# **PROLINE TUTORIAL**

## LABEL-FREE LC-MS QUANTITATION

## I/ START PROLINE

The same project as the one created for previous tutorials will be used. See Tutorial 1 *Proline Basic* for authentication and Tutorial 2 *Quantify by Spectral Counting* for dataset organization.

A. OPEN PROJECT

Select the desired project in the drop-down list.

⊳	
File Window Help	
Projects × MzDB Files	
< Select a Project >	v 11 2 4



The LC-MS label free quantitative analysis will be done on a sample of  $2\mu g$  of yeast cells lysate spiked with 10 fmol of UPS1 on one side and with 100 fmol of UPS1 on the other side. 3 replicates of each sample have been analysed on a VELOS ETD spectrometer.

### II/ QUANTIFY

A. QUANTITATION VIEW

Quantitation could be launched by using any of these 2 methods :

S S	Quantify >	Spectral Counting
т 💼	Add Quantitation Folder	Label Free
		Residue Labeling

From the Quantitation tree, at the left bottom of the Proline window. Right click on *Quantitations* node and select « Quantify> Label Free » in the drop down menu.



From *the identification* tree. Select the reference dataset containing the datasets to quantify and from which proteins sets list will be extracted. Right click and select « Quantify > Label Free... »

#### Step1- Experimental Design dialog.

On the left part the tree view shows the experimental design (groups, samples and replicates) that will be built from the identification datasets represented in the panel on the right. Drag and drop identification summaries from le right to the left to build the quantitation experimental design. Depending on the method used to run quantitation, only child datasets of reference dataset or all identification hierarchy will be shown. The experimental design is composed of :

- groups or biological conditions
- samples or biological replicates
- technical replicates

Note If you drag a dataset and drop it on the Quant node, the groups and samples nodes will be automatically generated, depending on the "group-biological replicate-technical replicate" tree.
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	Drag and drop the two datasets 100fmol et 10fmol to create 2 groups, a unique sample per
Action	group and 3 replicates per samples (see result below).



B. RENAME NODES OF THE EXPERIMENTAL DESIGN

Nodes of the experimental design could be renamed by one of the following actions:

- Select the node to rename and press the F2 key
- long click on the node to rename it
- Left click the node and choose "Rename" in the popup menu

It is recommended to rename the top level node "Quant" to choose a more appropriate name.

Action	Rename the node to quant_100vs10. Do the same with the samples according to the concentration of spiked UPS1.
Note	Nodes can also be deleted from the experimental design by right clicking on the node and choosing "Delete" in the popup menu.

#### C. Link datasets and $\ensuremath{\mathsf{MS}}$ files

To perform a quantitation, Proline needs the MS files from which identification results originated. The link between identification results and MS files must be specified by the user in the quantitation dialog (step 2). MS files are required to be supplied in mzDB format and uploaded to the server. Raw files are converted into mzDB format through a converter tool named *raw2mzDB*. This could be done in ProlineStudio via the MS Files tab but batch conversion and upload of raw files could also be automated by using MSAngel or mzdbWizard.

When quantifying an identification result Proline tries to find in the server database an mzDB file already linked to that result. If there is no mzDB file linked, the user must supply a file path by choosing a file from the right part of the panel and drag and drop this file on the corresponding row of the table.

NoteIf values are displayed in the peaklist column, Proline can match peaklist values to file names to link MS files and identification datasets. Drag and drop a batch of files in the Drop Zone area and let Proline associate files with identification results automatically.
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	Step 2: Associa	ate MS files to sample es from the file explorer (	e <b>analyses.</b> (right panel) to the dro	p zone or to the sample analyses	table to link files to sar	nple analyses.		
MS fi	les association							
Au	Group Group 10 fmol - 1% Group 10 fmol - 1% Group 10 fmol - 1% Group 10 0 fmol - 1% Group 100 fmol - 1% Group 100 fmol - 1% Group 100 fmol - 1%	Sample Sample 10 fmol - 1% Sample 10 fmol - 1% Sample 100 fmol - 1% Sample 100 fmol - 1% Sample 100 fmol - 1% Sample 100 fmol - 1%	Sample Analysis F083064 F083066 F083067 F083068 F083069 F083070	mzDB File OEMMA121101_36b.mzdb OEMMA121101_38b.mzdb OEMMA121101_61b.mzdb OEMMA121101_61b.mzdb OEMMA121101_65b.mzdb	Peaklist	Association Source	Server     mzdb_files     OFMMA121101_36b.mzdb     OFMMA121101_36b.mzdb     OFMMA121101_36b.mzdb     OFMMA121101_61b.mzdb     OFMMA121101_65b.mzdb     OFMMA121101_65b.mzdb     OFMMA121101_65b.mzdb     OFMMA12101_65b.mzdb     Sample_mascot_cdt     Sample_mascot_ECol.dat	
0 f								

