Proline

MS-Angel: an automated management of LC-MS/MS acquisition files, and a direct link to Proline

Introduction to MS-Angel

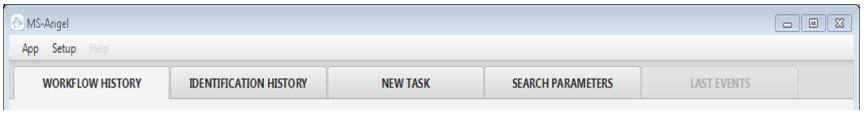
The MS Angel software allows you to easily manage your acquisition files. It offers several levels of file processing, including:
- file conversions, from RAW and WIFF files;
- peaklists identifications using one or several search engines (Mascot fully supported, OMSSA is being integrated);
- import of identification results within Proline.

The design of workflows and tasks provides a high level of automation and control.

Installation and administration

See the dedicated page.

The graphical interface in 5 tabs



- *Workflow history:* visualize tasks, giving details about the progression of the workflow on each file of the selected task.
- *Identification history:* visualize tasks including an MS identification step, giving details about the search engine, search parameters, and identification results for each file of the selected task.
- *New task:* design and launch a new task.
- *Search parameters:* create, import, visualize and modify search parameters templates.
- *Log events:* know about the last notable events in tasks execution [not yet implemented].

User case example

We will follow the example of a user willing to launch a task executing :
- the conversion of RAW acquisition files into MGF files (Mascot Generic Format),
- a peaklist identification using Mascot,
- the import of identification results into an existing Proline project.

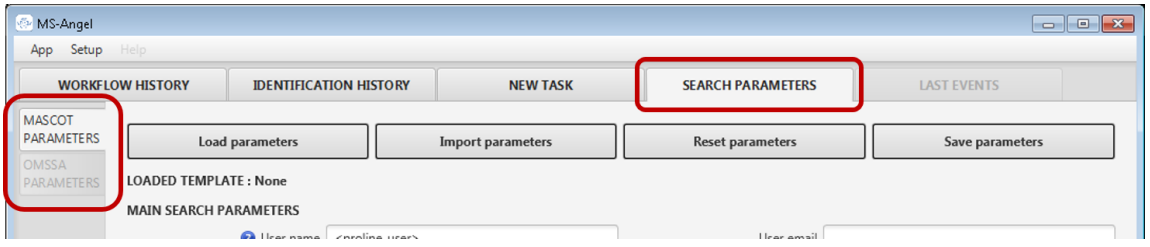
For this, we will see how to go through each step:
1. Create a search parameters template
2. Create and launch a task (input files, workflow…)
3. Visualize progression and results.

For some of these steps, several options will be suggested and explained.

NB: The tasks and templates created in MS-Angel are assigned to an owner, wich is a Proline user. If you don't have a profile on Proline yet, please create it first. If you wish to import your identification results in a Proline project, it also has to be already existing. See how to create a project in Proline.

1. Create a search parameters template

Go to the "Search parameters" tab, then to the search engine-specific subtab.

