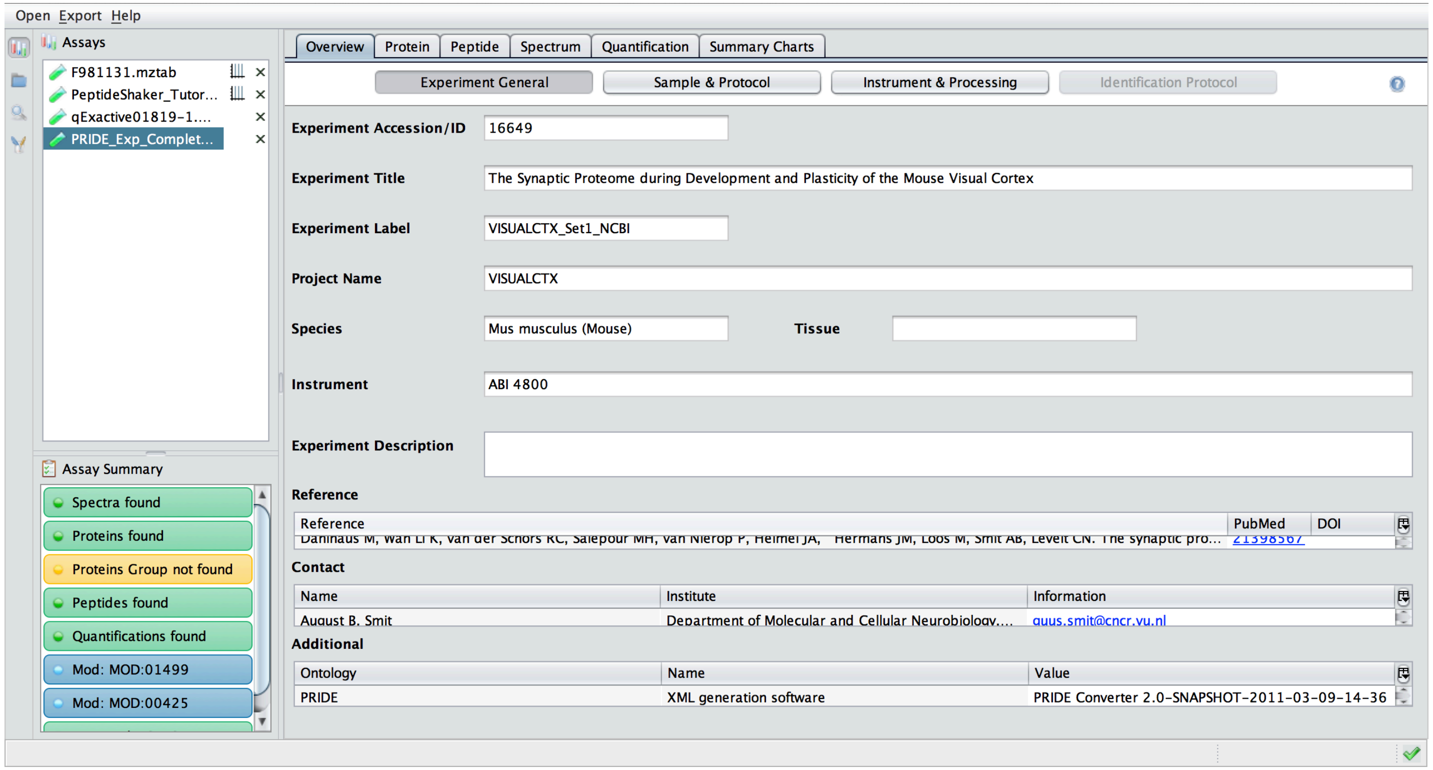
Perez-Riverol *et al.,* PRIDE Inspector Toolsuite: moving towards a universal visualization tool for proteomics data standard formats and quality assessment of ProteomeXchange datasets, Supp. Figures

Supplementary Figures



Experiment Accession/ID 16649

Experiment Title The Synaptic Proteome during Development and Plasticity of the Mouse Visual Cortex

Experiment Label VISUALCTX_Set1_NCBI

Project Name VISUALCTX

Species Mus musculus (Mouse) **Tissue**

Instrument ABI 4800

Experiment Description

Reference

Reference	PubMed	DOI
Dahlhaus M, Wan Li K, van der Schors RC, Saiepour MH, van Nierop P, Heimel JA, Hermans JM, Loos M, Smit AB, Levelt CN. The synaptic pro...	21398567	

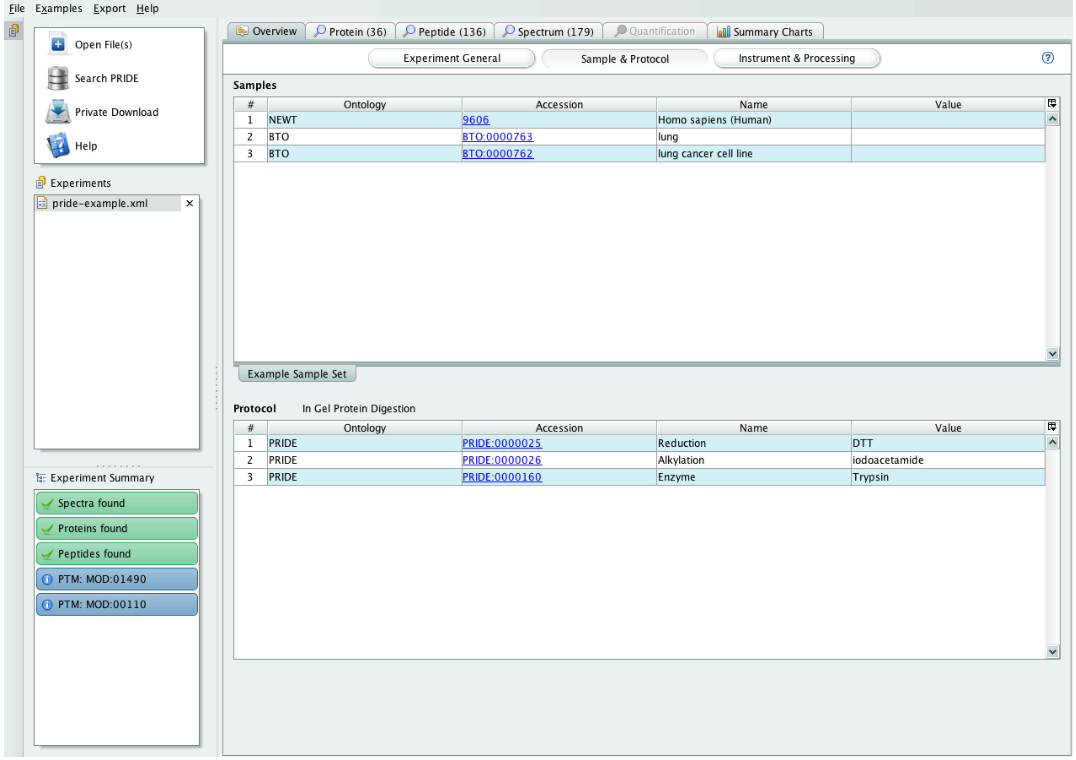
Contact

Name	Institute	Information
August B. Smit	Department of Molecular and Cellular Neurobiology....	guus.smit@cncr.vu.nl

Additional

Ontology	Name	Value
PRIDE	XML generation software	PRIDE Converter 2.0-SNAPSHOT-2011-03-09-14-36

Suppl. Figure 1: PRIDE Inspector 'Overview' panel: 'Experiment General View'. The tab contains basic metadata information about an experimental file: experiment and project titles, contact information, software used for the file generation, and original file format, amongst others.