Action

Make sure that each identification dataset is linked to an MS file.

#### D. QUANTIFICATION PARAMETERS

By clicking *Next*, the parameters dialog opens. Not all of the quantitation parameters are displayed at first. To access a complete set of parameter settings, click on *"Advanced Parameters"*.

**Extraction moz tolerance**: the error tolerance on m/z between the mass at the apex of the peak to extract from the mzDB file and the mass recorded in preceding or following scans.

**PSM/Peakel matching moz tolerance**: the error tolerance on m/z between the mass of the peakel and the PSMs experimental mass.

#### Clustering

Extracted elution peaks are clustered as soon as they are matched to the same identified ion and according to the following parameters.

Detection	Clustering	Alignment	Normalization	Cross Assignment	
Feat	ure Cluster	ization ru	es		
delta mo	z (ppm) <=	5.0			
delta RT (s) <=		15.0	15.0		
time com	putation:	Most In	tense		
intensity	computation	Most Intense			

**moz tolerance - time tolerance** : error tolerance applied to cluster detected features.

**time computation** : calculation method to be used to determine the elution time of created clusters (elution time of the most abundant feature or median of elution times)

**intensity computation :** calculation method to determine the intensity value of created clusters (most intense item of the cluster or sum)

#### **Alignment parameters**

#### Map Alignment :

- **method** : Two alignment methods can be used : *Iterative*: for the iterative algorithm, a reference map is first chosen randomly, then every other map is aligned against the reference and the algorithm computes the distance for each pair of maps. The map that has the shortest distance becomes the reference map. The 2 previous steps are re-iterated until either the reference map stays the same between two iterations or the maximum number of iterations is reached.
  - *Exhaustive*: the comprehensive algorithm computes the distance between maps for each possible pair of maps and selects the map with the lowest sum of distances to be the reference map. Then all other maps are aligned to this computed reference map and their retention times are corrected.

**max iteration**: this option is available only for the iterative method. This is a stop condition of this algorithm. When the algorithm has reached its maximum number of iterations, it stops

Parameters	uncer	<u> </u>				
Detection Clus	tering	Alignment	Normalization Cr	oss Assignment		-
Map Alignme	nt					
method:	Itera	tive			•	
max iteration:	3					
Smoothi	ng					
method:	ess				<b>.</b>	
<ul> <li>Feature method:</li> </ul>	Маррі	ng Peptide Ide	entity		•]	н
time toleranc	e (s):	600.0				
Ignore Alig	nment	Errors				

#### Smoothing

When the alignment is done, a trend can be extracted with a smoothing method permitting the correction of the aligned map retention time.

#### Number of landmarks/time interval:

- If the selected smoothing method is *landmark range*, the retention times in the aligned map are adjusted using the median computed on a sliding window whose size is determined by the number of landmarks it must contain. This is set up with the parameter *number of landmarks*. The smoothing method is applied considering the number of landmarks present in the window, and computes the median point for this window.
- If the selected smoothing method is set to *time window*, the retention times in the aligned map are adjusted using the median in a time window. You have to provide the fixed time interval. This time interval corresponds to the window size in which time median will be computed.

**Minimum number of landmarks in window:** this option is only available for time window smoothing method. This allows you to specify the minimum number of landmarks a window must contain to compute a median on it; it is not significant to compute a median on less landmarks.

