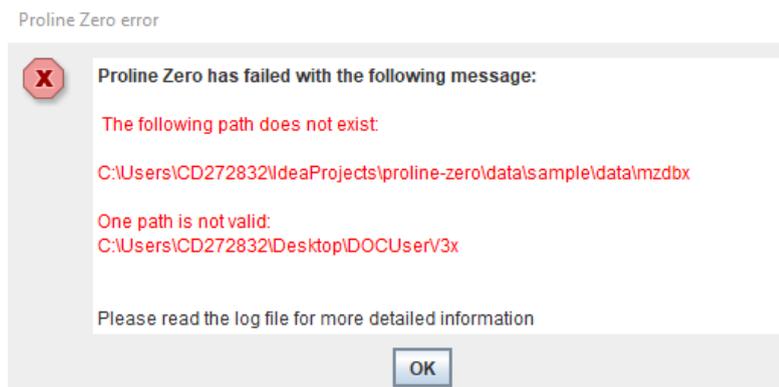
It is possible (and **required**) to repair an invalid path with the edit button. Proline also checks for the presence of at least one mount point. In case of failure a warning will be displayed.A warning is also displayed when a default mount point is missing although it is not considered an error.

Parsing Rules Tab

This tab is dedicated to the visualization and management of parsing rules used by "Sequence Repository" module.

A parsing rule has four elements:

1. a label,
2. two regular expressions (Fasta Version Rule and Protein accession Rule)
3. a list of "fasta name rules" of variable size.
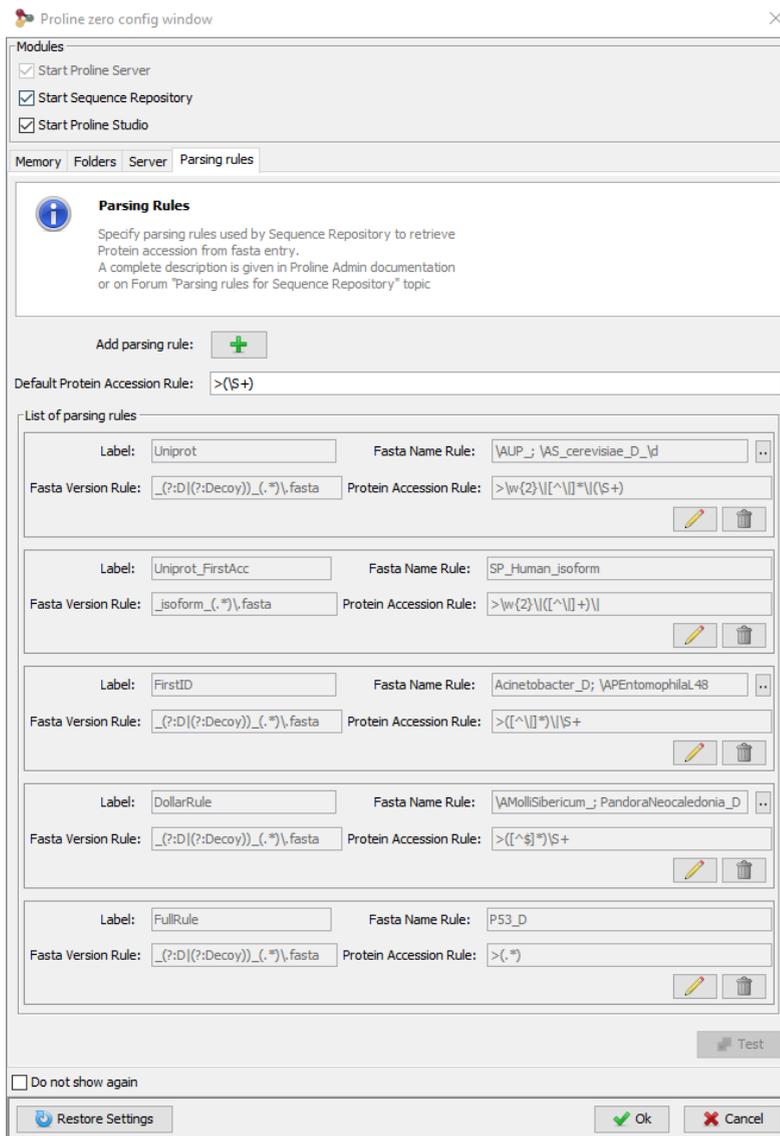
Add A Parsing Rule

