

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

- Introduction to MS-Angel
- Installation and administration
- The graphical interface in 5 tabs
- User case example

# 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

💮 MS-Angel					
App Setup Help					
WORKFLOW HISTORY	IDENTIFICATION HISTORY	NEW TASK	SEARCH PARAMETERS	LAST EVENTS	

- Workflow bistory: 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.

<u>NB</u>: 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.

MS-Angel	Help			
WORKFLO	W HISTORY IDENTIFICATION HI	STORY NEW TASK	SEARCH PARAMETERS	LAST EVENTS
MASCOT PARAMETERS	Load parameters	Import parameters	Reset parameters	Save parameters
PARAMETERS	LOADED TEMPLATE : None			
	MAIN SEARCH PARAMETERS			
	🗿 User name 🗌 zproli	a urar's	Licer email	

#### There a several ways to create a template:

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

#### Fields whose names are marked by a star are mandatory.

Keywords can be used (within diples) 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.

The MS-Angel					
App Setup Help					
WORKFLOW HISTORY IDENTIFICA	TION HISTORY	NEW TASK	SEARCH PARAMETERS		LAST EVENTS
MASCOT PARAMETERS Load parameters		Import parameters	Reset parameters		Save parameters
OMSSA PARAMETERS LOADED TEMPLATE : None					
MAIN SEARCH PARAMETERS					
(2) User name	<proline_user:< pre=""></proline_user:<>	>	User email		
3 Search title	<task_name></task_name>	<input_file_name></input_file_name>			
Database*	SwissProt		Enzyme*	Trypsin	n/p 👻
	Ubiquitine		Allow up to	1 -	missed cleavages.
	unipOryct_cun	iJL33	Protein mass		kDa
	Uniprot_Bos-ti	aurus	Precursor		m/z
	Uniprot_chick		v Precursor		11/2
Taxonomy*	All entries		Decoy	$\checkmark$	
Peptide tol. (+/-)*	0.8	Da	Report	AUTO	▼ top hits.*
Peptide charge*	2+ and 3+		Mass type	Mon	noisotopic
# 13C*	0			Aver	rage
Fixed			<	Disp	lay all modifications
modifications			>	Carban	nidomethyl (C)
Verieble	Oxidation (M)		<	Carban	nyl (K)
warable modifications	oxidation (m)			Carban	nyi (N-term)
MS/MS SEARCH PARAMETERS					
MS/MS ions search	$\checkmark$		Data format	Mascot	t generic 🔹
Error tolerant search			Quantitation*	None	•
MS/MS tol. (+/-)*	0.8	Da	. Instrument	Default	t 👻



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

#### 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.

WORKFLOW H	ISTORY IDEN	TIFICATION HISTORY	NEW TASK	SEARCH PARAMETERS	LAST EVENTS
ARAIVIL	Load paramete	rs	Import parameters	Reset parameters	Save parameter
ARAMETERS	ADED TEMPLATE : (adm	in) defaults [MODIFIED]			
M/	IN SEARCH PARAMETER	RS			
	🝞 User	name <proline_user></proline_user>		User email masco	t default user email
💷 Load param	eter set				
Owner : a	lmin		-		
	Name	Created by	Created on	Enzyme* V8-DE	
Mtb_R27_dea	midHexINLP1_2.par	admin	02/04/15, 15:46:22	Allow up to 1	missed cleavages.
defaults		admin	23/09/14, 13:32:19		

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

		CEARCH RADAMETERS	
WORKFLOW HISTORY IDENTIFICATION HISTORY	NEW TASK	SEARCH PARAMETERS	LASTEVENTS
Task	Wo	rkflow	
Name :* Some task		Add file co	onversion
Dwner :* Doisat		Add file	transfer
		Add peaklist i	identification
MsAngel_tests	• • • • • • • • • • • • • • • • • • •	Add Prolir	ne import
Start now         Real time monitoring         Start at         Input Data         inter your input files here :         \\tol-brandir\Masse\Data LTQ-Orbitrap\Standards\MelangeComplexeDi         \\tol-brandir\Masse\Data LTQ-Orbitrap\Standards\MelangeComplexeDi	#2 #3 igLiquide\OECCF1 igLiquide\OECCF1	rom: KAW To: MGP Using: ProteoWizz PEAKLIST IDENTIFICATION Using : Mascot Params for Mascot : classique swiss prof PROLINE IMPORT Peaklist software : Proline nstrument configuration : LTQ-ORBITR Decoy strategy : Software Decoy	t human (lambour)
	> >		
Marge MS/MS files into single search	Delete		
Fake task (debug mode)		Save as template	Load template

## 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 bistory' and 'Identification bistory' 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'. <u>Tip:</u> You are strongly recommanded to specify a project when possible, since it will later become a criteria to quikely 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  $(Setup)'(menu) \rightarrow Open setup dialog \rightarrow Preferences (first tab) \rightarrow File browsing (first section) \rightarrow Input files directory (first field).$ 

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).

