

<https://msda.unistra.fr>

MSDA tutorial: How to read *de novo* results

The *de novo* pipeline will generate for each peaklist one MSBlast html result file, plus one Excel file containing

- An overview of the search: settings, date, related informations...
- The PepNovo+ results
- The MSBlast results exported from the html file

All these files will be packaged in a single zipped file.

Results from PepNovo+

	A	B	C	D	E	F	G	H	I	J	K	L	M
	Spectrum name	PepNovo sequence tag	[M+H]	M/z	Charge	Rank score	PepNovo Score	N-Gap	C-Gap	PepNovo extended sequence for Blast	PepNovo+ 'MSBlast score'	Will be sent to MSBlast	Comments
1													
2	Cmpd 1, +MSn(519.62), 0.0 min												#could not read spectrum correctly...
3	Cmpd 2, +MSn(311.02), 0.1 min												#could not read spectrum correctly...
4	Cmpd 3, +MSn(387.32), 0.1 min	LVR	387,252	387,252	1	-1,06	32	0	0	BLVR	-1000000000	no	
5	Cmpd 4, +MSn(701.70), 0.2 min												#could not read spectrum correctly...
6	Cmpd 5, +MSn(650.23), 0.2 min												#could not read spectrum correctly...
7	Cmpd 6, +MSn(530.09), 0.3 min	QGLQQESLR	1058,549	529,778	2	5,014	35,918	0	0	BANXXXXXELSR	3,02774	no	
8	Cmpd 7, +MSn(553.77), 0.3 min	FLSW	552,282	552,282	1	0,361	-29,002	0	0	BLFLC	-1000000000	no	
9	Cmpd 8, +MSn(832.31), 0.3 min												#could not read spectrum correctly...
10	Cmpd 9, +MSn(521.44), 0.4 min	GAQEAEER	1041,539	521,273	2	7,574	43,339	281,126	0	BXXAQQEAEER	4,66799	yes	
11	Cmpd 10, +MSn(680.09), 0.4 min	QALGGPES	1358,683	679,845	2	0,731	61,968	0	619,33	BAQLGGPESAXXXXXXX	5,91309	yes	
12	Cmpd 11, +MSn(673.66), 0.4 min	PASYAQR	1345,675	673,341	2	-0,121	-0,614	553,262	0	BXXXXXXVPASSFKR	3,19684	no	
13	Cmpd 12, +MSn(397.27), 0.5 min	EEEKMK	793,415	397,211	2	3,016	31,53	0	0	BEEEEKMK	1,23434	no	
14	Cmpd 13, +MSn(595.64), 0.5 min	LNTLAFK	1189,599	595,303	2	1,564	26,046	383,179	0	BXXQLQNVDMK	3,45963	no	

Every PepNovo+ results are stored into an Excel spectrum report. The columns are the following:

Spectrum name	The title of the spectrum used by PepNovo+ to determined the sequence tag
PepNovo sequence tag	The tag determined by PepNovo+ with PTMs included
[M+H]	The mass in Dalton
M/z	The mass divided by the charge
Charge	The charge
Rank score	Relative score used by PepNovo+ to order the computed solutions
PepNovo Score	Score representing the quality of the spectrum
N-Gap	Mass of unknown amino acids at the left of the sequence tag (0 when peptide is N-terminal)
C-Gap	Mass of unknown amino acids at the right of the sequence tag (0 when peptide is C-terminal)
PepNovo extended sequence for Blast	Sequence formatted for a MSBlast process with X's instead of missing amino acids, tags for N-terminal and/or C-terminal peptides, etc. The selected sequence may be different than the PepNovo sequence tag !
PepNovo+ 'MSBlast score'	Score calculated by PepNovo+, a high score will indicate that the sequence has a good probability to match something in the following MSBlast process
Will be sent to MSBlast	Yes or No
Comments	Output message when PepNovo+ is unable to get something from a spectrum