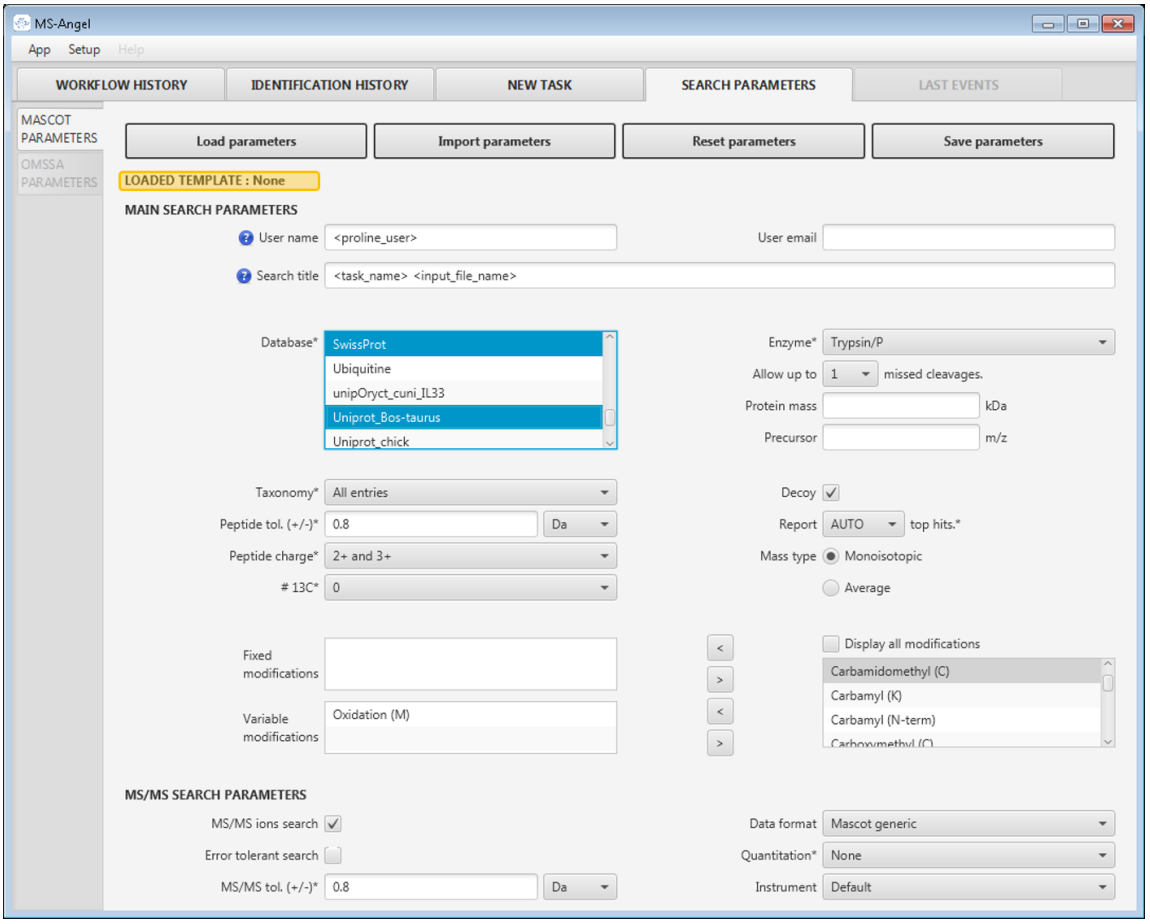


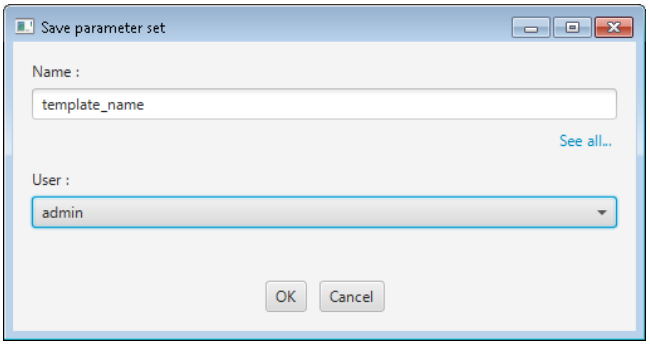
There a several ways to create a template:

- fill the form by hand
- modify an existing template
- import a Mascot Daemon .PAR file

Option A: Fill the form by hand

Fields whose names are marked by a star are mandatory.
Keywords can be used (within dipples) for the fields *'User name'* and *'Search title'*. The list of available keywords and their meaning is displayed by clicking on the help icon.
Several databases can be selected by clicking on the databases names while pressing the shift key (or the Ctrl key to select a range of entries).
To add some PTMs to the *'Fixed modifications'* list, select them in the complete list of modifications (on the right), then click on the top '<' button. To remove modifications from the *'Fixed modifications'* list, select them within the *'Fixed modifications'* list then use the top '>' button. This works the same way for *'Variable modifications'*, using the bottom '<' and '>' buttons.





Then save your new template by clicking *'Save parameters'*.
You must provide your template a name, and an owner within Proline users.

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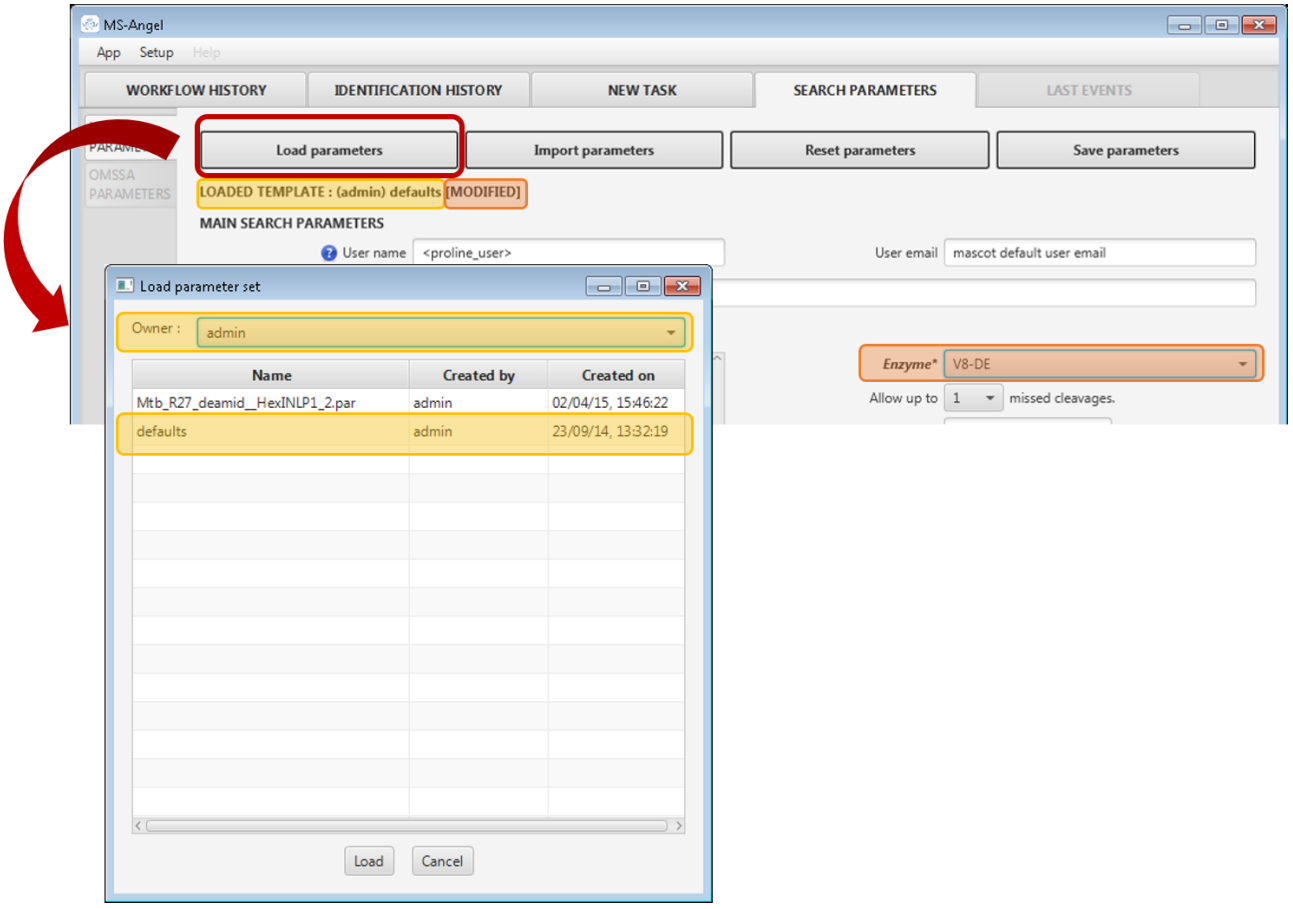
Option B: Modify an existing template

Click on *'Load parameters'*. Select the template you want to load. The template list can be filtered by template user, as seen on the screenshot below. You can see all the templates in the database by selecting *Owner: All users*.
Load the template by double-clicking on it, or clicking *'Load'*.

