A guide to ProteomeDiscoverer (1.4)/Mascot (2.4) based LC-MS/MS data analysis (Excel format).

This report format presents qualitative and quantitative details of matched proteins and peptides

Annotation callouts:
- Master protein acc. # (UniProt).
- Master protein description.
- Total % protein sequence coverage.
- # of proteins in a group.
- Total # of peptides unique to the protein group.
- Total # of peptides.
- Total # of Peptide Spectrum Matches.
- *Optional* protein annotations.
- Average area of the 3 most intense peptides for a protein group per sample.
- Mascot protein score for sample **A**. Higher score => higher confidence in match.
- % protein sequence coverage for sample **A**.
- # of peptides matched to the protein in sample **A**.
- Total # of Peptide Spectrum Matches in Sample **A**.
- # of amino acids.
- Master protein MW.
- pI
- Specific to Sample A
- Specific to Sample B.
- Potential contaminating proteins are marked CON_
- Singly charged mass of peptide.
- Posterior Error Probability (PEP) is the probability that the observed PSM is incorrect. Lower is better.
- Sample B: False Discovery Rate group: **High: <1%** or better, **Medium: 1-5%**, **Low: >5%**.
- Mascot peptide score for best scored PSM for the particular peptide. Higher score, higher confidence.
- Click + to see peptide details.
- # of proteins that the peptide matches.
- Modification(s) included in search and matched to peptide.
- Area of peptide in Sample A
- Area of peptide in Sample B
- # of missed cleavages. in the peptide.

	Accession	Description	ΣCoverage	Σ# Proteins	Σ# Unique Peptides	Σ# Peptides	Σ# PSMs	Molecular Function	Cellular Component	Biological Process	Pfam IDs	Gene IDs	A 5: Area	B 5: Area	Score A 15	Coverage A 15	# Peptides A 15	# PSM A 15	Score B 15	Coverage B 15	# Peptides B 15	# PSM B 15	# AAs	MW [kDa]	calc. pI
2	A2AMW0	Capping protein (Actin filament) muscl	52.69	7	11	11	15	protein binding	on; membrane	ogical process	Pf01115	12345	7.6E+07	1.4E+08	95.6	15.8	4	4	217.2	49.6	10	11	260	29.3	6.9
15	A2A547	Ribosomal protein L19 OS=Mus muscu	25.77	3	6	6	11	; RNA binding	ne; membrane	bolic process	Pf01280	19921	1.4E+08	2.0E+08	150.8	21.1	5	5	87.5	22.7	4	6	194	23.2	11.5
23	Q80SW1	Putative adenosylhomocysteinase 2	20.94	8	5	10	13	protein binding	ol; membrane	se to stimulus	Pf006		1.0E+08	1.7E+08	124.2	9.8	5	6	141.7	12.6	6	7	530	58.9	6.9
35	Q78ZM0	Sorting nexin 3 OS=Mus musculus GN=	57.41	4	7	9	19	protein binding	ol; membrane	ogical process	Pf007			1E+08	197.0	57.4	9	11	105.2	51.9	8	8	162	18.8	8.7
46	Q61411	GT	3.49	5	2	9	15	porter activity	mbrane; Golgi	nd biogenesis	Pf0000			2.1E+08	83.1	40.2	5	6	203.6	56.6	8	9	189	21.3	5.3
57	Q9D6F9	Tu	5.18	1	3	21	60	olecule activity	on; membrane	nd biogenesis	Pf00091;	22153	8.1E+08	1.9E+09	507.5	44.8	18	28	750.8	45.1	16	32	444	49.6	4.9
86	P99024	Tu	2.16	2	5	26	79	protein binding	on; membrane	nd biogenesis	Pf00091;	22154	1.5E+09	1.7E+09	787.3	51.8	23	41	872.5	55.4	19	38	444	49.6	4.9
124	Q62159	Rho-rel GTP-binding protein RhoC	46.11	2	2	9	15	protein binding	ol; memb		Pf0000			7.1E+08	56.5	18.7	3	3	186.6	37.3	7	12	93	22.0	6.6
135	CON_0000	SWISS-PROT:P13647 Tax_Id=9606 G	18.98	25	6	15	22							2.0E+07	358.2	19.0	15	20	68.2	3.4	2	2	5	62.3	7.7
152	CON_0070	(Bos taurus) Gene_Symbol=YWHAQ 1	57.96		2	1	12	21						8.1E+08	272.3	38.0	8	11	244.9	45.3	9	10		
167	Q6ZWV3	60S ribosomal protein L10 OS=Mus mu	56.54	4	14	14	23	; RNA binding	ne; memb				8.3E+08	119.0	23.4	5	6	217.6	55.6	13	17		
183	Q6ZWN5	40S ribosomal protein S9 OS=Mus mu	46.39	6	17	17	24	ulator activity	ne; memb				3.6E+08	98.3	38.7	11	11	158.8	37.1	12	13		
202	P51150	Ras-related protein Rab-7a OS=Mus	80.68	1	19			protein binding	gi; membrane	nd biogenesis	Pf0025;		1.9E+09	7.6E+08	397.4	62.8				13	16	207	23.5	6.7
	O01853	Transitional endoplasmic reticulum ATP	30.65	7	17			activity	rane; cytosol	nd biogenesis	Pf0004;							17	18	806	89.3	5.3
		slation initiation factor	24.49	1	10			ein binding	m; membrane	ogical process	Pf01399;							7	8	445	52.2	6.0
		mic 1 OS=		14					bran		0022						24	60	375	41.7	5.5
		ation fact		5					ran		0270;						19	21	406	46.1	5.5
319	P61021	Ras-related protein Rab		3							0009;					6	117.5	21.9	4	5	215	23.7	8.1
328	P61027	Ras-related protein Rab-10 OS=Mus	27.50	19			12	protein binding	ne; Golgi	tion	Pf0025;		2.2E+08	2.9E+08		24.0	5	7	70.7	18.0			8.4

