https://msda.unistra.fr

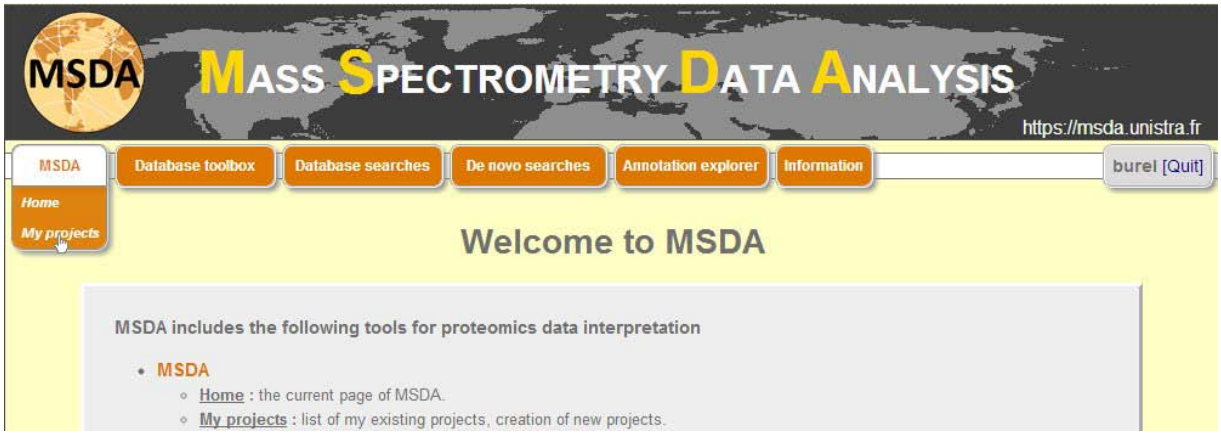
MSDA tutorial: How to start a *de novo* search

To start a new *de novo* search, you have to:

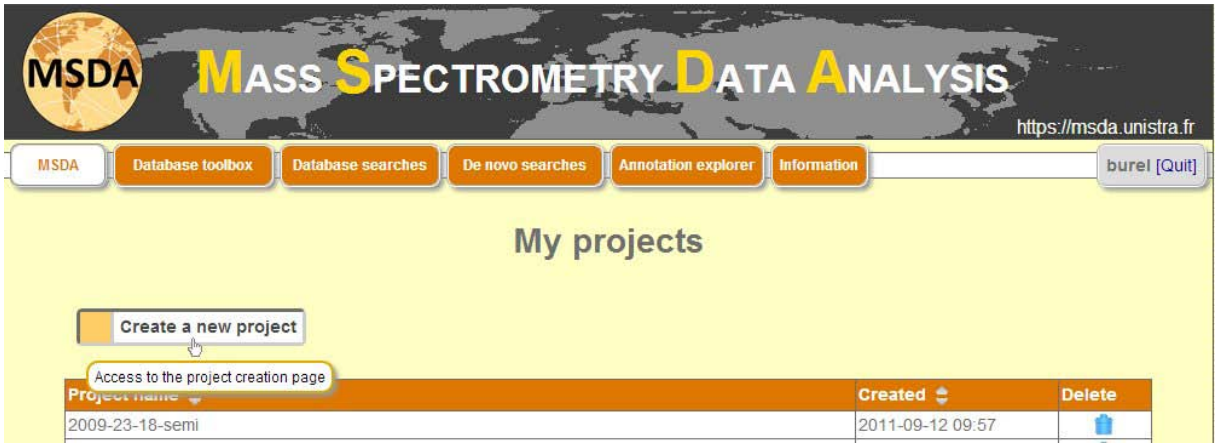
1. upload your peak lists into a new project
2. set PepNovo+ settings
3. set MSBlast settings
4. start the search