The form fields will then auto-fill with the template values; and the template name and owner will be displayed at the top of the form (yellow zone on screenshot).

You can edit any field. When a value is changed and differs from the actual template, the field name becomes bold and italic. If any value changes in the template, the text *'[MODIFIED]'* will appear near the template name (orange zones).

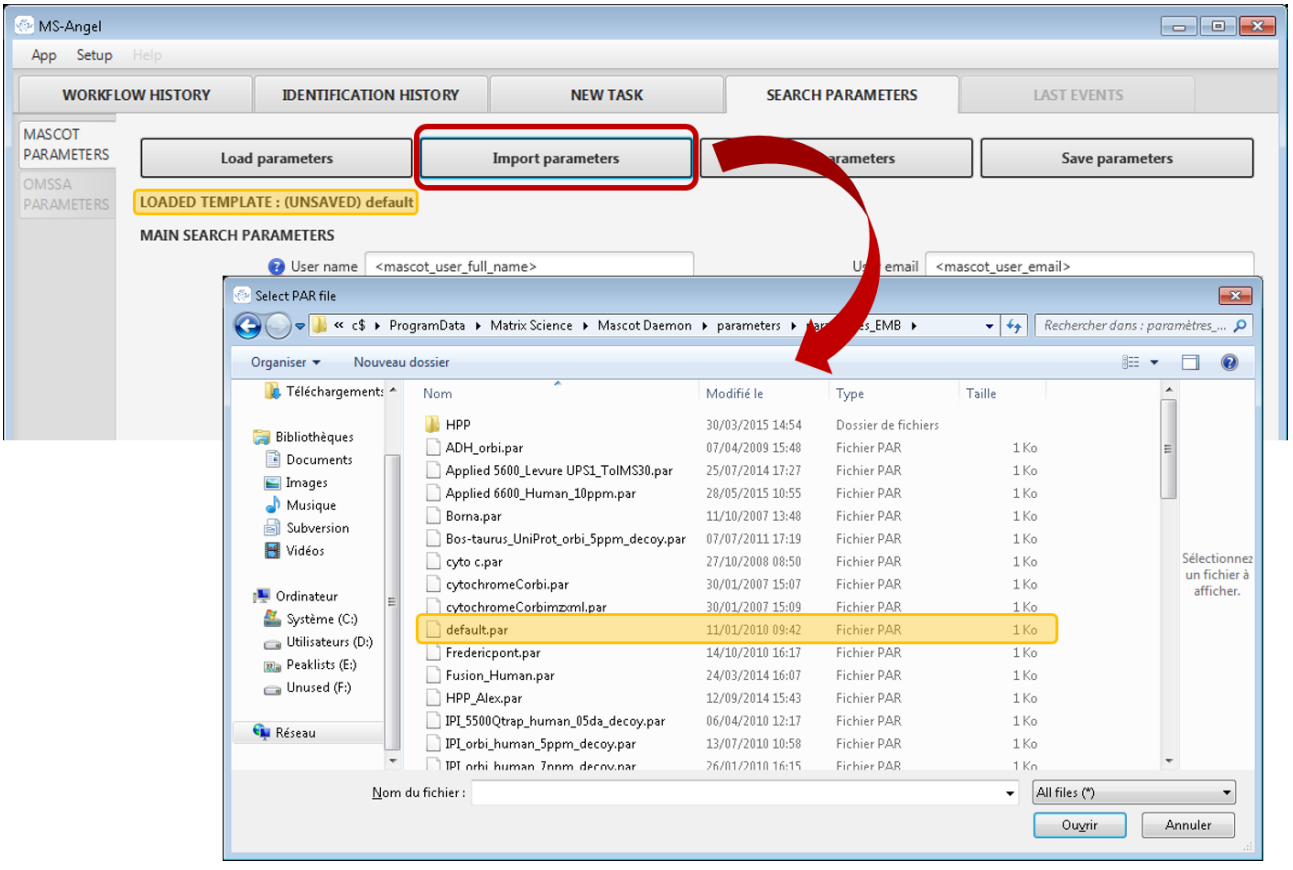
When your changes are done, you can either:
- save it as a new form: click on *'Save parameters'*, change the template name and/or owner.
- override the existing form: click on *'Save parameters'*, and don't change the template name and owner. A confirmation will be asked, since this operation is irreversible.