	Sequence	# PSMs	# Proteins	# Protein Groups	Protein Group Accessions	Modifications	MH+ [Da]	A5: Area	B5: Area	q-Value	PEP	A15	IonScore A 15	Exp Value A15	B15	IonScore B 15	Exp Value B15	# Missed Cleavages
330	LLLIGDSGVGK	2	12	7	P61027;P628		1071.64092	1.1E+08	7.0E+08	0	0.0009095	High	28	0	High	32	0.02542	0
331	LQIWDTAGQER	4	43	12	P61027;Q91V		1316.65898	6.3E+07	4.3E+07	0	0.0001339	High	51	0	High	49	0.00068	0
332	NIDEHANEDVER	2	1	1	P61027		1440.63506	3.0E+08	0.0E+00	0	1.042E-08	High	57	0				0
333	FFETSAK	2	3	2	P61027;Q9DD		829.40978	2.0E+08	1.5E+08	0.002	0.02878	High	20	0	High	29	0.03185	0
334	TYDLLFK	1	1	1	P61027		899.48754	0.0E+00	2.2E+07	0.002	0.01741				High	17	0.68086	0
335	ANINIEK	1	1	1	P61027		801.44548	1.6E+08	0.0E+00	0.004	0.04421	High	37	0				0
336	Q91V41 Ras-related protein Rab-14 OS=Mus	67.91	18	14	15	32	talytic activity Golgi; cytosol nd biogenesis Pf0009;	68365	4.5E+08	2.0E+08	####	55.81		13	19	226.62	50.70	9 13 215 23.9 6.2

Good to know ● Unique (**Σ# Unique Peptides**) and all peptides (**Σ# Peptides**) together with sequence coverage (**Σ Coverage**) are used to understand sequence representation of the particular protein. ● Peptide Spectrum Matches (**Σ# PSMs**) indicates how many MS/MS spectra that were matched to a particular protein or peptides. PSMs can be used as a quantitative metric. When comparing same protein, higher number is an indication of higher abundance. The robustness of this metric increases with greater numbers. ● **Area**s assigned to proteins is calculated as the average-area-of-the-3-most-intense-peptides-signal. Uniqueness or not of a peptide is not taken into account. The ability to gauge changes increases with increased with fold difference and signal. A peptide or protein assigned an 'area' of 0 was either not matched or could not be quantified. ● A peptide match False Discovery Rate (FDR) is calculated per searched data set. Peptides can be assigned as **High** (FDR < 1%), **Medium** (FDR: 1%-5%) or **Low** (FDR >5%) confidence based on statistical calculations.