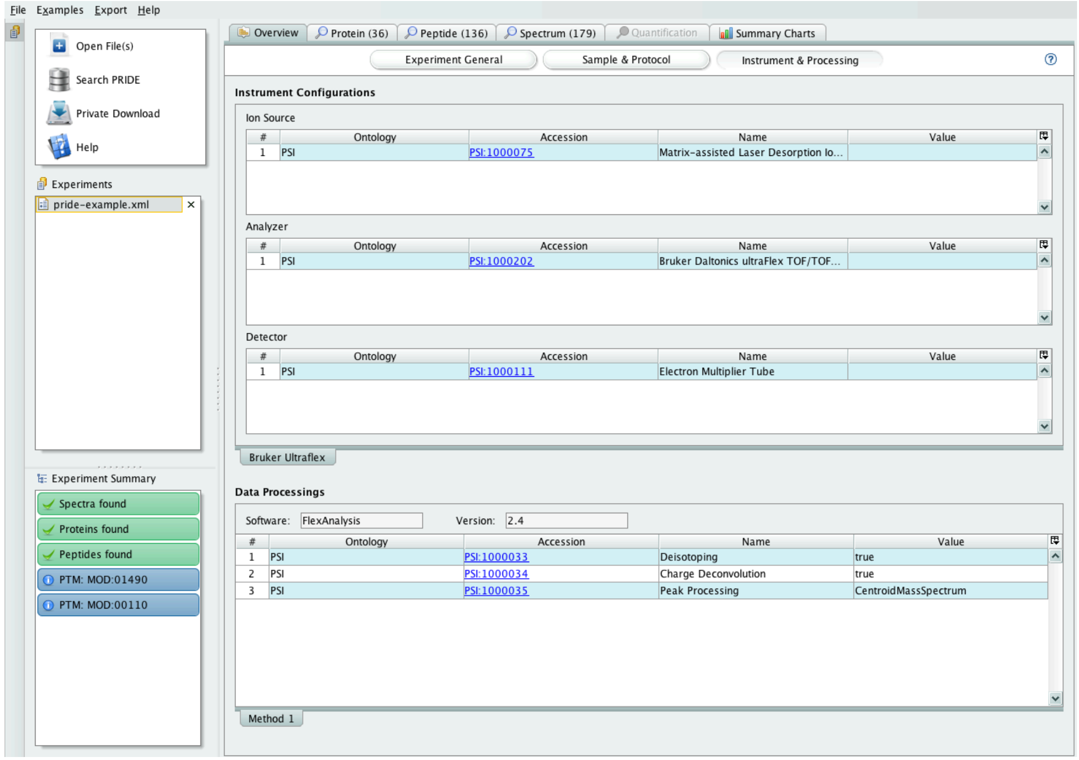
Samples

#	Ontology	Accession	Name	Value
1	NEWT	9606	Homo sapiens (Human)	
2	BTO	BTO:0000763	lung	
3	BTO	BTO:0000762	lung cancer cell line	

Protocol In Gel Protein Digestion

#	Ontology	Accession	Name	Value
1	PRIDE	PRIDE:0000025	Reduction	DTT
2	PRIDE	PRIDE:0000026	Alkylation	iodoacetamide
3	PRIDE	PRIDE:0000160	Enzyme	Trypsin

Suppl. Figure 2: PRIDE Inspector ‘Overview’ panel: ‘Sample & Protocol View’. This tab contains metadata information about the sample (species, tissues, etc) and the experimental protocol.



Instrument Configurations

Ion Source

#	Ontology	Accession	Name	Value
1	PSI	PSI:1000075	Matrix-assisted Laser Desorption Io...	

Analyzer

#	Ontology	Accession	Name	Value
1	PSI	PSI:1000202	Bruker Daltonics ultraFlex TOF/TOF...	

Detector

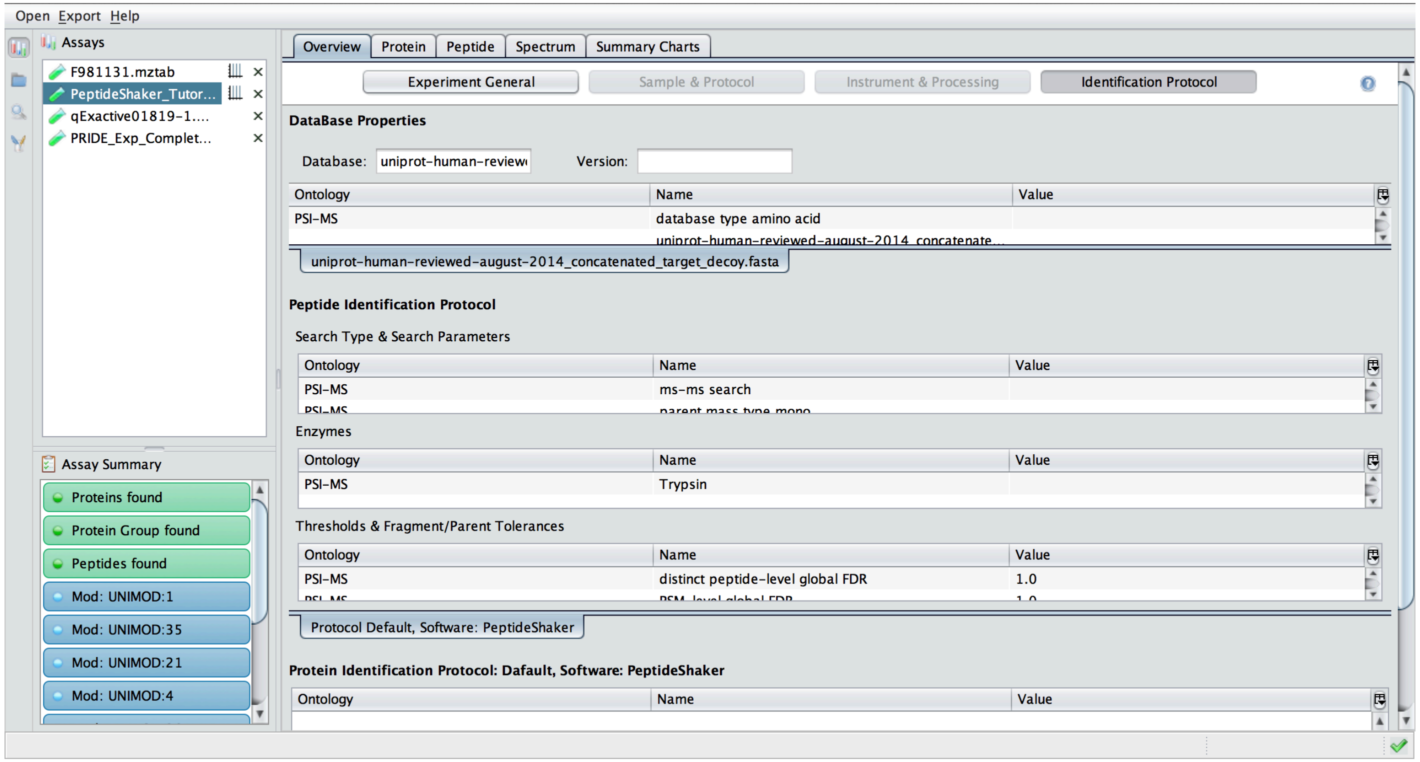
#	Ontology	Accession	Name	Value
1	PSI	PSI:1000111	Electron Multiplier Tube	

Data Processings

Software: FlexAnalysis
Version: 2.4

#	Ontology	Accession	Name	Value
1	PSI	PSI:1000033	Deisotoping	true
2	PSI	PSI:1000034	Charge Deconvolution	true
3	PSI	PSI:1000035	Peak Processing	CentroidMassSpectrum

Suppl. Figure 3: PRIDE Inspector ‘Overview’ panel: ‘Instrument & Processing View’. This tab contains metadata information about the instrument configuration and software used.