Option C: Import a Mascot Daemon .PAR file (Mascot parameters only)

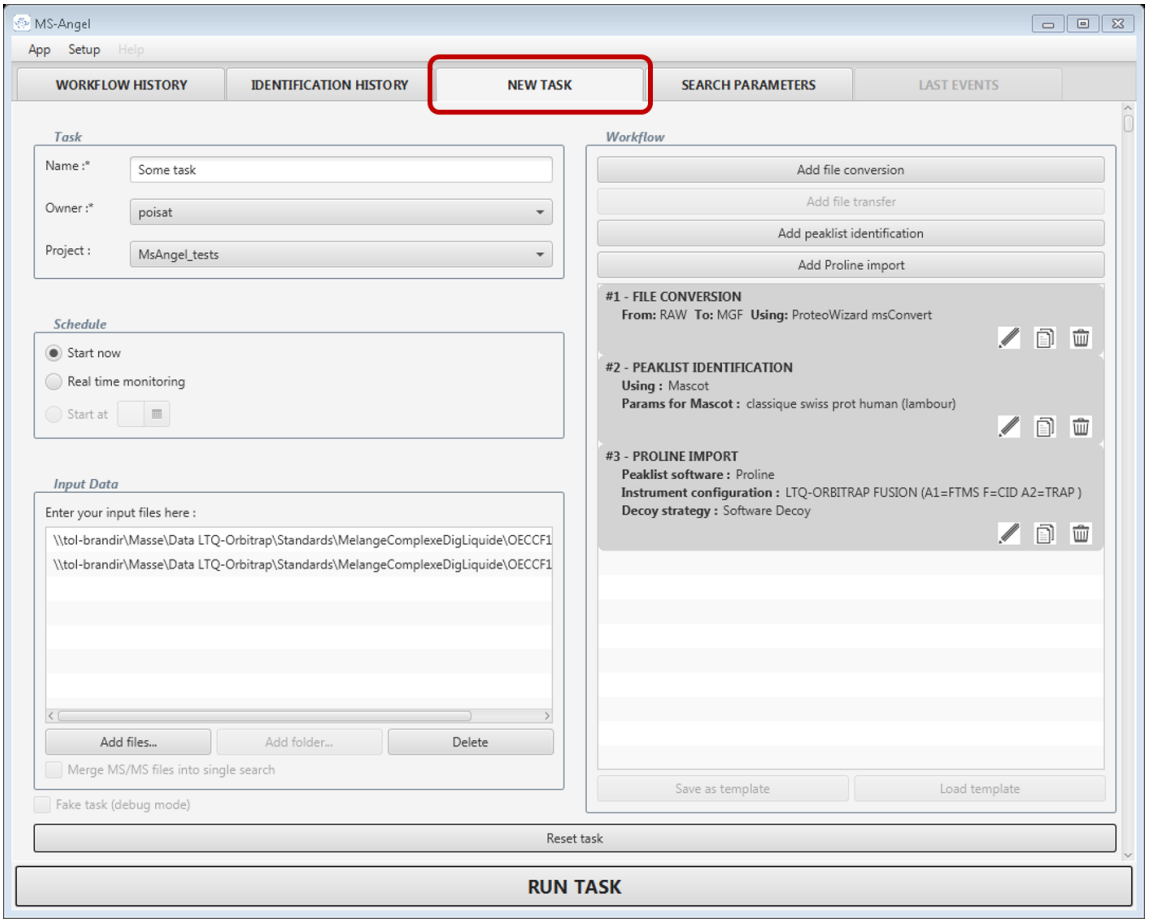
Click on *'Import parameters'*. A file browser will open. The default folder for Mascot Daemon .PAR files can be registered in the 'Setup' menu.
The form will auto-fill when a .PAR file is selected. Note that the default template name will be the .PAR file name, and that no owner is attributed to the template.

As said before, you can edit this form before saving it by clicking *'Save parameters'*.



2. Create and launch a task

Select the '*New task*' tab.



a. What is a task, what is a search

The tasks and searches are organized as in Mascot Deamon:
- a **search** refers to a single file or, more widely, to the execution of the workflow on this input file.
- a **task** refers to a set of searches: a set of input files that will be processed together, with the same workflow and the same parameters.

b. Define the task global parameters

Consider the '*Task*' part of the '*New task*' tab.

- First, give your task an arbitrary name. This is the name that will represent the task in the '*Workflow history*' and '*Identification history*' tabs.

- Select the task owner (you). This is a Proline user, which means you *must* have an account on your Proline installation already (see how to create a Proline user).

- Select the Proline project on which the task depends. As for the owner, it must be already existing (see how to create a project in Proline).
A project is mandatory if you wish to automatically import your search results in Proline. If you don't wish to use this feature, though, you can select 'None'.
Tip: You are strongly recommanded to specify a project when possible, since it will later become a criteria to quikcly filter and find tasks in the history.

c. Schedule type and input data

There are two types of task execution in MS-Angel:
- *Start now*: workflow execution in batch on a given set of input files.
- *Real time monitoring*: monitoring of a given data folder; the workflow is executed on each input file appearing in this folder (as soon as it is created).

The '*Input data*' panel depends on the selected schedule type.

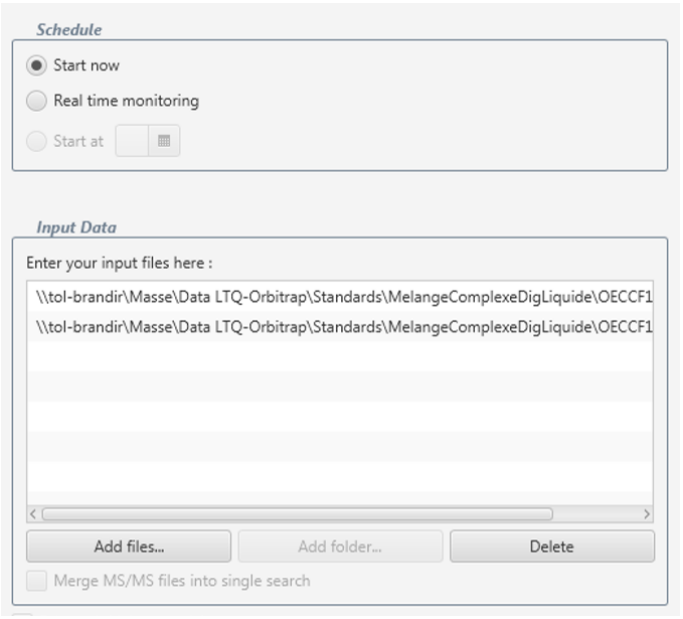
Mode 'Start now'

In the '*Schedule*' part, select *Start now*.