To add a parsing rule click on the button ![+]. Following dialog will be opened.
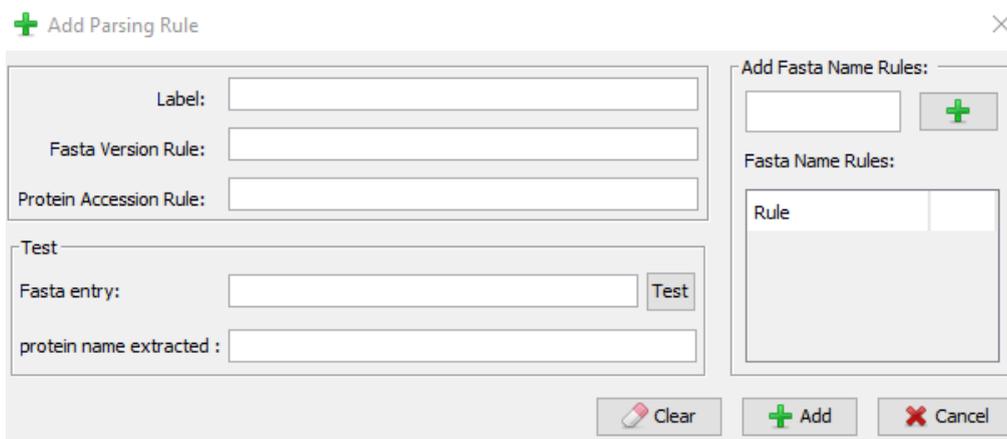
It is possible to enter as many fasta names as you want, they are displayed dynamically in a table :

After filling in the four fields, click on the button . If the input is valid the parsing rule will be saved and displayed.

Visualization of the Parsing rules in a block with the four fields :
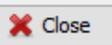
Visualization of Fasta Name Rules: If the number of rules is low, the rules are concatenated into a single element. Otherwise an additional button is present, by clicking on it a window opens with all the rules displayed in a list:

Edit Parsing Rules

Editing and deleting parsing rules is possible by clicking on the edit button and the delete button

The editing is done in a dialog box :

The fields are pre-filled with the initial values. It is possible to safely cancel the changes at any time with the cancel button

After clicking on update Proline checks if all fields are completed and if the label is not already allocated to another parsing rule. If everything is correct the parsing rule is updated and displayed in the GUI. If not, pop-ups will guide you to solve the problem.

Testing one parsing rule (local test)

It is common to make errors when using regular expressions, so Proline offers the possibility to test if they are correct.

The user can test the parsing rule in the dialog box. Just click on the test button. A new window is displayed and it is possible to submit a line of identification of a fasta file. If the regular expression is valid, the protein name is displayed. If the match is not correct, the user can modify the regular expression and run the test again.

Global test

To perform this test click on the button test at the bottom of the Parsing Rule Panel.

This test is applied to all fasta files in the directories specified in the configuration file. The files are analyzed one by one.

For each file, Proline tries to find a parsing rule that contains a regular expression that matches with the name of the file.

The fasta file is parsed and three lines are selected then protein names are extracted using the regular expression.