DataBase Properties

Database: uniprot-human-reviewe

Version:

Ontology	Name	Value
PSI-MS	database type amino acid	
	uniprot-human-reviewed-august-2014_concatenate...	

uniprot-human-reviewed-august-2014_concatenated_target_decoy.fasta

Peptide Identification Protocol

Search Type & Search Parameters

Ontology	Name	Value
PSI-MS	ms-ms search	
PSI-MS	parent mass type mono	

Enzymes

Ontology	Name	Value
PSI-MS	Trypsin	

Thresholds & Fragment/Parent Tolerances

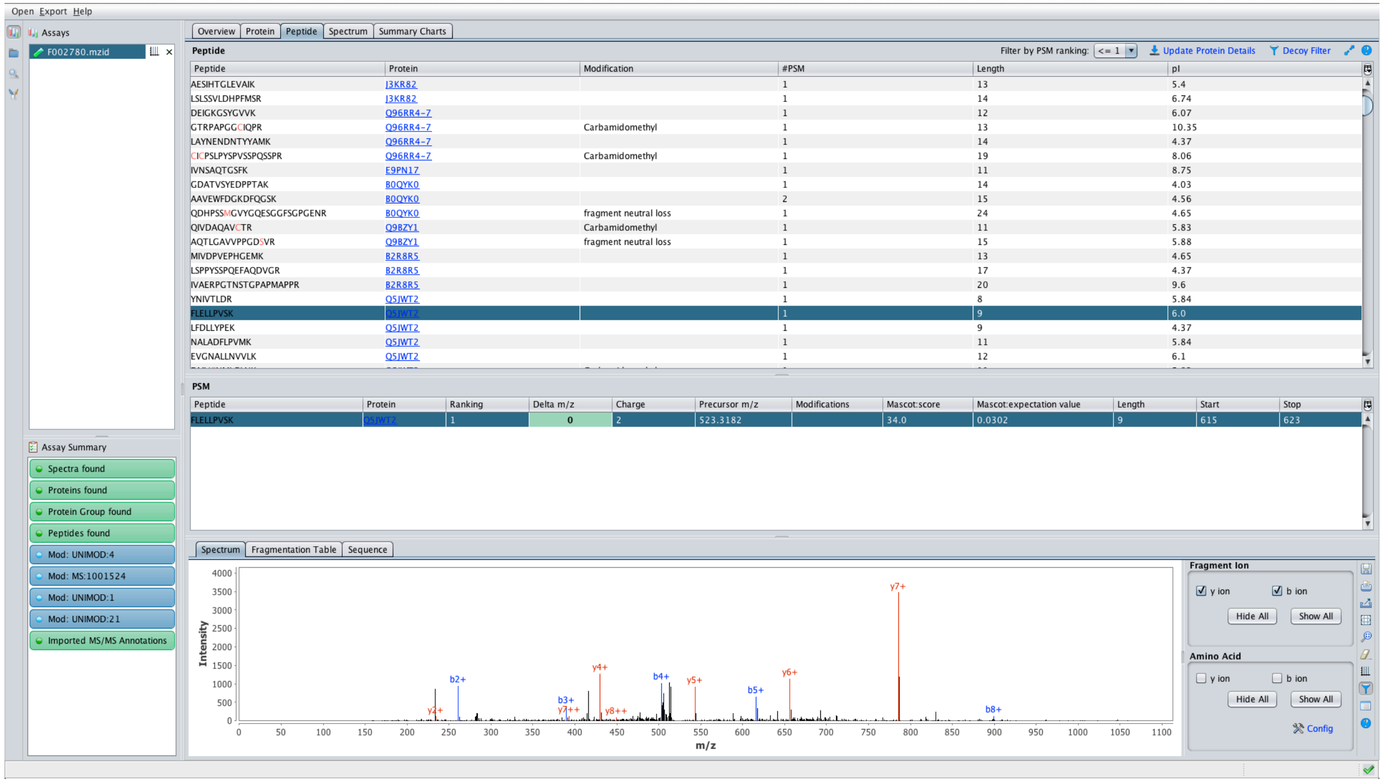
Ontology	Name	Value
PSI-MS	distinct peptide-level global FDR	1.0
PSI-MS	PSM-level global FDR	1.0

Protocol Default, Software: PeptideShaker

Protein Identification Protocol: Dafault, Software: PeptideShaker

Ontology	Name	Value

Suppl. Figure 4: PRIDE Inspector 'Overview' panel: 'Identification Protocol View'. This tab contains metadata information about the peptide/protein identification protocols such as search parameters, databases, search engines and software used.



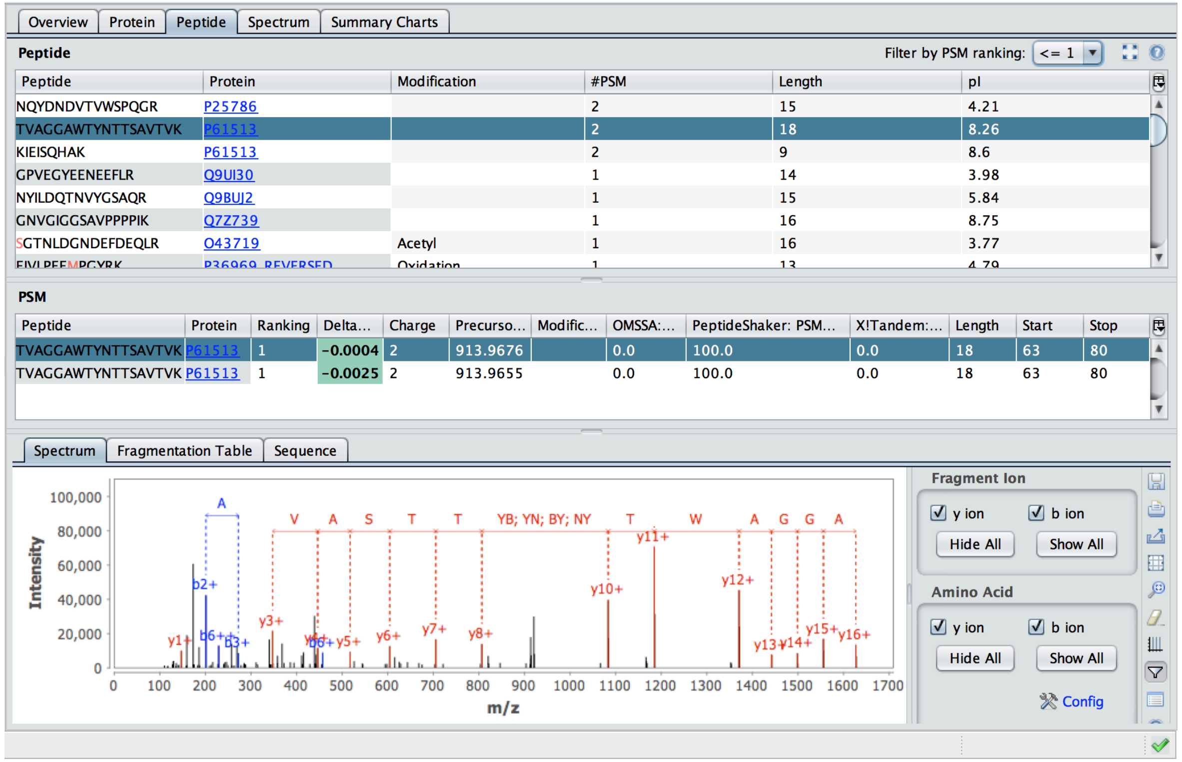
Peptide

Peptide	Protein	Modification	#PSM	Length	pI
AESIHTGLEVAIK	J3KR82		1	13	5.4
LSLSSVLDHPFMSR	J3KR82		1	14	6.74
DEIGKGSYGVVK	Q96RR4-7		1	12	6.07
GTRPAPGGCIQPR	Q96RR4-7	Carbamidomethyl	1	13	10.35
LAYNENDNTYYAMK	Q96RR4-7		1	14	4.37
CICPSLPYSPVSSPQSSPR	Q96RR4-7	Carbamidomethyl	1	19	8.06
IVNSAQTGSFK	E9PN17		1	11	8.75
GDATVSYEDPPTAK	B0QYK0		1	14	4.03
AAVEWFDGKDFQGSK	B0QYK0		2	15	4.56
QDHPSSMGVYGQESGGFSGPGENR	B0QYK0	fragment neutral loss	1	24	4.65
QIVDAQAVCTR	Q9BZY1	Carbamidomethyl	1	11	5.83
AQTLGAVVPPGDSVR	Q9BZY1	fragment neutral loss	1	15	5.88
MIVDPVEPHGEMK	B2R8R5		1	13	4.65
LSPPYSSPQEFAQDVGR	B2R8R5		1	17	4.37
IVAERPGTNSTGPAPMAPPR	B2R8R5		1	20	9.6
YNIVTLDR	Q5JWT2		1	8	5.84
FLELLPVSK	Q5JWT2		1	9	6.0
LFDLLYPEK	Q5JWT2		1	9	4.37
NALADFLPVMK	Q5JWT2		1	11	5.84
EVGNALLNVVLK	Q5JWT2		1	12	6.1