**Sliding window overlap:** overlap is used to compute the step to move the smoothing window forward to calculate a smoothing point for this new smoothing window. This parameter gives the percentage of overlapping between two consecutive windows. For example, if the window size is 200 (seconds or landmarks depending on which smoothing method is selected) and overlap is 20%, the step forward is 200\*((100-20)/100) = 160 seconds or landmarks, i.e. the smoothing window is moved forward by a step of 160, so two successive windows overlap each other by a step of 40 seconds or landmarks corresponding to 20% of 200.

#### **Feature Mapping**

**method**: controls how feature mapping will be performed: by matching feature coordinates (mz, rt) or by using peptide identity associated with identified and quantified features.

**Moz tolerance (ppm)** -time tolerance : mass and time tolerance used to match features coordinates (only used if method is set to feature coordinates, ignored if the method is based on peptide identity).

#### Normalization

During this step, map intensities could be normalized using three different methods :

C Param	eters		
Detection	Clustering Alignme	nt Normalization Cross Assignment	
Map inter	isities Normalization	Nedian Ratio Median Ratio Intensity Sum Median Intensity	

Intensity sum : compute feature intensities sums for each map, set the reference map to the median map, normalization factor for map M = intensities sum of reference map / intensities sum of map M Median intensity: compute median intensity for each map, set the reference map to median map, normalization factor for map M = reference map median intensity / map M median intensity Median ratio: compute sum of feature intensities for each map of the map set and sort maps by computed intensities. The map ranking nearest from

the median is taken as the reference map. Then for each master map feature, compute ratio as reference map feature intensity / feature intensity

for the considered map. The normalization factor corresponds to the median of the computed ratios

#### Cross assignment(Master map creation):

This step consists in creating the "master map" (also called consensus map). This map results in the superimposition of all compared maps.

Detection Church	wing A	Imment Normalization Cross Assignment
Cross Assignm	ment	
Allow cross assig	nment	Between all runs
- Filtering		Between all runs
T neering		Within groups only
Use only o	contident	t features
Intensity	Filtering	1
intensity:	Intensit	
operator:	~	
operator.		*
value:	0.0	
Feature M	lapping	1
moz tolerance	(ppm):	5.0
RT tolerance (	s);	60.0

**Retain only reliable cross assigned features**: if checked, features found by cross assignment will be assessed by checking monoisotopic mass and charge state.

**Feature filter :** optional parameter to filter detected features. This option can be useful to ignore features of low intensity.

#### **Feature Mapping**

**moz tolerance (ppm)/ time tolerance** : error tolerance used to match features between maps. This procedure is also known as "match between runs" or "cross assignment" in other quantification software.

Astuce

Parameter settings can be saved and reused to configure a new quantification process.



Click OK to start the quantification process.

<b>III/</b>	VISUALIZE THE QUANTIFICATION	N RESULTS
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A. EXPORT QUANTIFICATION RESULTS

Export of the quantification includes separate tabs, some providing general information about the analysis, and some giving several levels of information about the results: the « Protein Set » level, the « Protein Match » level, and the peptidic and ionic levels.

Right-click on the quantification to display this menu:



#### **Display Abundances :**

**Peptide Ion/ Peptides/ Proteins Sets**: visualize the ions intensity (with redundancy on the charge), the peptides intensity and the protein abundance.

**Modification Sites/Modification Clusters:** Identify Modification Sites should have been run before. Visualize modification sites or modification clusters (grouping sites) with corresponding abundance data.

**Display Identification summary**: same as for the identifications.

**Display Exp.Design** : visualize the parameters that were used to realize the quantification (experimental design - parameters). Map alignments for all runs or between 2 specific ones could also be visualized.

## Rename

Delete

ComputePostProcessingonAbundances:post-processthe data (performs statistics). Also knownas Profilizer, this will be further detailed.

**Clone & Extract Abundances**: re-launch the quantification on this dataset with updated quantification parameters.

**Identify Modification Sites:** identify all modification sites in the dataset and cluster these sites according to specified parameters.