The extracted protein names are displayed in a dialog box:
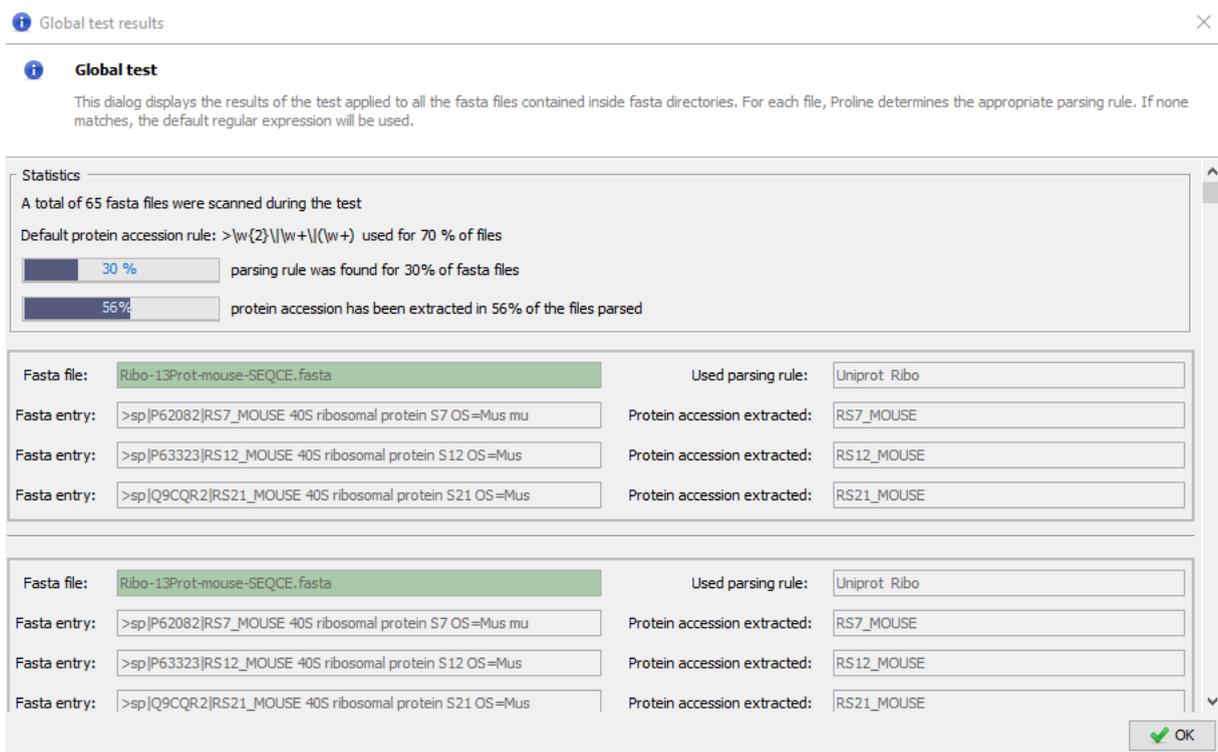
Some statistics are displayed.

Error handling:

If no parsing rule is recorded, a warning is displayed, so it is recommended to enter at least one parsing rule.

Server Tab

Server tab deals with server parameters, please consider that some settings are complex to manage and you should only change them if you are an advanced user.

Folder

Specify datastore (Postgresql or H2) port to be used.
WARNING : once datastore has been initialized this SHOULD NOT be changed.
It may cause Proline Zero to be unstable. This may be done only in some special cases