Schedule	
Start now	
Real time monitoring	
Start at	
Input Data	
Enter your input files here :	
\\tol-brandir\Masse\Data LTQ-Orbitrap\Standards\Melange	ComplexeDigLiquide\OECCF1
\\tol-brandir\Masse\Data LTQ-Orbitrap\Standards\Melange	ComplexeDigLiquide\OECCF1
< (	>
Add files Add folder	Delete
Merge MS/MS files into single search	

## Mode 'Real time monitoring'

Schedule
Start now
Real time monitoring
Start at
Input Data
Path to data folder :*
\\tol-brandir\Masse\Data LTQ-Orbitrap Select
Optional wildcard for file(s) name :
*JPO.raw
New flag and
New files only
Include sub-folders
Ending options
Max. files count : 12
Max. creation date :
Max. interval between files creation :

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  $\rightarrow$  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.



#### Proline import

Peaklist software :	
Proline 1.0	
Instrument configuration :	
LTQ-ORBITRAP VELOS ETD (A1=FTMS F=CID A2=TRAP)	
Decoy parameters	
Decoy strategy :	
Software Decoy	
Protein Match Decoy Rule :	
Parser parameters	
Ion score cut-off :	
Subset threshold :	

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 inferred. (NB: If you used the option 'Use Proline 1.0 parsing rule4, 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.

# e. Launch the task

Click on 'RUN TASK' at the bottom.

# **RUN TASK**

Task submitted

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.

The task "Some task	k" has been successfully subm	itted to Proline server.
response code: 200		
response message:	Task successfully submitted.	

X

## 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

WORKFLOW HISTORY	IDENTIFICATION HISTORY	NEW TASK	SEARCH PARA	METERS	LAST EVENTS
358: LpqH WI&NG Digest	TASK : MMA_IP mouse	pour TP			
360: TBL_MC_ETD_150929 361 /MYC_ANR_Projet 3_Serie 363: MYC_ANR_Projet 3_Serie 363: MYC_MC RKO_Fusion_ITC 364: MYC_MC RKO_Fusion_ITC 364: MYC_ANR_Projet 3_Serie 367: MYC_ANR_Projet 3_Serie 368: MMA_IP mouse pour TP QEMMA140604_22.raw QEMMA140604_24.raw	Status : running Progression : 3 / 18 search(es) Start : 14/10/15, 09:39:20 Stop : Owner : admin Project : None Fake task : false Scheduling type : Start now Worfklow template : false		(#1 - FILE COI From: RAV See more #2 - PEAKLIS Using : M Params fo See more	NVERSION W To: MGF Using: Proteo it IDENTIFICATION ascot r Mascot : None	Wizard msConvert
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QEMMA140604_27.raw QEMMA140604_28.raw QEMMA140604_28.raw QEMMA140604_29.raw QEMMA140604_32.raw QEMMA140604_33.raw QEMMA140604_95.raw QEMMA140604_95.raw QEMMA140604_97.raw QEMMA140604_101.raw QEMMA140604_101.raw QEMMA140604_105.raw QEMMA140604_105.raw	Input file .urme\QEMMA140604_22.raw lurme\QEMMA140604_23.raw .urme\QEMMA140604_23.raw .urme\QEMMA140604_28.raw .urme\QEMMA140604_28.raw .urme\QEMMA140604_28.raw .urme\QEMMA140604_33.raw .urme\QEMMA140604_33.raw .urme\QEMMA140604_34.raw .urme\QEMMA140604_34.raw	Status succeeded succeeded succeeded running created created created created created created	Progression operation #2 (PeaklistIdentif operation #2 (PeaklistIdentif operation #2 (PeaklistIdentif operation #1 (FileConversion) operation #1 (FileConversion) operation #1 (FileConversion) operation #1 (FileConversion) operation #1 (FileConversion) operation #1 (FileConversion)	Start time           14/10/15, 09:39:20           14/10/15, 10:08:48           14/10/15, 10:39:40           14/10/15, 10:59:50	Stop time           14/10/15, 10:08:48           14/10/15, 10:39:40           14/10/15, 10:59:50

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 Massot task' / 'Go to OMSSA task'.