PSM

Peptide	Protein	Ranking	Delta m/z	Charge	Precursor m/z	Modifications	Mascot:score	Mascot:expectation value	Length	Start	Stop
FLELLPVSK	Q5JWT2	1	0	2	523.3182		34.0	0.0302	9	615	623

Suppl. Figure 5: ‘Peptide View’: It shows the peptides identified in the experiment and the corresponding PSMs including different properties such as peptide scores, isoelectric point and sequence length.



Peptide

Filter by PSM ranking: <= 1

Peptide	Protein	Modification	#PSM	Length	pI
NQYDNDVTVWSPQGR	P25786		2	15	4.21
TVAGGAWTYNTTSAVTVK	P61513		2	18	8.26
KIEISQHAK	P61513		2	9	8.6
GPVEGYEENEEFLR	Q9UI30		1	14	3.98
NYILDQTNVYGSAQR	Q9BUJ2		1	15	5.84
GNVGIGGSAVPPPPIK	Q7Z739		1	16	8.75
SGTNLDGNDEFDEQLR	O43719	Acetyl	1	16	3.77
EIVLPEEMPGYRK	P36969_REVERSED	Oxidation	1	13	4.79

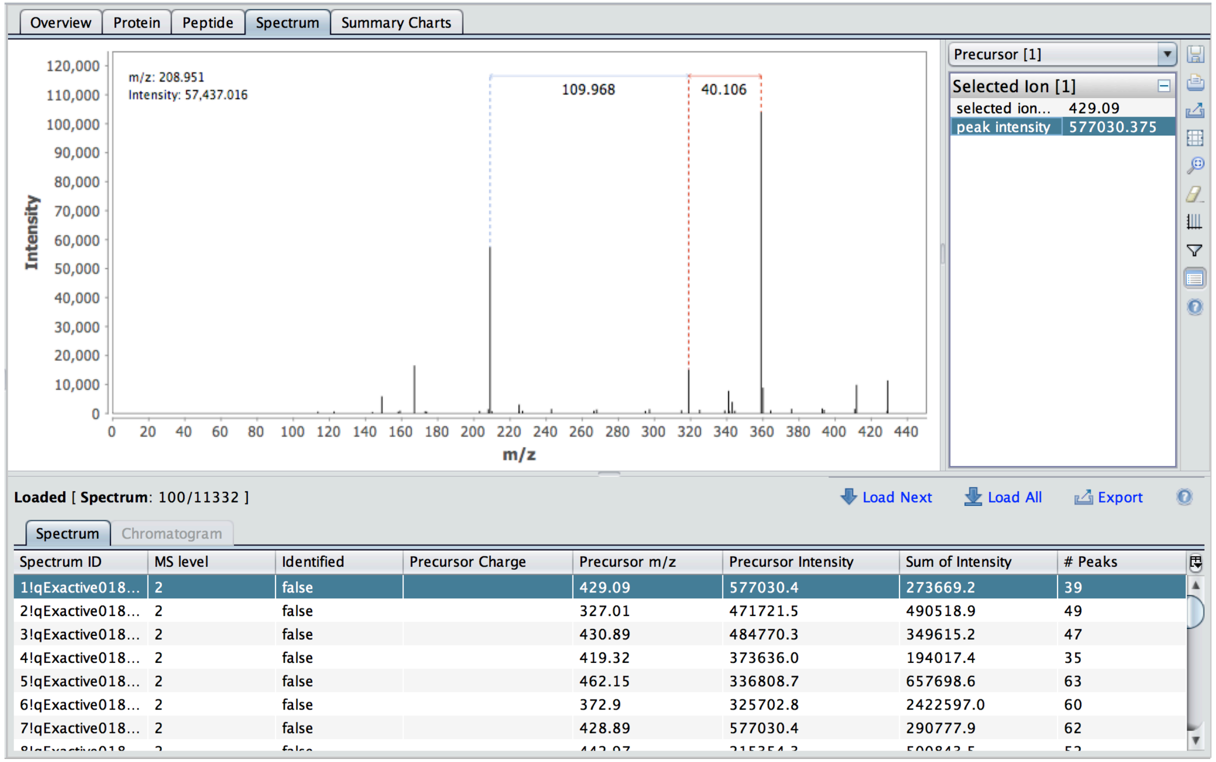
PSM

Peptide	Protein	Ranking	Delta...	Charge	Precurso...	Modific...	OMSSA:...	PeptideShaker: PSM...	X!Tandem:...	Length	Start	Stop
TVAGGAWTYNTTSAVTVK	P61513	1	-0.0004	2	913.9676		0.0	100.0	0.0	18	63	80
TVAGGAWTYNTTSAVTVK	P61513	1	-0.0025	2	913.9655		0.0	100.0	0.0	18	63	80

Fragment Ion: ☑ y ion ☑ b ion — Hide All / Show All

Amino Acid: ☑ y ion ☑ b ion — Hide All / Show All

Suppl. Figure 6: The ‘Peptide View’ tab including the mass spectrum fragment annotation viewer: the selected amino acid sequences are highlighted.