In the '*Input data*' part, click on *Add files*. A file browser will open for you to select all your input files. It can be .RAW, .WIFF, or .MGF files. All input files must have the same extension.

The default folder for this file browser can be set in *'Setup' (menu)* → *Open setup dialog* → *Preferences (first tab)* → *File browsing (first section)* → *Input files directory (first field)*.

As long as you task is not started, you can modify this list by adding more input files, or select and remove some (*Delete* button).



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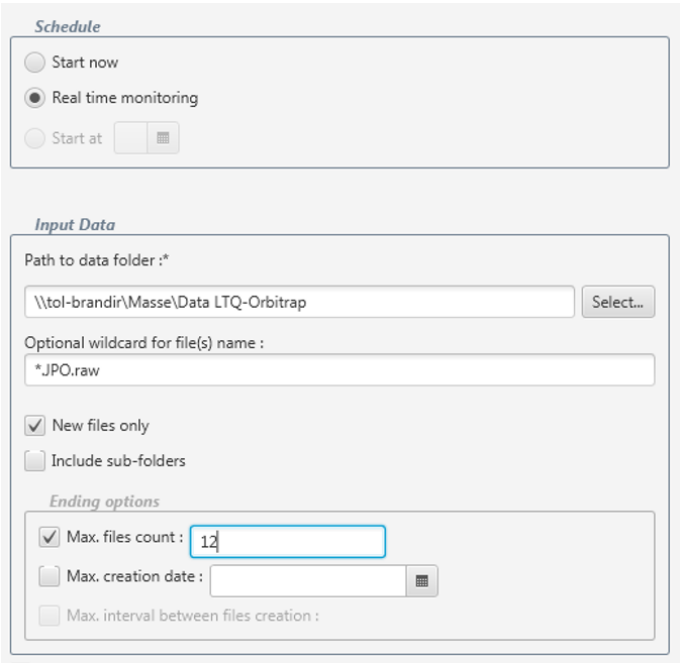
Mode 'Real time monitoring'



In the '*Schedule*' part, select *Real time monitoring*. In the '*Input data*' part, you will be able to set up many parameters:

- *Path to data folder*: the **absolute** path to the folder you want to monitor, e.g. where the input files will be created then handled by MS-Angel. You are advised to use the '*Browse*' button to select your folder.

- *Optional wildcard for file(s) name*: you can use this textfield to filter the input files name and/or extension. A star means 'anything'. In the given example, only files whose name is ending with ".JPO.raw" will be taken into account. Only one expression can be described in this field (don't use comma-separated list of expressions). If you don't want to apply any filter, you can just leave this field blank or with '*' or the initial '*.*'.

- *New files only*: if this option is checked, all files already existing before the task is launched will be ignored.

- *Include sub-folder*: if this option is checked, files created in folders under the chosen data folder will be processed.

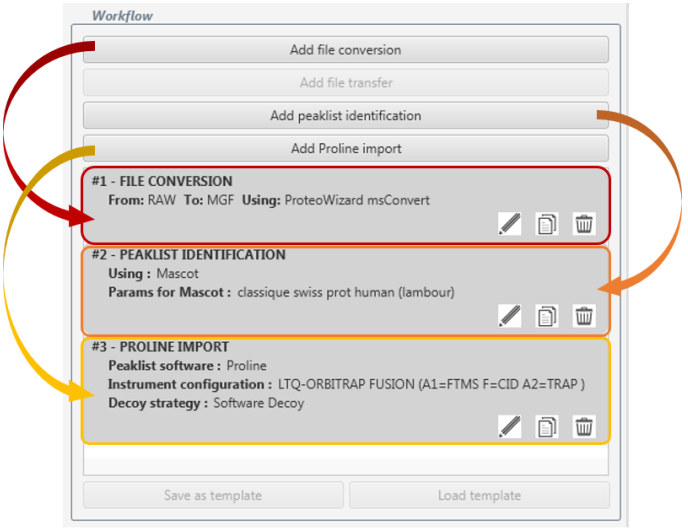
- *Ending options*: select the criterium to end up the task. It can be either a finite number of processed files, or a given date, or (if the two are selected) the first to be reached. It is currently impossible to launch a task in Real-time monitoring mode without ending parameters.

d. Design the workflow

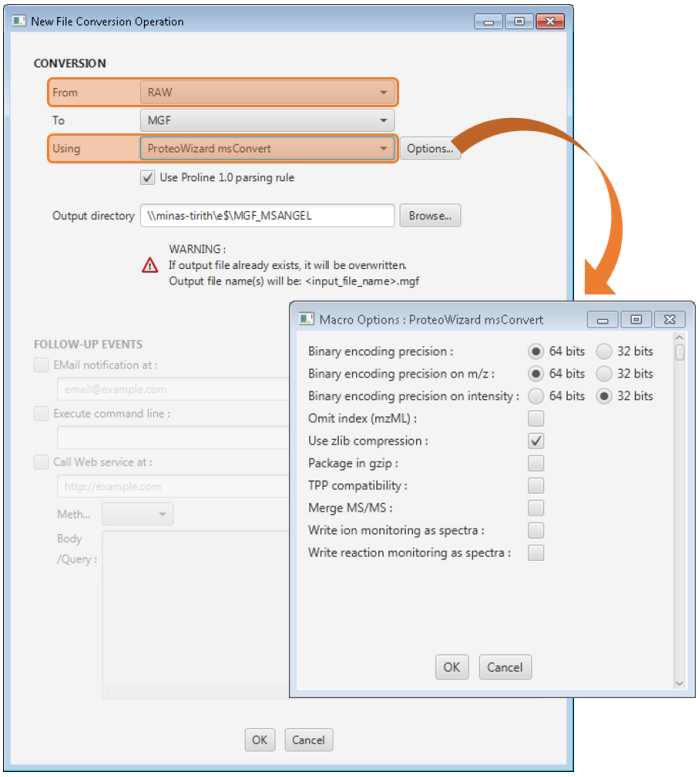
Let's focus on the '*Workflow*' part. Here you will design the workflow applied on the input files. Three types of operations are currently available:
- File conversion
- Peaklist identification (on one or many search engines)
- Proline import: import of Peaklist identification results in the Proline suite.