Input file		Status	P
\OVEMB150205_1	2.raw.mgf	succeeded	operation
\OVEMB150205_1	Copy sele	cted cell(s)	operation
	Copy sele	cted cell(s) with headers	
	Copy tabl	e content	
	Copy tabl	e content with headers	

Identification history

WORKFLOW HISTORY	IDENTIFICATION HISTO	NEW NEW	TASK	SEARCH PARAMETERS	LAST	EVENTS
353: MYC_ANR_Projet 3_Serie						
354: MYC_ANR_Projet 3_Serie		use pour rr				
355: MYC_MC RKO_Fusion_ITC	Status : succeeded Progression : 18 / 18 sea	rch(es)				
356: MYC_MC RKO_Fusion_ITC	Start : 14/10/15, 10:07:08	3				
357: MYC_ANR_Projet 3_Serie	Stop : 14/10/15, 18:46:18	3				
358: MYC_ANR_Projet 3_Serie	Owner : admin					
359: MYC_ANR_Projet 3_Serie	Search engine : Mascot					
360: MMA_IP mouse pour TP	Fake task · false					
QEMMA140604_22.raw.mgf	Take task Taise					
QEMIMA140604_23.raw.mgf	Parameters template : M	MA_Qex_mouse (admin)				
QEMINA140604_24.raw.mgf	Database(s) : SwissProt					
QEMMA140004_27.raw high	Taxonomy : Mus muscule	us (house mouse)				
OEMMA140604_29.raw.m.f	Cleavage enzyme: Trypsi Fixed modifications : Car	n/P bamidomethyl (C)				
OEMMA140604_32.raw.mc	Variable modifications : 0	Oxidation (M),Acetyl (Prote	ein N-term)			
QEMMA140604_33.raw.mgf	Rotein mass : (kDa)					
QEMMA140604_34.raw.mgf	Input file	Result file	Status	Progression	Start time	Stop time
QEMMA140604_34.raw.mgf QEMMA140604_95.raw.mgf	Input file MA140604_22.raw.mgf	Result file 20151014/F075083.dat	Status succeeded	Progression 100%	Start time 14/10/15, 10:07:08	<b>Stop time</b> 14/10/15, 10:08:48
QEMMA140604_34.raw.mgf QEMMA140604_95.raw.mgf QEMMA140604_96.raw.mgf	Input file MA140604_22.raw.mgf	Result file 20151014/F075083.dat 20151014/F075084.dat	Status succeeded succeeded	Progression           100%           100%	Start time           14/10/15, 10:07:08           14/10/15, 10:38:05	Stop time           14/10/15, 10:08:48           14/10/15, 10:39:39
QEMMA140604_34.raw.mgf QEMMA140604_95.raw.mgf QEMMA140604_96.raw.mgf QEMMA140604_97.raw.mgf	Input file MA140604_22.raw.mgf .MA140604_23.raw.mgf .MA140604_24.raw.mgf	Result file           20151014/F075083.dat           20151014/F075084.dat           20151014/F075085.dat	Status succeeded succeeded succeeded	Progression           100%           100%           100%	Start time           14/10/15, 10:07:08           14/10/15, 10:38:05           14/10/15, 10:58:00	Stop time           14/10/15, 10:08:48           14/10/15, 10:39:39           14/10/15, 10:59:50
QEMMA140604_34.raw.mgf QEMMA140604_95.raw.mgf QEMMA140604_95.raw.mgf QEMMA140604_97.raw.mgf QEMMA140604_100.raw.mgf QEMMA140604_100.raw.mgf	Input file MA140604_22.raw.mgf I.MA140604_23.raw.mgf MA140604_24.raw.mgf MA140604_27.raw.mgf	Result file           20151014/F075083.dat           20151014/F075084.dat           20151014/F075085.dat           20151014/F075087.dat	Status succeeded succeeded succeeded succeeded	Progression           100%           100%           100%           100%           100%	Start time           14/10/15, 10:07:08           14/10/15, 10:38:05           14/10/15, 10:58:00           14/10/15, 11:36:48	Stop time           14/10/15, 10.08:48           14/10/15, 10:39:39           14/10/15, 10:59:50           14/10/15, 11:38:20