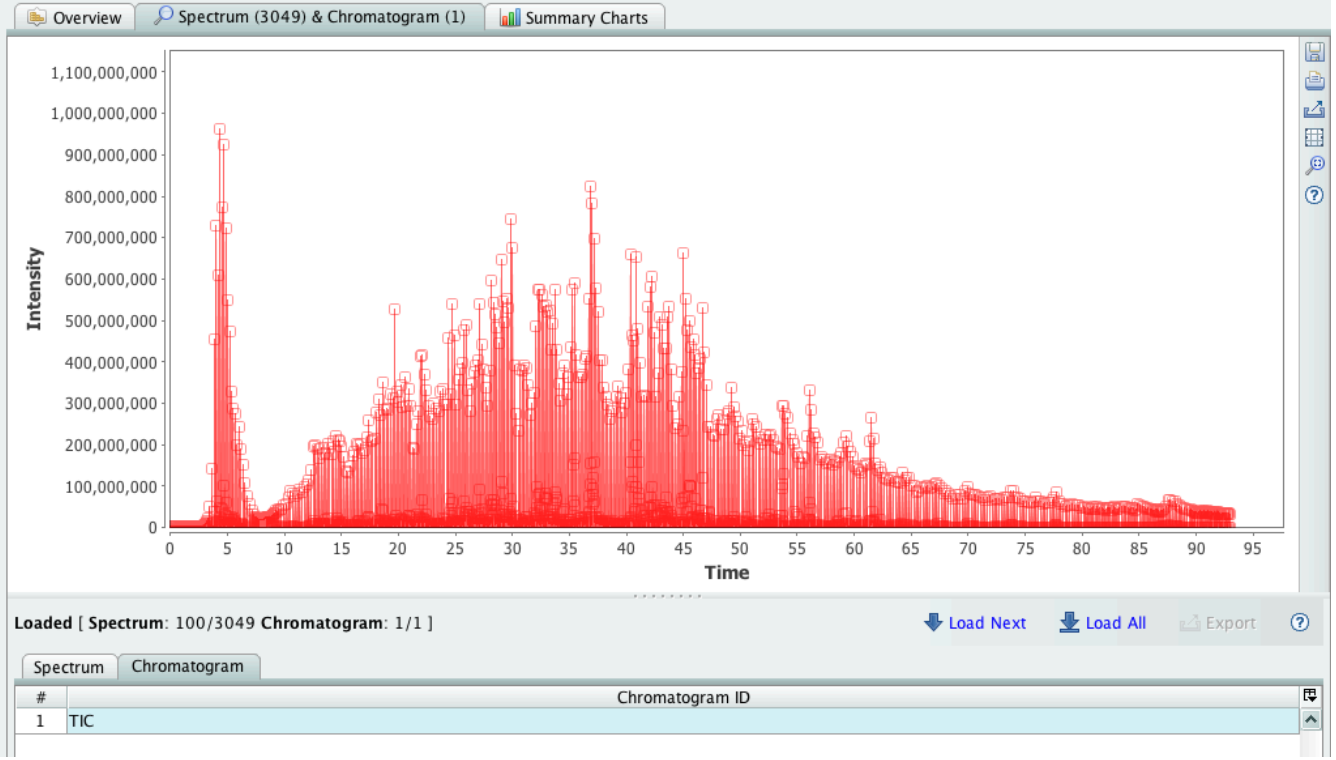


selected ion...	429.09
peak intensity	577030.375

Loaded [**Spectrum**: 100/11332]

Spectrum ID	MS level	Identified	Precursor Charge	Precursor m/z	Precursor Intensity	Sum of Intensity	# Peaks
1!qExactive018...	2	false		429.09	577030.4	273669.2	39
2!qExactive018...	2	false		327.01	471721.5	490518.9	49
3!qExactive018...	2	false		430.89	484770.3	349615.2	47
4!qExactive018...	2	false		419.32	373636.0	194017.4	35
5!qExactive018...	2	false		462.15	336808.7	657698.6	63
6!qExactive018...	2	false		372.9	325702.8	2422597.0	60
7!qExactive018...	2	false		428.89	577030.4	290777.9	62

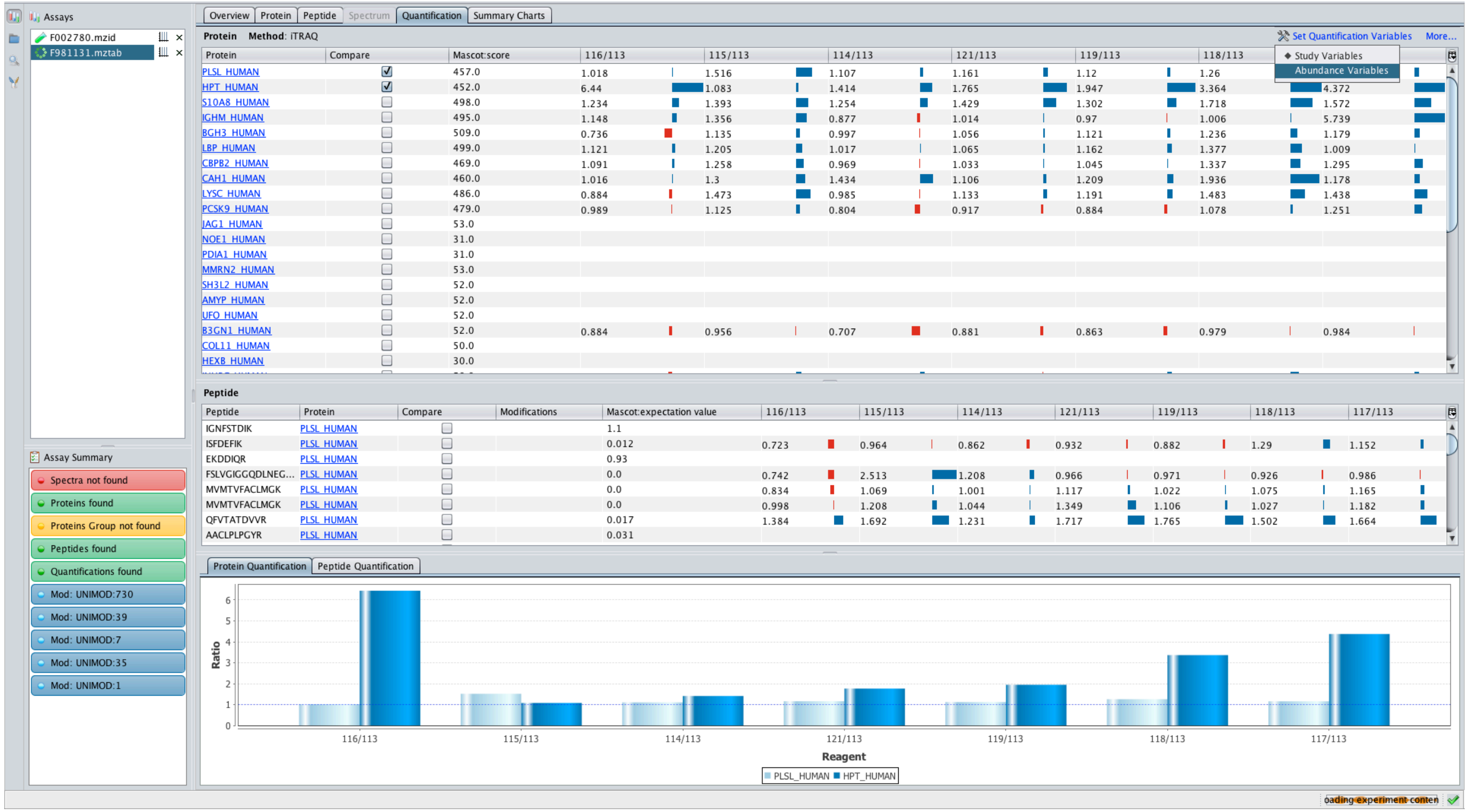
Suppl. Figure 7: ‘Mass Spectrum View’. This tab shows all mass spectra (identified + unidentified) included in the experiment. Mass spectrum details and the related scan and precursor information are accessible from the upper right window. In addition it is possible to perform *de novo* sequencing (not shown).



Loaded [**Spectrum**: 100/3049 **Chromatogram**: 1/1]

#	Chromatogram ID
1	TIC

Suppl. Figure 8: ‘ Mass Spectrum View’: If chromatograms are included in the mzML file, PRIDE Inspector can display them in this tab. It must be noticed that chromatograms cannot be included in PRIDE XML and/or mzTab files.