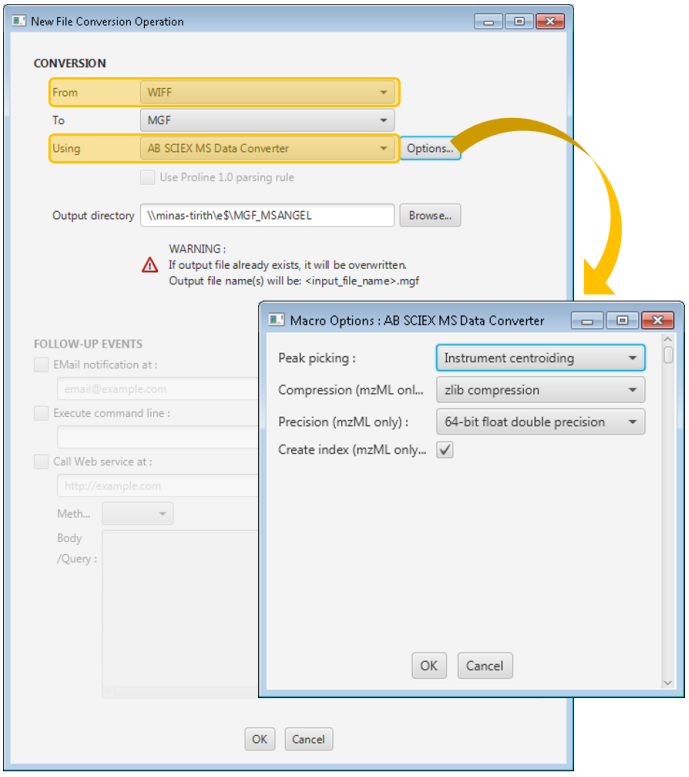
The buttons at the top allow you to create and design new operations.

WARNING: The operations order is crucial: the operations will be chained in this order, so it must be coherent with your file format, and in-between operations. For example, you must convert RAW files into MGF files before submitting them to Mascot, and must run a search on Mascot before import its results in Proline.
When you create an operation, it is placed at the end of the workflow. You can change its position by dragging and dropping it.



File conversion





Click on '*Add file conversion*'. Select the input format of your files (depending on the Schedule mode, it may be pre-selected), then the format in which they will be converted. You can then select a conversion tool. If none is displayed, then the conversion you wish to do is not yet handled by MS-Angel. The available tools are:

- ProteoWizard MsConvert (typically for RAW → MGF conversions)
- ABSciex MS Data Converter (typically for WIFF → MGF conversions).

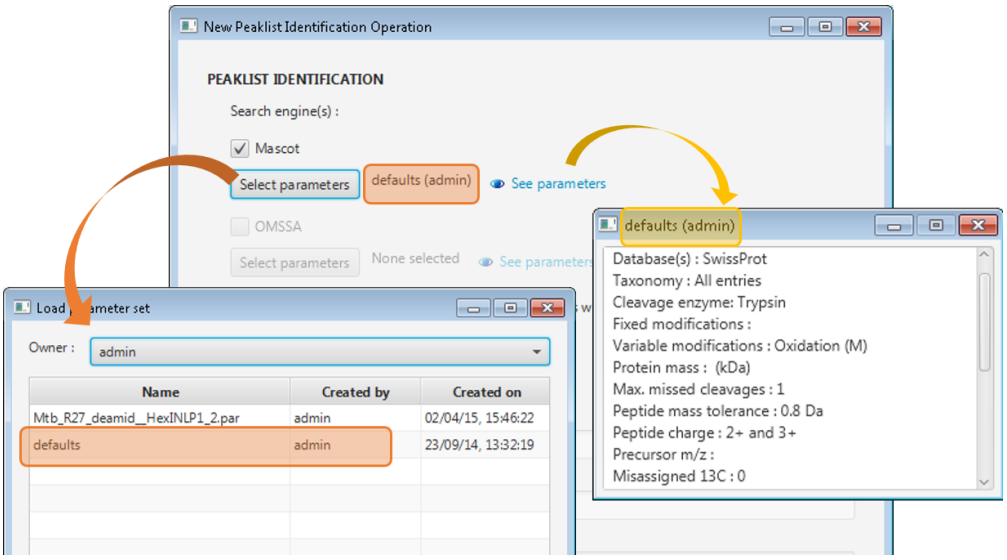
You can see and change the conversion settings by clicking *Options*.

When using MsConvert, you can (and are recommanded to) use the Proline rule for generated spectrum titles by selecting '*Use Proline 1.0 parsing rule*'. Using this rule, your MGF file will contain all the information needed by Proline for further analysis.

Peaklist identification

Select the search engine(s) you desire for peaklist identification.

For each, selected a parameter set by clicking the corresponding '*Select parameters*' button. When a template is chosen, its name and owner will be displayed, and you will be able to click '*See parameters*' to have a quick look at it.