QEMMA140604_34.raw.mgf QEMMA140604_95.raw.mgf QEMMA140604_96.raw.mgf QEMMA140604_100.raw.mgf QEMMA140604_100.raw.mgf QEMMA140604_101.raw.mgf QEMMA140604_102.raw.mgf	Input file MA140604_22.raw.mgf IMA140604_23.raw.mgf MA140604_24.raw.mgf MA140604_27.raw.mgf MA140604_28.raw.mgf	Result file           20151014/F075083.dat           20151014/F075084.dat           20151014/F075085.dat           20151014/F075087.dat           20151014/F075089.dat	Status succeeded succeeded succeeded succeeded succeeded	Progression           100%           100%           100%           100%           100%           100%	Start time           14/10/15, 10:07:08           14/10/15, 10:38:05           14/10/15, 10:58:00           14/10/15, 11:36:48           14/10/15, 12:07:41	Stop time           14/10/15, 10:08:48           14/10/15, 10:39:39           14/10/15, 10:59:50           14/10/15, 11:38:20           14/10/15, 12:09:13
QEMMA140604_34.raw.mgf QEMMA140604_95.raw.mgf QEMMA140604_95.raw.mgf QEMMA140604_97.raw.mgf QEMMA140604_100.raw.mgf QEMMA140604_101.raw.mgf QEMMA140604_102.raw.mgf	Input file MA140604_22.raw.mgf MA140604_23.raw.mgf MA140604_24.raw.mgf MA140604_27.raw.mgf MA140604_28.raw.mgf MA140604_29.raw.mgf	Result file 20151014/F075083.dat 20151014/F075084.dat 20151014/F075087.dat 20151014/F075089.dat 20151014/F075089.dat	Status succeeded succeeded succeeded succeeded succeeded succeeded	Progression           100%           100%           100%           100%           100%           100%           100%           100%	Start time           14/10/15, 10:07:08           14/10/15, 10:38:05           14/10/15, 10:58:00           14/10/15, 11:36:48           14/10/15, 12:07:41           14/10/15, 12:43:53	Stop time           14/10/15, 10.08.48           14/10/15, 10.39.39           14/10/15, 10.59.50           14/10/15, 11.38.20           14/10/15, 12.09.13           14/10/15, 12.45.52
QEMMA140604_34.raw.mgf QEMMA140604_95.raw.mgf QEMMA140604_96.raw.mgf QEMMA140604_97.raw.mgf QEMMA140604_100.raw.mgf QEMMA140604_101.raw.mgf QEMMA140604_105.raw.mgf QEMMA140604_105.raw.mgf	Input file MA140604_22.raw.mgf MA140604_23.raw.mgf MA140604_24.raw.mgf MA140604_27.raw.mgf MA140604_28.raw.mgf MA140604_29.raw.mgf MA140604_32.raw.mgf	Result file           20151014/F075083.dat           20151014/F075084.dat           20151014/F075085.dat           20151014/F075087.dat           20151014/F075089.dat           20151014/F075089.dat           20151014/F075089.dat           20151014/F075090.dat	Status succeeded succeeded succeeded succeeded succeeded succeeded	Progression           100%           100%           100%           100%           100%           100%           100%           100%           100%	Start time           14/10/15, 10:07:08           14/10/15, 10:38:05           14/10/15, 10:58:00           14/10/15, 11:36:48           14/10/15, 12:07:41           14/10/15, 12:43:53           14/10/15, 13:14:24	Stop time           14/10/15, 10.0848           14/10/15, 10.39.39           14/10/15, 10.59.50           14/10/15, 11.38.20           14/10/15, 12.09.13           14/10/15, 12.45.52           14/10/15, 13.15.58
QEMMA140604_34.raw.mgf QEMMA140604_95.raw.mgf QEMMA140604_95.raw.mgf QEMMA140604_97.raw.mgf QEMMA140604_100.raw.mgf QEMMA140604_102.raw.mgf QEMMA140604_102.raw.mgf QEMMA140604_105.raw.mgf QEMMA140604_107.raw.mgf	Input file MA140604_22.raw.mgf MA140604_23.raw.mgf MA140604_27.raw.mgf MA140604_27.raw.mgf MA140604_28.raw.mgf MA140604_29.raw.mgf MA140604_32.raw.mgf	Result file           20151014/F075083.dat           20151014/F075084.dat           20151014/F075087.dat           20151014/F075087.dat           20151014/F075089.dat           20151014/F075090.dat           20151014/F075090.dat           20151014/F075093.dat	Status succeeded succeeded succeeded succeeded succeeded succeeded succeeded	Progression           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%	Start time           14/10/15, 10:07:08           14/10/15, 10:38:05           14/10/15, 10:58:00           14/10/15, 11:36:48           14/10/15, 12:07:41           14/10/15, 12:43:53           14/10/15, 13:14:24           14/10/15, 13:51:14	Stop time           14/10/15, 100848           14/10/15, 103939           14/10/15, 103939           14/10/15, 103930           14/10/15, 113820           14/10/15, 120913           14/10/15, 124552           14/10/15, 131558           14/10/15, 132524