**Change Typical Protein/ Generate Spectrum Matches/ Retrieve Protein Sequences:** same as for the identifications.

**Export** : Excel format or list of spectra (list of transitions)

Action	<ul> <li>Compute Post Processing on Abundances with the following parameters:</li> <li>Use specific peptides only (in pep. selection tab)</li> <li>Do not Apply Normalization for peptides nor for protein sets (in Pep. configuration and Prot. configuration tabs)</li> <li>Use Sum for Abundance Summarizer Method (in Prot. configuration tab).</li> </ul>

Compute PostProcessing on Pr	roteins Sets Abundances	×
Pep. selection Pep. configuration P	rot. configuration	
Peptides Selection Method:	Specific	$\sim$
Discard Miss Cleaved Peptides		
Discard Modified Peptides		
Acetyl (Protein N-term)		
Carbamidomethyl (C)		
Oxidation (M)		
Modified Peptide Filtering Method:	Discard all forms	~
Discard Pep Ions Sharing Peakels		
Save 🕕 Load	V OK X Cancel	0

Action	Export the quantification results in an .xls file (version 2003) with the Protein sets tab checked (in addition to the 3 first tabs, checked by default).
Note	In the export configuration tabs, you will find 2 values for the abundance, depending on the profilizer setup: the raw abundance and the modified abundance (named only 'abundance').

Second Second											
cort to file:											
port Type: Excel (.xlsx)								~			
Custom Options											
Date format: vvvv:MM:dd	HH:mm:ss V Protein set	ts: Validated only									
Number separator:	<ul> <li>Export pro</li> </ul>	file: Best									
Search settings and infos	Import and filters	Quant config	Protein sets	Protein matches in protein sets	Best PSM from protein set	s Quantified peptide ions	PTM Clusters	Dataset statistics			
Orientation: rows				protein_match Rename the t	itle by Right click to Enable/Di	able	Select/Unselect al	fields 🗸			
Internal field name			Displayed field na	ame (editable)	Ex	port					
intormation_searcn_date			searcn_date				$\bowtie$				
nformation_raw_file_name			raw_file_name								
nformation_peaklist_file_path			peaklist_file_path			$\checkmark$					
nformation_result_file_name			result_file_name								
nformation_result_file_directory			result_file_directo	огу							
nformation_job_number			job_number								
nformation_user_name			user_name				$\checkmark$				
formation_user_email			user_email				$\leq$				
formation_queries_count			queries_count								
formation_searched_sequences	_count		searched_sequen	ices_count			$\leq$				
nformation_software_name			software_name								
formation_software_version			software_version								
nformation_instrument_config			instrument_config	1							
formation_database_names			database_names								
formation_database_releases	Contract of		database_release	:S							
formation_database_sequences	_count		uatabase_sequer	ices_count							
nformation_taxonomy			taxonomy								
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			peptide_charge_a	, 1							
ave 🕕 Load							🖌 Expor	t 🔀 Cancel			

## B. VISUALIZE QUANTIFIED PROTEINS AND PEPTIDES

Action

Use the Display Abundances menu to display the quantified proteins and peptides tables.



Action

Select the yeast proteins and the UPS1 proteins showing a variation between the two conditions 100 fmol and 10 fmol.