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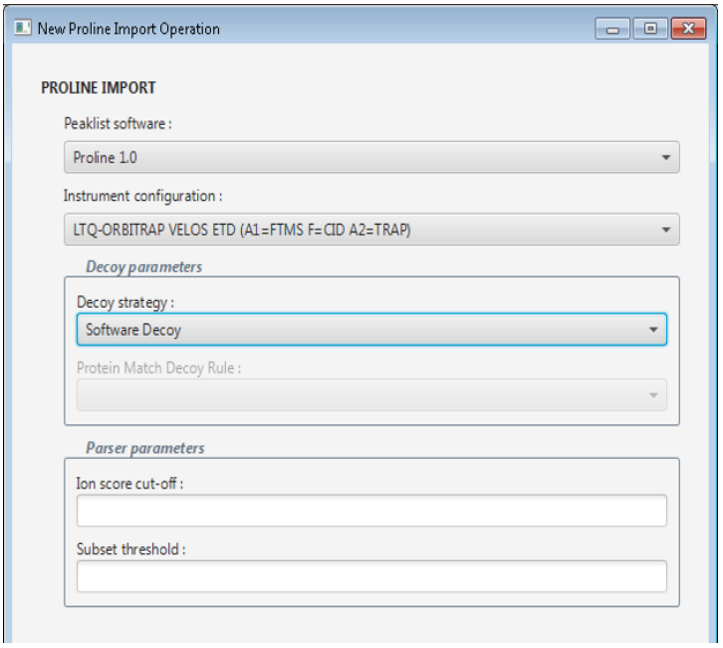
Proline import



This feature allows you to import each identification result in Proline, as soon as it is created. The parameters are the same than in ProlineStudio and in ProlineWeb.

Peaklist software: the software that was used to create the peaklists (i.e. MGF files). If you used MS-Angel for this conversion, this value will be infered. (NB: If you used the option '*Use Proline 1.0 parsing rule*4, then select '*Proline 1.0*' here.)

Instrument configuration: on which the samples were run

Decoy strategy: if you ran a classic target/decoy search on Mascot, select '*Software Decoy*'.

Protein Match decoy rule: these rules must be defined in Proline before (TODO: how to)

Ion score cutoff and *Subset threshold* are optional.

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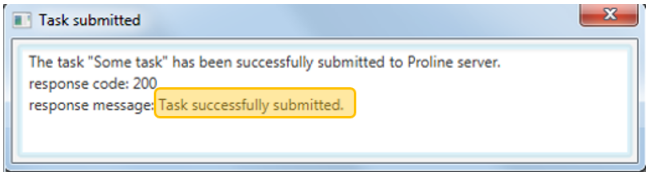
e. Launch the task

Click on '*RUN TASK*' at the bottom.

A popup window will open to let you know if the task was well launched. Close this window, you will be redirected to the *Workflow History* tab.



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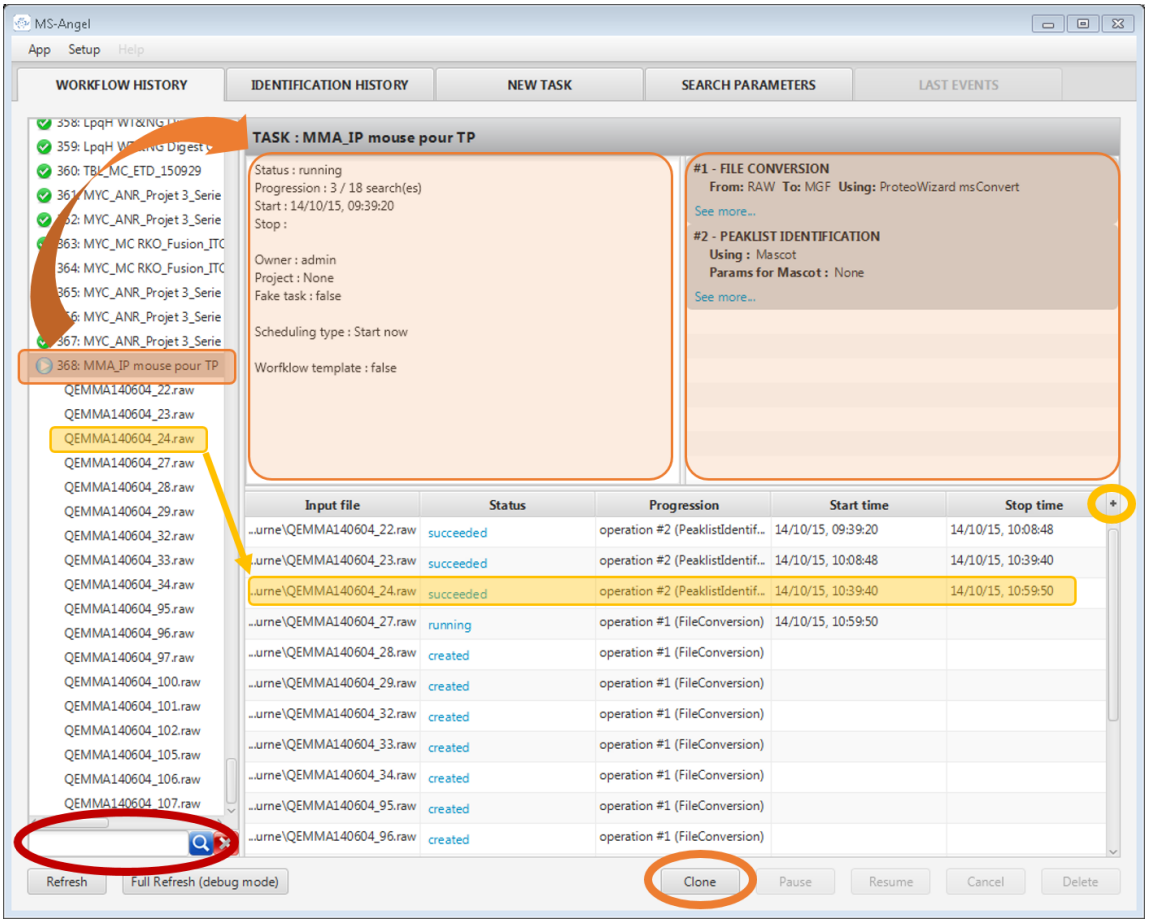
3. Visualize progression and results

Two tabs are dedicated to tasks visualization.
In the *Workflow History* tab, all tasks are displayed, and the progression of the workflow can be followed.
In the *Identification History* tab, only tasks with a Peaklist Identification are displayed. The information given in this tab is related to the peaklist identification.