Create a new project and upload your peak lists in it

Click on the menu and select the "My projects" page



Then click on **"Create a new project"**



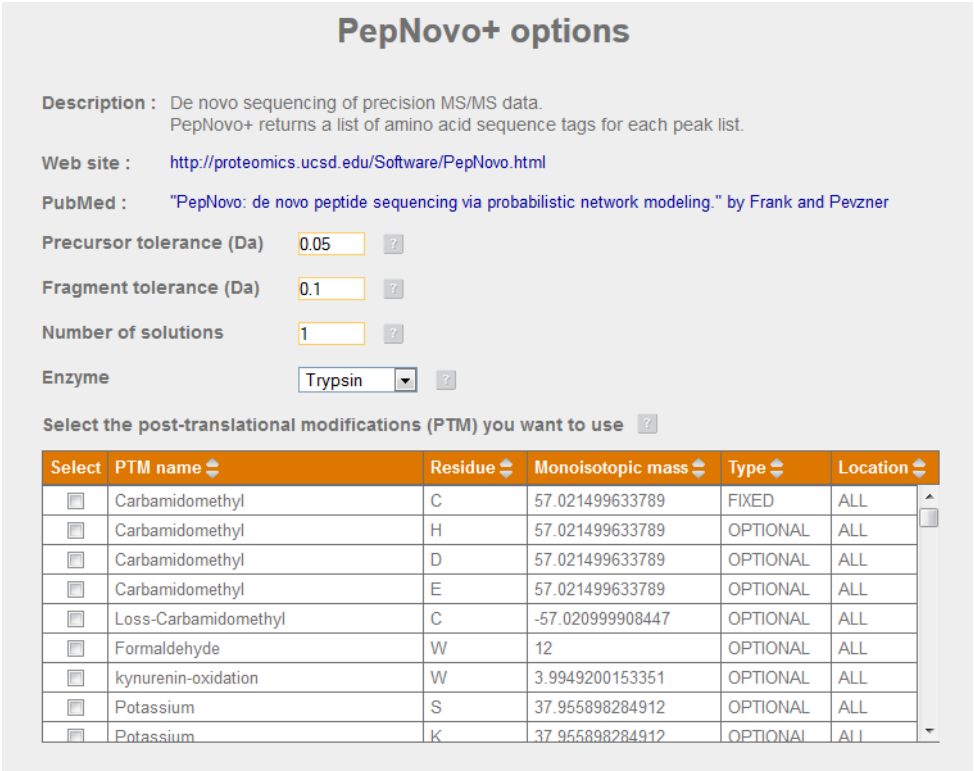
Set PepNovo+ settings

Note that the list of PTMs is specific to PepNovo+. You will not find the PTMs you may have created for your OMSSA database searches.

PepNovo+ reads peaklists and tries to determine the most probable peptide sequences for each spectrum, allowing a user-defined mass tolerance on precursor and fragments. PepNovo+ will return the best solution for each spectrum, but you can ask for more solutions.

The quality of a solution is given by a "MSBlast score" calculated by PepNovo+. A high score will indicate that the sequence has a good probability to match something in the following MSBlast process. **Despite a confusing name, this score is calculated by PepNovo+ and must not be considered as a protein match!**

PepNovo+ complete results will be written into an Excel file.



PepNovo+ options

Description : De novo sequencing of precision MS/MS data.
PepNovo+ returns a list of amino acid sequence tags for each peak list.

Web site : http://proteomics.ucsd.edu/Software/PepNovo.html

PubMed : "PepNovo: de novo peptide sequencing via probabilistic network modeling." by Frank and Pevzner

Precursor tolerance (Da) 0.05

Fragment tolerance (Da) 0.1

Number of solutions 1

Enzyme Trypsin

Select the post-translational modifications (PTM) you want to use

Select	PTM name	Residue	Monoisotopic mass	Type	Location
	Carbamidomethyl	C	57.021499633789	FIXED	ALL
	Carbamidomethyl	H	57.021499633789	OPTIONAL	ALL
	Carbamidomethyl	D	57.021499633789	OPTIONAL	ALL
	Carbamidomethyl	E	57.021499633789	OPTIONAL	ALL
	Loss-Carbamidomethyl	C	-57.020999908447	OPTIONAL	ALL
	Formaldehyde	W	12	OPTIONAL	ALL
	kynurenin-oxidation	W	3.9949200153351	OPTIONAL	ALL
	Potassium	S	37.955898284912	OPTIONAL	ALL
	Potassium	K	37.955898284912	OPTIONAL	ALL

Set MSBlast settings

The MSBlast process takes every sequence generated by PepNovo+ with a 'MSBlast score' bigger than the given threshold. MSBlast will try to match these sequences to the selected database. This step is optional though: select the first entry if you do not wish to run a MSBlast on your sequences.

MSBlast will generate a classic html file with the search results for each peptide sequence. These results will also be exporter in the output Excel file, after the PepNovo+ sheet.