DataStore port : 4569   Test available   ✔
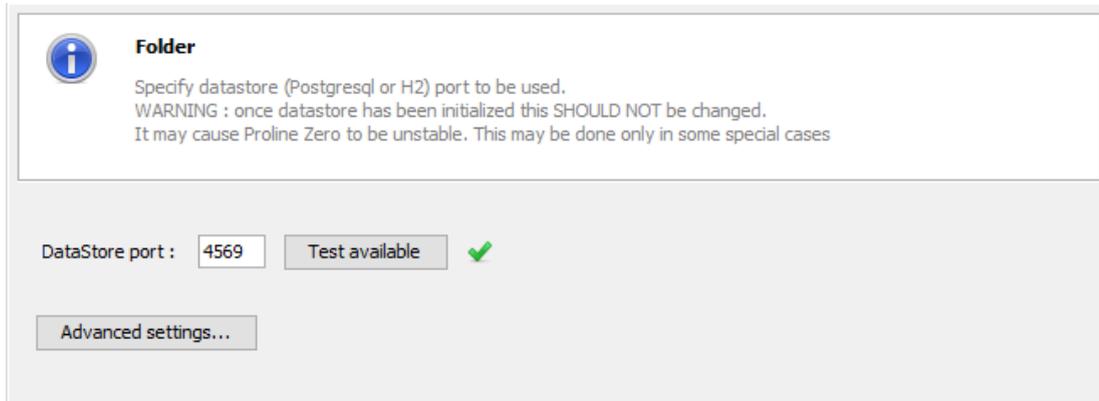
Advanced settings...

At first the current datastore port is displayed :

DataStore port : 4569   Test available   ✔
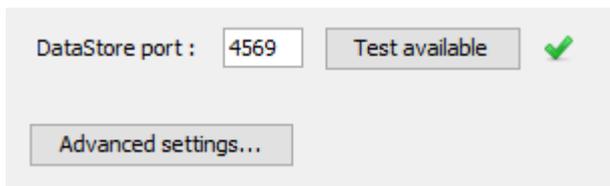
Advanced settings...

Datastore represents the database used, it can be either PostgreSQL or H2.
If the port is unavailable a cross ✖ will appear in place of the green label ✔.

By clicking on the advanced settings button a new dialog box opens :

Proline zero advanced config window   ✖

Folder

Specify different ports to be used by JMS Server (this is usefull when 2 ProlineZero may run at the same time).
Other server specific settings are also available such as "Server Thread pool size" which specify the number of process running at the same time on server side.
Note: This parameter depends on computer configuration, if too high the computer may stop responding.

Ports choice

JMS Server Port :	5445	Test available	✔
JMS Batch Server Port :	5455	Test available	✔
JNP Server Port :	1099	Test available	✔
JNP RMI Server Port :	1098	Test available	✔

Server default timeout (s) : 120

Server thread pool size : 1

JVM path : C:\Christophe\logiciels\jdk-17

☐ Force DataStore update

✔ Ok   ✖ Cancel

In that tab you can visualize the ports to be used by JMS Server (this can be useful when two ProlineZero run at the same time).

A test is possible for each configurable port, simply click on the test available button, this will tell you if the port is already in use or available.

JMS Server Port : 5445   Test available ✔

The green label ✔ on the right indicates that the JMS server is available (here on port 5445). If not a cross ✖ will appear.

Server default timeout :

Server default timeout (s) : 120

This is the time in seconds before considering a component is unavailable.

Server thread pool size :

Server thread pool size : 1

Server thread pool size specifies the number of processes running at the same time on the server side.

It is also possible to specify the path for the JVM on your pc. The JVM is the java virtual machine used to run Proline. If you need to change that parameter , simply click on the folder icon 📁 and choose the path of the JVM on your machine.

JVM path : C:\Christophe\logiciels\jdk-17   📁
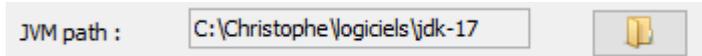
Finally a checkbox allows you to force the update of the database.

☐ Force DataStore update

Error management

Proline will check if the JVM path is well configured, then it will verify that ports are not used by two servers at the same time. Then it will test the availability of the ports for the database JMS, JMS batch,JNP and JNP RMI.

Conclusion

You have read the entire document, congratulations!!! By now you know how to configure Proline using the GUI. You can click on the Ok button ✔ Ok to launch Proline. Proline will check if there are errors. If this is not the case you have finished configuration otherwise you still have to fix the fatal errors. You can launch Proline if configuration contains only minor errors.
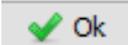
From now on you can refer to this documentation for further learning: Proline User Doc