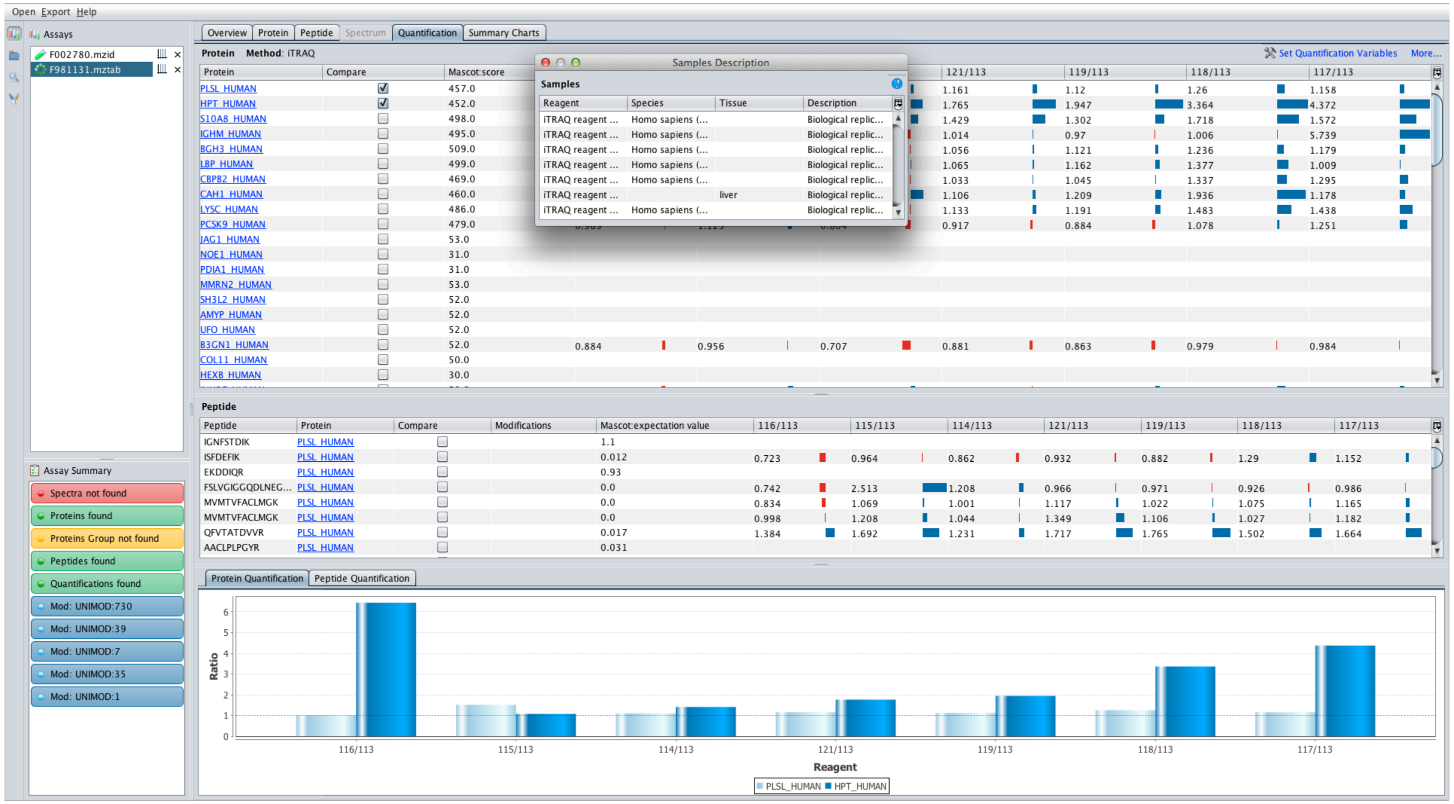
Protein **Method**: iTRAQ

Protein	Compare	Mascot:score	116/113	115/113	114/113	121/113	119/113	118/113	
PLSL_HUMAN	☑	457.0	1.018	1.516	1.107	1.161	1.12	1.26	
HPT_HUMAN	☑	452.0	6.44	1.083	1.414	1.765	1.947	3.364	4.372
S10A8_HUMAN	☐	498.0	1.234	1.393	1.254	1.429	1.302	1.718	1.572
IGHM_HUMAN	☐	495.0	1.148	1.356	0.877	1.014	0.97	1.006	5.739
BGH3_HUMAN	☐	509.0	0.736	1.135	0.997	1.056	1.121	1.236	1.179
LBP_HUMAN	☐	499.0	1.121	1.205	1.017	1.065	1.162	1.377	1.009
CBPB2_HUMAN	☐	469.0	1.091	1.258	0.969	1.033	1.045	1.337	1.295
CAH1_HUMAN	☐	460.0	1.016	1.3	1.434	1.106	1.209	1.936	1.178
LYSC_HUMAN	☐	486.0	0.884	1.473	0.985	1.133	1.191	1.483	1.438
PCSK9_HUMAN	☐	479.0	0.989	1.125	0.804	0.917	0.884	1.078	1.251
JAG1_HUMAN	☐	53.0							
NOE1_HUMAN	☐	31.0							
PDIA1_HUMAN	☐	31.0							
MMRN2_HUMAN	☐	53.0							
SH3L2_HUMAN	☐	52.0							
AMYP_HUMAN	☐	52.0							
UFO_HUMAN	☐	52.0							
B3GN1_HUMAN	☐	52.0	0.884	0.956	0.707	0.881	0.863	0.979	0.984
COL11_HUMAN	☐	50.0							
HEXB_HUMAN	☐	30.0							

Peptide

Peptide	Protein	Compare	Modifications	Mascot:expectation value	116/113	115/113	114/113	121/113	119/113	118/113	117/113
IGNFSTDIK	PLSL_HUMAN	☐		1.1							
ISFDEFIK	PLSL_HUMAN	☐		0.012	0.723	0.964	0.862	0.932	0.882	1.29	1.152
EKDDIQR	PLSL_HUMAN	☐		0.93							
FSLVGIGGQDLNEG...	PLSL_HUMAN	☐		0.0	0.742	2.513	1.208	0.966	0.971	0.926	0.986
MVMTVFACLMGK	PLSL_HUMAN	☐		0.0	0.834	1.069	1.001	1.117	1.022	1.075	1.165
MVMTVFACLMGK	PLSL_HUMAN	☐		0.0	0.998	1.208	1.044	1.349	1.106	1.027	1.182
QFVTATDVVR	PLSL_HUMAN	☐		0.017	1.384	1.692	1.231	1.717	1.765	1.502	1.664
AACLPLPGYR	PLSL_HUMAN	☐		0.031							

Suppl. Figure 9: “Quantitation View”. This panel shows quantitative information at the protein and peptide level. The “Set quantitation variables” option shows the study variables and abundance variables following the mzTab model.



Protein **Method**: iTRAQ

Protein	Compare	Mascot:score				121/113	119/113	118/113	117/113
PLSL_HUMAN	☑	457.0				1.161	1.12	1.26	1.158
HPT_HUMAN	☑	452.0				1.765	1.947	3.364	4.372
S10A8_HUMAN	☐	498.0				1.429	1.302	1.718	1.572
IGHM_HUMAN	☐	495.0				1.014	0.97	1.006	5.739
BGH3_HUMAN	☐	509.0				1.056	1.121	1.236	1.179
LBP_HUMAN	☐	499.0				1.065	1.162	1.377	1.009
CBPB2_HUMAN	☐	469.0				1.033	1.045	1.337	1.295
CAH1_HUMAN	☐	460.0				1.106	1.209	1.936	1.178
LYSC_HUMAN	☐	486.0				1.133	1.191	1.483	1.438
PCSK9_HUMAN	☐	479.0				0.917	0.884	1.078	1.251
JAG1_HUMAN	☐	53.0							
NOE1_HUMAN	☐	31.0							
PDIA1_HUMAN	☐	31.0							
MMRN2_HUMAN	☐	53.0							
SH3L2_HUMAN	☐	52.0							
AMYP_HUMAN	☐	52.0							
UFO_HUMAN	☐	52.0							
B3GN1_HUMAN	☐	52.0	0.884	0.956	0.707	0.881	0.863	0.979	0.984
COL11_HUMAN	☐	50.0							
HEXB_HUMAN	☐	30.0							

