



<https://msda.unistra.fr>

MSDA tutorial: How to refine OMSSA search parameters

MSDA and OMSSA enable all search parameters to be user-adjusted. A set of settings is stored into a method named by the user. You can generate your own protein databases and post-translational modifications, save and store your methods to reuse them for further searches. Every user has a predefined default method.

Create your own method

You need to enter a method name and set your parameters at adapted values for your searches. The grey boxes with an interrogation mark contain a definition of the parameter. A method is divided into five parts: the main settings, modifications, precursor & product ion handling, and advanced settings.

Method name

Description

Main settings

Select the database you want to use

Select	Database	Decoy	Trypsin	Keratin	Date	Main
<input type="radio"/>	azerty	✓	✓	✓	2011-04-05	SP
<input type="radio"/>	homo	✓	✓	✓	2010-07-16	SP
<input type="radio"/>	homo	✗	✓	✓	2011-04-05	SP
<input type="radio"/>	homo	✗	✓	✓	2011-04-13	NC
<input type="radio"/>	homoDC	✗	✓	✓	2011-04-13	NC
<input type="radio"/>	mynewdb	✓	✓	✓	2011-03-02	NC
<input type="radio"/>	rattus	✗	✓	✓	2010-04-20	NC
<input type="radio"/>	SSP	✗	✓	✓	2011-04-21	SP
<input type="radio"/>	SWISSPROT	✗	✓	✓	2011-05-04	SP

Enzyme

Maximum allowed missed cleavages

Maximum peptide hitlist length per spectrum

E-value cutoff

Modifications

Precursor ion handling

Product ion handling

Advanced settings



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Adapt a method to your search

If you want to run a search with parameters close to an existing method, select this method and click "Adapt the method". This will open the method and allows you to change any parameter in it. **The adapted method will only be used in your search.**

Project settings

Project name:

Description:

Input files	Size
W13381CC.pkl	19.94 MB
W13384CC.pkl	19.28 MB
W13387CC.pkl	13.87 MB
W13390CC.pkl	13.17 MB

Search settings

Search name:

Select an existing method or adapt one

Select	Method	Enzyme	Database	Created
<input type="radio"/>	Default method	trypsin	SWISSPROT	2011-04-30


Merge the results ?

Receive an e-mail at the end of the search ?

Description:

Use your own databases or generate a new one

The database toolbox is a set of tools designed to generate any databases you want. You can **generate** a database including selected taxonomies, add sequences and/or accession numbers. You can **upload** your own FASTA files into MSDA. You can also **merge** your databases. The toolbox can generate decoy entries, add trypsin and/or keratins to your database. The toolbox will also remove any redundant entries in the file (redundancy based on identical accession numbers).



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My databases


Click on a database to get detailed information

Generate a database Upload a database Merge databases

Database name	Decoy	Trypsin	Keratins	Date	Ref. database	Status	Download	Delete
droso	✗	✓	✓	2012-10-08	Swiss-Prot	🔒	⬇️	🗑️
humanNR	✓	✓	✓	2011-10-06	NCBI	🔒	⬇️	🗑️
humanSP	✓	✓	✓	2011-10-05	Swiss-Prot	🔒	⬇️	🗑️
rattus	✓	✓	✓	2011-10-06	Swiss-Prot	🔒	⬇️	🗑️
SWISSPROT	✗	✓	✓	2013-05-13	Swiss-Prot	🔒	⬇️	🗑️
TAIRwb	✗	✓	✓	2013-04-25	UniProt	🔒	⬇️	🗑️
wb	✗	✓	✓	2012-06-22	Swiss-Prot	🔒	⬇️	🗑️

Create your own post-translational modifications

The default protein modifications listed on MSDA are extracted from Unimod (<http://www.unimod.org>), but you can define and insert your own modifications if necessary.



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Modification list

Click on a modification to get detailed information

Create a new modification

Access the modification creation page

Modification name	Monoisotopic mass	Average mass	Author	Used	Delete
TMPP C	572.181134	572.5401	Alexandre Burel	36	🗑️
2-propenal	56.026215	56.0633	Alexandre Burel	10	🗑️
TMPP K	572.181134	572.5401	Alexandre Burel	6	🗑️
TMPP Y	572.181134	572.5401	Alexandre Burel	6	🗑️
Malonaldehyde	54.010565	54.0474	Alexandre Burel	3	🗑️