#### Protein Set: TRFL\_HUMAN\_UPS

Protein Set: ANXA5\_HUMAN\_UPS

ts × Ms Files	Logs	* 👲 Quant_100vs10	rotein Sets ×												
roline_Project 🗸 🖉 💌	M	× Protein Set	✓ Protein Set = ✓	MKAS_HUMAN_UPS	at otide	#Quant. Peptide		#Quant. PSM F083064	45	Abundance 1083064	#Quant. PSMs F083066	Abundance     F083066	<ul> <li>#Quant. PSMs</li> <li>F083067</li> </ul>	Abundance     F083067	#Quant. PSMs F083068
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Al Imported	TB.	05 ARO8_YEAST		sp P53090 ARO8_YE		21	21		34	29 171 01	0	27 28 29	1 096	22 26 166	338
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Trash		71 CISY1_YEAST		sp P00890 CISY1_YE	-	20	20		56	58 055 28	8	43 57 162	7 236	44 56 843	792
		72 ANXA5_HUMAN_		P08758ups(ANXA5_H.		20	20		0	5 301 37	2	1 3 674	1 569	0 4043	750
		73 BMH2_YEAST		sp[P34730]BMH2_YE		17	4		12	5 321 63	7	9 507	9 229	13 5 039	898
instations		74 RL8A_YEAST	8-8-1	sp/P17076/RL8A_YEA.		20	3		6	1 337 30	3	5 518	3 002	4 1640	078
SC Compare 1%		10 SAPPLITEAST		spipostspipost year		10	10		30	57 390 97 40 702 65	2 c	19 40 051	1 11/2	32 34034	307
Craul Trovaro		27 B PHSC YEAST		eniP06738IDHSC YE		27	27		36	24 203 31	2	4 24.46	718	33 22 795	024
Identification reference : Comparaison 100 vs 10 1%		78 GRP78 YEAST		spiP 16474 GRP 78 YE.		20	18		27	30 459 34	D	30 29 092	2 352	25 29 218	508
Group 10 mill - 1%		<													
E- Sampe 10 mol - 1%									-						
E PLASSING	m								R Gra	aphic : Linear Plot 、	X Axis: Quant. Ch	annel 🗸 Y Axis:	Abundance 🗸 🗸		
() C Engine 7	T	Status	Peptide Sequence	PTMs	Score	Charge	m	1/z 🗘	-						
Course 100 feed - 181	50	10	LIVALMKPSR			4.05	3	0	-	1.307			1		•
Group 100 mol - 1%		2 4	DLLDDLK			16.26	2		2)	1/12/7					-5
Er a Sample 100 mild - 198	12	2 🗳	QEISAAFK			27.21	2		冊						
(g)- PUS3068	12	4 🖒	FITIFGTR			40.40	2		100	1.467 -					
E-0 P083089		3 10	NEATSLYSICK	Oxidation (M9)		47.40	2		Ξ.						
E-OFERSONO		10	SIPAYLAETLYYAMK			33.90	3		📼 🦉	0.460					
Quar		4	DPDAGLDEAQVEQUA	Oxidation (M1)	_	91.32	2		- Pe	6.8F6 -					3
Quart_100vs10_2		4	G GTDEESILTH TSR	Oxdator (H1)		26.08	-		- q				11/2-		
(Tesz)		10 13	LYDAYELK			27.43	2		-	4.066 -					
		11 6	SIPAYLAETLYYA'K	Oxidation (M14)		61.84	2						11/		
		12 🖒	LIVALMK			12.58	2			2.0E6 -					
		13 🙆	ALLLEGEDD	Carbamidomethyl (C6)		5.56	2			() ()	8				
		14 0	QVYEEEYGSSLEDOWV			43.90	3							<u></u>	
		15 0	SEIDLENIR			45.98	2	· ·		P083064	F083166	F083057	F083268	F083059	F083270
												Qua	ant. Channel		
	Que	nti. Peptides Ions XIC Fe	atures						A Gr	aphic : Linear Plot	/ X Axis: RT	V Y Axis: Intens	ty 🗸		
	n	Peptide Sequence	Status	PTMs	Score	Charge		m/z tu		8.086					
	I	I GLGTDEESILTILTSR	á		13	95.84	2			7,0E6 -		Δ.			
		2 GLGTDEESILTLLTSR	4			36.08	3		1941	6.056 -		AR			
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								~						a	
		<						>		\$5,4	35,8 96	96,2 96,4	96.6 96.8	97 97,2 97,4	97,6 97,
													RT		

Example: peptidic view (top) with the table of the peptide ions (bottom) associated with the selected peptide:

Status	Peptide Sequence	PTMs	Score	Charge	m/z	RT	Protein	. Protein S	Sets	Overview	Quant.     PSMs	<ul> <li>Abundance</li> <li>F083064</li> </ul>	Quant.     PSMs	<ul> <li>Abundance</li> <li>F083066</li> </ul>	Quant     PSMs	<ul> <li>Abundance</li> <li>F083067</li> </ul>	Quant.     PSMs	Abundance     F083068	Qua Abunda PSMs F083069	ance F
17	MPAISLTS IK	Oxidation (MA)	47.40		2 043.8240	/8.2		1_CANVAL	UMAN_UPS		. 0	242 845	. 0	U		154.075	1 2	1 23/ 3/5	3	1 /55 82*
0	DPDAGIDEAQVEQDAQA		41.32		2 1329.6350	94.3		1 ANXA5_H	IUMAN_UPS	10	0	0	0	0	(	0	0 0	747 719	0	1 086 201
0	GLGTDEESILTLLTSR		36.08		3 568.9735	5 96.53		1 ANXA5_H	IUMAN_UPS		0	196 364	0	0	(	0	) 3	2 085 402	4	2 329 266
6	SEIDLFNIR		45.98		2 553.7957	83.32		1 ANXA5_H	IUMAN_UPS		0	543 434	0	682 872	0	555 717	7 2	6 788 921	2	6 056 654
6	GAGTDDHTLIR		63.33		2 578.2910	17.29		1 ANXA5_H	IUMAN_UPS		0	196 195	0	232 610	0	206 115	5 2	2 444 841	1	2 424 022
-	MLVVLLQANRDPDAGIDEAQ	Oxidation (M1)	59.44		3 1271.3130	95,84		1 ANXA5_F	HUMAN_UPS		0	264 074	0	277 259		312 170	0 1	2 601 544	2	2 545 243
6	SIPAYLAETLYYA	Oxidation (M14)	61.84		2 875.4431	92.21		1 ANXA5_H	IUMAN_UPS		0	0	0	0	(	0	3	1 734 762	2	1876 411
6	QVYEEEYGSSLEDDVVGD		36.32		2 1444.6230	0.08		1 ANXA5_H	IUMAN_UPS		0	103 818	0	0	0	( C	1	979 418	2	1017 122
6	LYDAYELK		27.43		2 507.7601	44.81		1 ANXA5_H	IUMAN_UPS		0	523 377	0	521 367	(	542 732	2 0	5 712 158	0	5 968 464
3	VLTEIIASR.		62.35		2 501.3029	49.53		1 ANXA5_H	IUMAN_UPS		0	984 817	0	983 957	(	1 128 651	1 2	12 245 631	1	12 891 288
6	FVDQNPGVFSK		29.96		2 619.3141	42.21		1 SEC7_YE	AST		0	301 916	0	0	(	263 360	0 0	275 602	0	351 730
6	IEDDILVTK		35.27		2 523.2917	45.80		1 YFH6_YE	AST	and the	1	528 030	0	505 534	1	596 495	5 1	745 704	1	785 907
6	VKDLLLNR		38.44		485.8055	66.29		1 YFH6 YE	AST	Con State	1	1 372 311	1	1 319 226	0	1 278 718	3 2	1 686 754	3	1 682 715
B	WDGSSGGVIR		43.03		2 517.2561	30.42		1 PSB6 YE	AST		2	1 087 848	1	988 684	(	981 606	5 2	1 128 706	0	0
13	TTTGAYLANR		52.02		2 534.2766	18.05		1 PSB6 YE	AST	Con State	0	744 435	1	700 167		678 234	1	994 291	1	940 712
13	GNOFLOENK		32.46		2 539,2693	21.73		1 SYMC YE	AST	and the	2	557 734	2	563 103		615 460	2	822 356	1	722 416
6	GVGVEGNNAODSGISPSV		94.36		2 1024.0040	81.92		1 SYMC YE	AST	Contract.	2	804 936	1	711 029		703 530	1	761 918	4	620 932
6	AI FEGYTPR		28.13		2 486 2605	20.25		1 SYMC YE	AST		0	651 535	0	679.953		674 307	7 0	927 787	0	912 159
6	DSETL PKPNER		26.91		2 649.3405	26.46		1 SYMC YE	AST		0	629.059	1	637 420		691 259	0	761 117	0	715 825