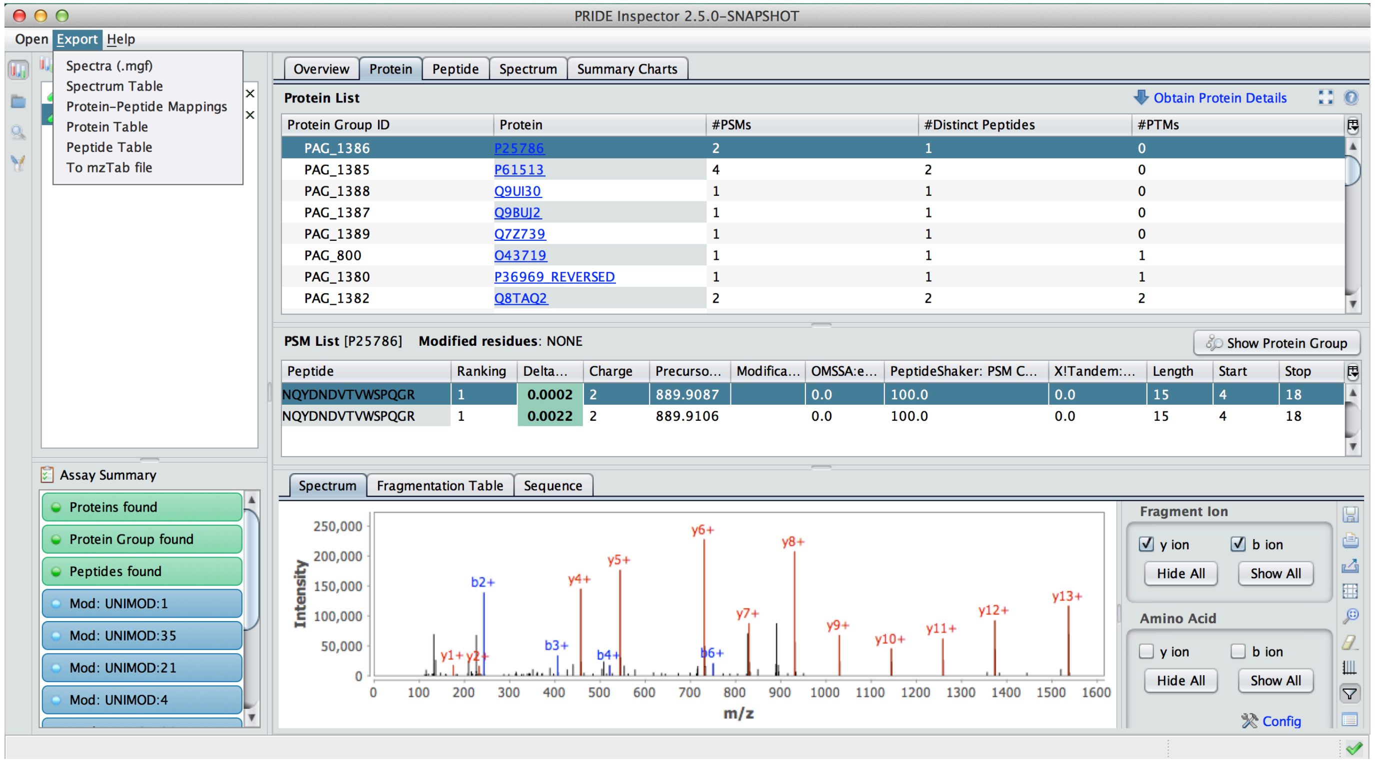
Samples

Reagent	Species	Tissue	Description
iTRAQ reagent ...	Homo sapiens (...		Biological replic...
iTRAQ reagent ...	Homo sapiens (...		Biological replic...
iTRAQ reagent ...	Homo sapiens (...		Biological replic...
iTRAQ reagent ...	Homo sapiens (...		Biological replic...
iTRAQ reagent ...	Homo sapiens (...		Biological replic...
iTRAQ reagent ...		liver	Biological replic...
iTRAQ reagent ...	Homo sapiens (...		Biological replic...

Peptide

Peptide	Protein	Compare	Modifications	Mascot:expectation value	116/113	115/113	114/113	121/113	119/113	118/113	117/113
IGNFSTDIK	PLSL_HUMAN	☐		1.1							
ISFDEFIK	PLSL_HUMAN	☐		0.012	0.723	0.964	0.862	0.932	0.882	1.29	1.152
EKDDIQR	PLSL_HUMAN	☐		0.93							
FSLVGIGGQDLNEG...	PLSL_HUMAN	☐		0.0	0.742	2.513	1.208	0.966	0.971	0.926	0.986
MVMTVFACLMGK	PLSL_HUMAN	☐		0.0	0.834	1.069	1.001	1.117	1.022	1.075	1.165
MVMTVFACLMGK	PLSL_HUMAN	☐		0.0	0.998	1.208	1.044	1.349	1.106	1.027	1.182
QFVTATDVVR	PLSL_HUMAN	☐		0.017	1.384	1.692	1.231	1.717	1.765	1.502	1.664
AACLPLPGYR	PLSL_HUMAN	☐		0.031							

Suppl. Figure 10: “Quantitation Panel”. This panel also shows the information about the samples and assays used for quantification purposes (for example, reagents, tissues, and description).

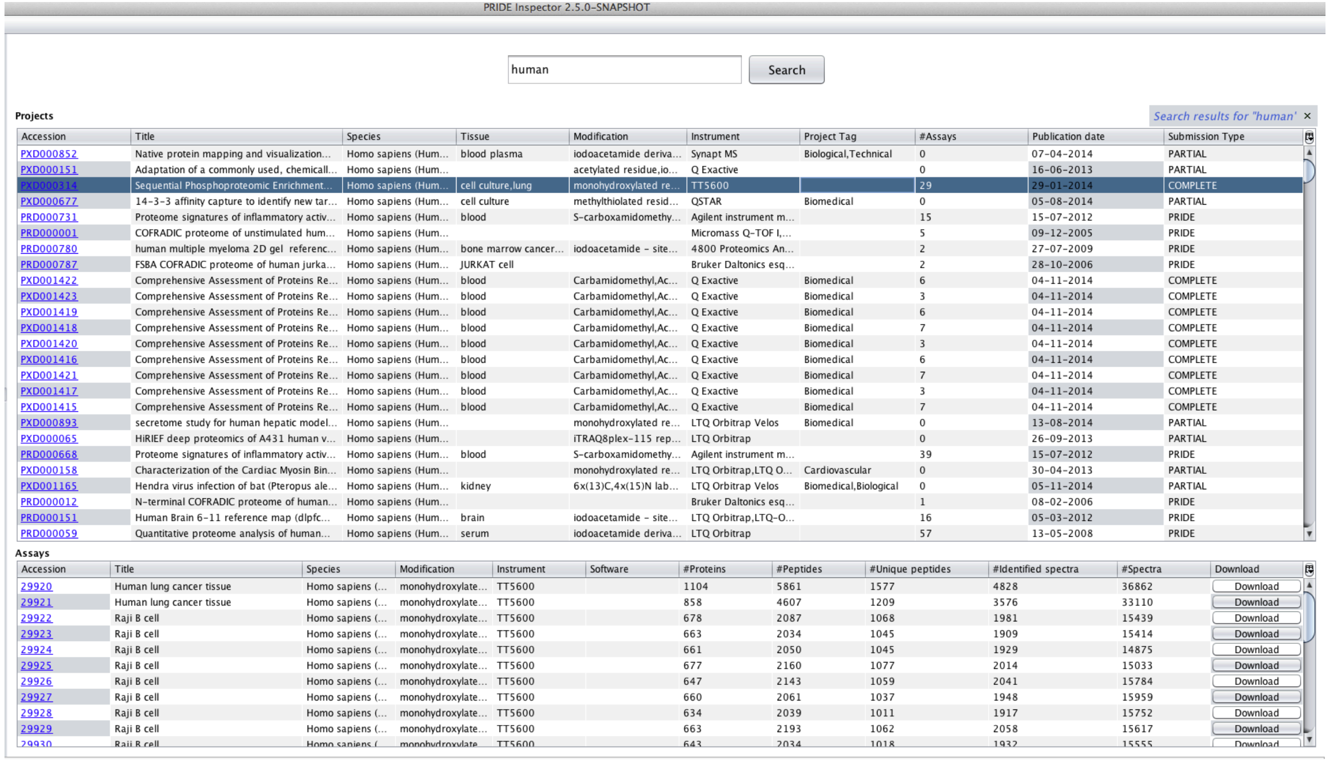


Protein Group ID	Protein	#PSMs	#Distinct Peptides	#PTMs
PAG_1386	P25786	2	1	0
PAG_1385	P61513	4	2	0
PAG_1388	Q9UI30	1	1	0
PAG_1387	Q9BUJ2	1	1	0
PAG_1389	Q7Z739	1	1	0
PAG_800	O43719	1	1	1
PAG_1380	P36969_REVERSED	1	1	1
PAG_1382	Q8TAQ2	2	2	2

PSM List [P25786] **Modified residues**: NONE

Peptide	Ranking	Delta...	Charge	Precurso...	Modifica...	OMSSA:e...	PeptideShaker: PSM C...	X!Tandem:...	Length	Start	Stop
NQYDNDVTVWSPQGR	1	0.0002	2	889.9087		0.0	100.0	0.0	15	4	18
NQYDNDVTVWSPQGR	1	0.0022	2	889.9106		0.0	100.0	0.0	15	4	18

Suppl. Figure 11: PRIDE Inspector tool Export Options. The following export options are available: mass spectra can be exported in Mascot Generic File (mgf) format and as a mass spectrum table. Additionally, the peptide and protein identifications can be exported as 'Protein-Peptide Mappings', and as detailed protein or peptide tables in a tab-delimited format, or in mzTab format.