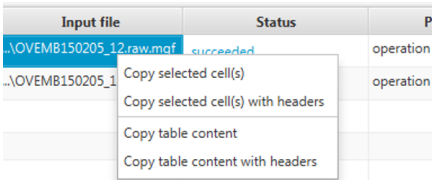
Workflow history



In the tree at the left, all tasks are displayed with an icon pointing out the tasks status (running, succeeded, failed…). By double-clicking the task name (orange), the input files appear in the tree (yellow).
A selected task can be cloned by clicking *Clone*.
The displayed tasks can be filtered on their name using the tool circled in red above.

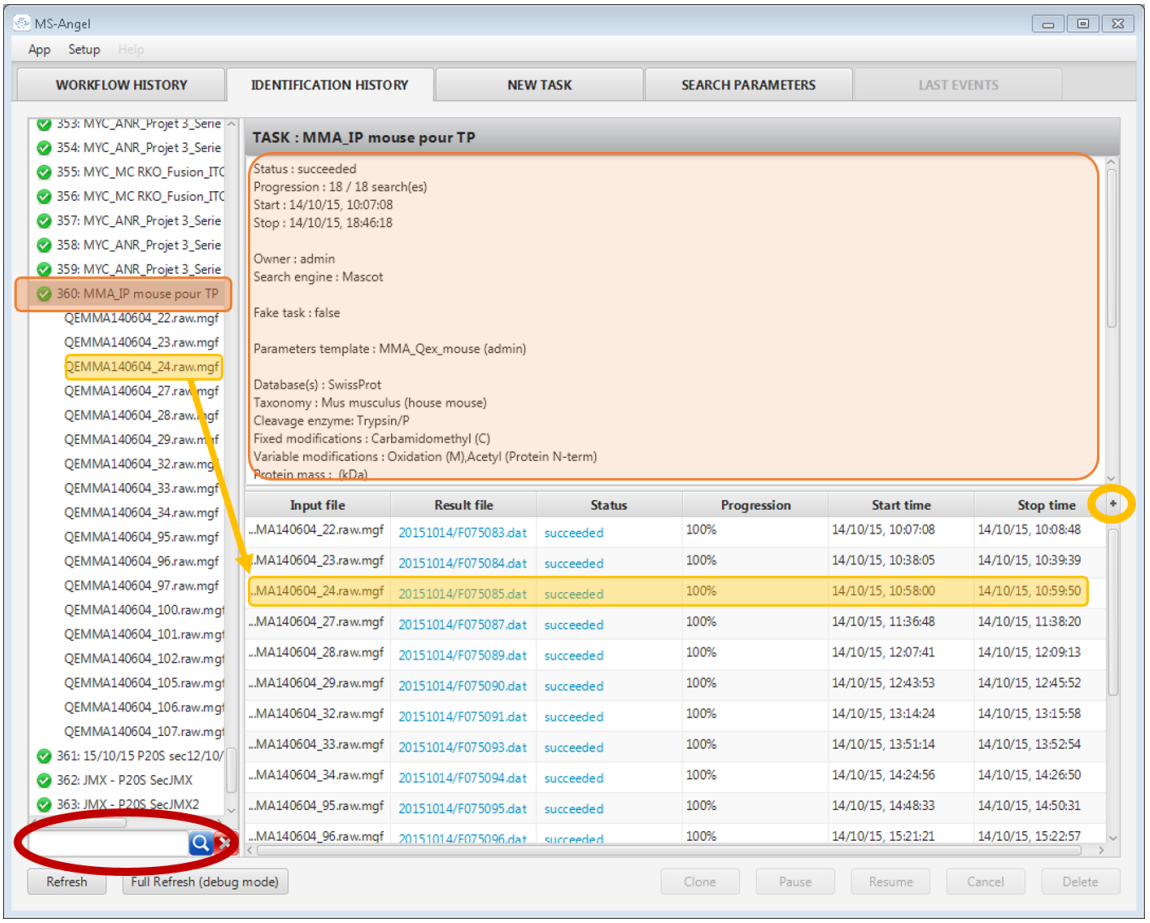
The top-right parts (pale orange) are related to the tasks. It gives detailled information on the parameters (left) and workflow operations (right). The bottom-right table is search-related: one line per input file. Texts in blue are hyperlinks, offering much details on the search progression. Some columns may be shown or hidden ('+' icon, circled in yellow).

The table can be copied, without or without the column names (*headers*), by right-clicking on the table.
You can also select only some cells to be copied (use the shift key to select a range of cells).



You can switch to *Identification History* while keeping the focus on a given task. To do that, right click on the task name in the tree, then on '*Go to Mascot task*' / '*Go to OMSSA task*'.

Identification history



The tasks in the tree are only those containing a Peaklist Identification in the workflow. So be aware that task number in the two history tabs may be different for a same task. If a search is run on *n* search engines, then there will be *n* associated identification tasks.

The top-right part (pale orange) is related to the identification task: you can se the search parameter template that was used, and the details of these parameters (useful in case the template has been updated since).

In te bottom-right table, search-related, you can see the details of the peaklist identification progression. For Mascot tasks, as in Mascot Daemon, you can click on a result file name (xxx.dat) to be redirected in your default web browser, on the Mascot result page.

As for *Workflow History*, you can copy the table (whole or selected cells), show or hide columns, and filter the displayed tasks. You can also switch to the */Workflow History* while keeping the focus on a given task; by right-clicking on the task name in the tree, and then on '*Go to Workflow task*'.