3	SELISEDY	Acetul (Protein	26.28		2 400 7641	04.75		1 SYMC VE	AST		0	029039	0	037 120		071255	1	273 529	0	713025
4	NENEOU TEDEVALUE	Access (Fronterin	42.45		012.0655	57.54		1 ADDC4 N	EACT		2	610.050	2	614.065		607.243		752 242	2	740.059
1	COSLODING TAND	Acatal Photoin	AC 40		716 9090	60.01		1 ADDCA V	EACT		3	1 317 497	2	1 207 719		1 245 061		1 626 461	2	1 445 036
4	CADMALCID	Acetyl (Protein	20.26		2 710.0303	101.60		LADOR VE	LAST		2	1217 907	2	1 307 710		243 901	1 2	1 012 497	3	1 113 930
4	GREDWILLGER		70.20		2 603.3394	101.60		TAKUS_TE	CAST			870 483	2	799 404		850 082		1012 487		10128/0
4	GITAAVSPEK		54.20		2 511.7607	17.24		TARUS_TO	LAST		1	1 909 992	1	1/114/2		1 622 571		2 345 093	1	2022814
0	ULYTIPTGQNPTGTSTADHR		74.92	2	2 10/8.0620	63.88		1 AROS_TE	AST		1	463 195	2	588 895		612 506	0	766 040	0	935 891
0	DTHPWDNLSVDSPRPPPPQG	Carbamidometh	34.22		3 1215.5840	93.3		1 AROS_TE	AST		1	1 686 646	1	1 552 878	1	1 /30 654	+ 1	1 213 053	0	1 292 104
0	SANPSNDIPLSR		50.80		2 635.8222	2 35.05		1 AROS_TE	:AST		2	2 205 696	3	2 551 328		2 328 861	0	2 826 378	1	2 798 844
0	YDFLIVEDEPYYFLQMNPYIK		30.15		2 1350.6520	102.38		1 ARO8_YE	EAST		1	350 967	0	434 946	6	290 755	5 0	296 549	0	275 091
6	GWLVVPGSWFK		33.96		2 594.8427	89.26		1 ARO8_YE	EAST		1	3 452 304	1	3 954 183		3 592 186	5 2	3 741 522	1	3 972 242
6	LGWITGSSK		33.66		2 474.7607	45.61		1 ARO8_YE	EAST		3	1 111 213	1	991 540	1	909 290	0 0	0	0	1 238 931
6	SEGETEPPQPAESK		70.02		2 743.3387	13.15		1 AROS_YE	AST		3	587 386	4	623 315	2	542 044	1 2	818 217	5	690 398
0	ALQYGFSAGQPELLNFIR		96.63	-	2 1012.5360	94.33		1 ARO8_YE	EAST		2	2 608 365	2	2 796 080	2	2 625 916	5 2	2 624 530	3	2 392 827
6	TCIHLFQDPNIIFLGGGLPLK	Carbamidometh	47.78		3 785.0992	97.38		1 AROS_YE	AST		0	556 378	0	706 708		735 877	3	635 303	1	945 364
6	LGDTLYEEFGISK		44.54		2 736.3702	81.25		1 ARO8_YE	AST	a-sist.	0	454 255	0	333 379	1	470 039	1	779 482	0	599 522
6	SLANTFLSLDTEGR		82.72		2 762.3890	85.15		1 ARO8_YE	AST		1	3 444 122	0	3 689 210	(	0	0 0	0	0	3 742 638
6	EVSNPNIIFFR		43.97		2 668.3563	8 81.57		1 AROS_YE	EAST		0	2 932 420	0	2 754 924	(	2 709 621	1 1	3 101 035	2	2 857 619
<	DEPUT CONTRACT					30.01		11000.07				1 20.4 400				1 204 021				>
ptide Se	quence	Status	PTMs	Score	Charge	m/z R	Pr	Pro	Pep. match	Abundance F083064	Pep. mat	ch Abundanc F083066	e Pep count	match Abu	undance 067	Pep. match count	Abundanc     F083068	e Pep. # A match F0	bundance P 33069 ma	ep. Abund tch F083070

Each column can be sorted. The tables can be exported to XLS (Excel) or TSV files.