Projects

Accession	Title	Species	Tissue	Modification	Instrument	Project Tag	#Assays	Publication date	Submission Type
PXD000852	Native protein mapping and visualization...	Homo sapiens (Hum...	blood plasma	iodoacetamide deriva...	Synapt MS	Biological,Technical	0	07-04-2014	PARTIAL
PXD000151	Adaptation of a commonly used, chemicall...	Homo sapiens (Hum...		acetylated residue,io...	Q Exactive		0	16-06-2013	PARTIAL
PXD000314	Sequential Phosphoproteomic Enrichment...	Homo sapiens (Hum...	cell culture,lung	monohydroxylated re...	TT5600		29	29-01-2014	COMPLETE
PXD000677	14-3-3 affinity capture to identify new tar...	Homo sapiens (Hum...	cell culture	methylthiolated resid...	QSTAR	Biomedical	0	05-08-2014	PARTIAL
PRD000731	Proteome signatures of inflammatory activ...	Homo sapiens (Hum...	blood	S-carboxamidomethy...	Agilent instrument m...		15	15-07-2012	PRIDE
PRD000001	COFRADIC proteome of unstimulated hum...	Homo sapiens (Hum...			Micromass Q-TOF I,...		5	09-12-2005	PRIDE
PRD000780	human multiple myeloma 2D gel referenc...	Homo sapiens (Hum...	bone marrow cancer...	iodoacetamide – site...	4800 Proteomics An...		2	27-07-2009	PRIDE
PRD000787	FSBA COFRADIC proteome of human jurka...	Homo sapiens (Hum...	JURKAT cell		Bruker Daltonics esq...		2	28-10-2006	PRIDE
PXD001422	Comprehensive Assessment of Proteins Re...	Homo sapiens (Hum...	blood	Carbamidomethyl,Ac...	Q Exactive	Biomedical	6	04-11-2014	COMPLETE
PXD001423	Comprehensive Assessment of Proteins Re...	Homo sapiens (Hum...	blood	Carbamidomethyl,Ac...	Q Exactive	Biomedical	3	04-11-2014	COMPLETE
PXD001419	Comprehensive Assessment of Proteins Re...	Homo sapiens (Hum...	blood	Carbamidomethyl,Ac...	Q Exactive	Biomedical	6	04-11-2014	COMPLETE
PXD001418	Comprehensive Assessment of Proteins Re...	Homo sapiens (Hum...	blood	Carbamidomethyl,Ac...	Q Exactive	Biomedical	7	04-11-2014	COMPLETE
PXD001420	Comprehensive Assessment of Proteins Re...	Homo sapiens (Hum...	blood	Carbamidomethyl,Ac...	Q Exactive	Biomedical	3	04-11-2014	COMPLETE
PXD001416	Comprehensive Assessment of Proteins Re...	Homo sapiens (Hum...	blood	Carbamidomethyl,Ac...	Q Exactive	Biomedical	6	04-11-2014	COMPLETE
PXD001421	Comprehensive Assessment of Proteins Re...	Homo sapiens (Hum...	blood	Carbamidomethyl,Ac...	Q Exactive	Biomedical	7	04-11-2014	COMPLETE
PXD001417	Comprehensive Assessment of Proteins Re...	Homo sapiens (Hum...	blood	Carbamidomethyl,Ac...	Q Exactive	Biomedical	3	04-11-2014	COMPLETE
PXD001415	Comprehensive Assessment of Proteins Re...	Homo sapiens (Hum...	blood	Carbamidomethyl,Ac...	Q Exactive	Biomedical	7	04-11-2014	COMPLETE
PXD000893	secretome study for human hepatic model...	Homo sapiens (Hum...		monohydroxylated re...	LTQ Orbitrap Velos	Biomedical	0	13-08-2014	PARTIAL
PXD000065	HiRIEF deep proteomics of A431 human v...	Homo sapiens (Hum...		iTRAQ8plex-115 rep...	LTQ Orbitrap		0	26-09-2013	PARTIAL
PRD000668	Proteome signatures of inflammatory activ...	Homo sapiens (Hum...	blood	S-carboxamidomethy...	Agilent instrument m...		39	15-07-2012	PRIDE
PXD000158	Characterization of the Cardiac Myosin Bin...	Homo sapiens (Hum...		monohydroxylated re...	LTQ Orbitrap,LTQ O...	Cardiovascular	0	30-04-2013	PARTIAL
PXD001165	Hendra virus infection of bat (Pteropus ale...	Homo sapiens (Hum...	kidney	6x(13)C,4x(15)N lab...	LTQ Orbitrap Velos	Biomedical,Biological	0	05-11-2014	PARTIAL
PRD000012	N-terminal COFRADIC proteome of human...	Homo sapiens (Hum...			Bruker Daltonics esq...		1	08-02-2006	PRIDE
PRD000151	Human Brain 6-11 reference map (dlpfc...	Homo sapiens (Hum...	brain	iodoacetamide – site...	LTQ Orbitrap,LTQ-O...		16	05-03-2012	PRIDE
PRD000059	Quantitative proteome analysis of human...	Homo sapiens (Hum...	serum	iodoacetamide deriva...	LTQ Orbitrap		57	13-05-2008	PRIDE

Assays

Accession	Title	Species	Modification	Instrument	Software	#Proteins	#Peptides	#Unique peptides	#Identified spectra	#Spectra	Download
29920	Human lung cancer tissue	Homo sapiens (...	monohydroxylate...	TT5600		1104	5861	1577	4828	36862	Download
29921	Human lung cancer tissue	Homo sapiens (...	monohydroxylate...	TT5600		858	4607	1209	3576	33110	Download
29922	Raji B cell	Homo sapiens (...	monohydroxylate...	TT5600		678	2087	1068	1981	15439	Download
29923	Raji B cell	Homo sapiens (...	monohydroxylate...	TT5600		663	2034	1045	1909	15414	Download
29924	Raji B cell	Homo sapiens (...	monohydroxylate...	TT5600		661	2050	1045	1929	14875	Download
29925	Raji B cell	Homo sapiens (...	monohydroxylate...	TT5600		677	2160	1077	2014	15033	Download
29926	Raji B cell	Homo sapiens (...	monohydroxylate...	TT5600		647	2143	1059	2041	15784	Download
29927	Raji B cell	Homo sapiens (...	monohydroxylate...	TT5600		660	2061	1037	1948	15959	Download
29928	Raji B cell	Homo sapiens (...	monohydroxylate...	TT5600		634	2039	1011	1917	15752	Download
29929	Raji B cell	Homo sapiens (...	monohydroxylate...	TT5600		663	2193	1062	2058	15617	Download
29930	Raji B cell	Homo sapiens (...	monohydroxylate...	TT5600		643	2034	1018	1932	15555	Download

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