QEMMA140604_34.raw.mgf QEMMA140604_95.raw.mgf QEMMA140604_95.raw.mgf QEMMA140604_07.raw.mgf QEMMA140604_100.raw.mgf QEMMA140604_102.raw.mgf QEMMA140604_102.raw.mgf QEMMA140604_105.raw.mgf QEMMA140604_107.raw.mgf 361: 15/10/15 P205 sec12/10/ 362: IXX P205 sec12/10/	Input file MA140604_22.raw.mgf .MA140604_23.raw.mgf MA140604_24.raw.mgf MA140604_27.raw.mgf MA140604_28.raw.mgf MA140604_32.raw.mgf MA140604_33.raw.mgf MA140604_33.raw.mgf	Result file           20151014/F075083.dat           20151014/F075084.dat           20151014/F075087.dat           20151014/F075087.dat           20151014/F075089.dat           20151014/F075090.dat           20151014/F075093.dat           20151014/F075093.dat           20151014/F075093.dat	Status succeeded succeeded succeeded succeeded succeeded succeeded succeeded succeeded	Progression           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%	Start time           14/10/15, 10:07:08           14/10/15, 10:38:05           14/10/15, 10:58:00           14/10/15, 11:36:48           14/10/15, 12:47:41           14/10/15, 12:43:53           14/10/15, 13:14:24           14/10/15, 13:51:14	Stop time           14/10/15, 1008:48           14/10/15, 1039:39           14/10/15, 1039:39           14/10/15, 1039:39           14/10/15, 1039:30           14/10/15, 1138:20           14/10/15, 1209:13           14/10/15, 1245:52           14/10/15, 13:15:58           14/10/15, 13:25:44           14/10/15, 14:26:50
QEMMA140604_34.raw.mgf QEMMA140604_95.raw.mgf QEMMA140604_95.raw.mgf QEMMA140604_96.raw.mgf QEMMA140604_100.raw.mgf QEMMA140604_100.raw.mgf QEMMA140604_105.raw.mgf QEMMA140604_105.raw.mgf QEMMA140604_106.raw.mgf QEMMA140604_107.raw.mgf 361: 15/10/15 P205 sec12/10/ 362: JMX - P205 SecJMX2	Input file MA140604_22.raw.mgf I.MA140604_23.raw.mgf MA140604_24.raw.mgf MA140604_27.raw.mgf MA140604_28.raw.mgf MA140604_29.raw.mgf MA140604_33.raw.mgf MA140604_33.raw.mgf MA140604_34.raw.mgf	Result file           20151014/F075083.dtal           20151014/F075084.dtal           20151014/F075087.dtal           20151014/F075087.dtal           20151014/F075089.dtal           20151014/F075091.dtal           20151014/F075093.dtal           20151014/F075094.dtal           20151014/F075093.dtal           20151014/F075093.dtal           20151014/F075094.dtal           20151014/F075094.dtal	Status succeeded succeeded succeeded succeeded succeeded succeeded succeeded succeeded succeeded	Progression           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%           100%	Start time           14/10/15, 10:07:08           14/10/15, 10:38:05           14/10/15, 10:58:00           14/10/15, 11:36:48           14/10/15, 11:36:48           14/10/15, 12:43:53           14/10/15, 13:14:24           14/10/15, 13:51:14           14/10/15, 13:54:56	Stop time           14/10/15, 1008:48           14/10/15, 1039:39           14/10/15, 1039:39           14/10/15, 1039:39           14/10/15, 1039:30           14/10/15, 11:38:20           14/10/15, 12:09:13           14/10/15, 12:45:52           14/10/15, 13:45:58           14/10/15, 13:25:44           14/10/15, 14:26:50           14/10/15, 14:26:50

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*'.

msangelworkflow.txt · Dernière modification: 2015/10/19 18:48 par 193.48.0.3