

Publishing Proteomics Data: How to Win Reviewers and Influence Editors

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at San Antonio**

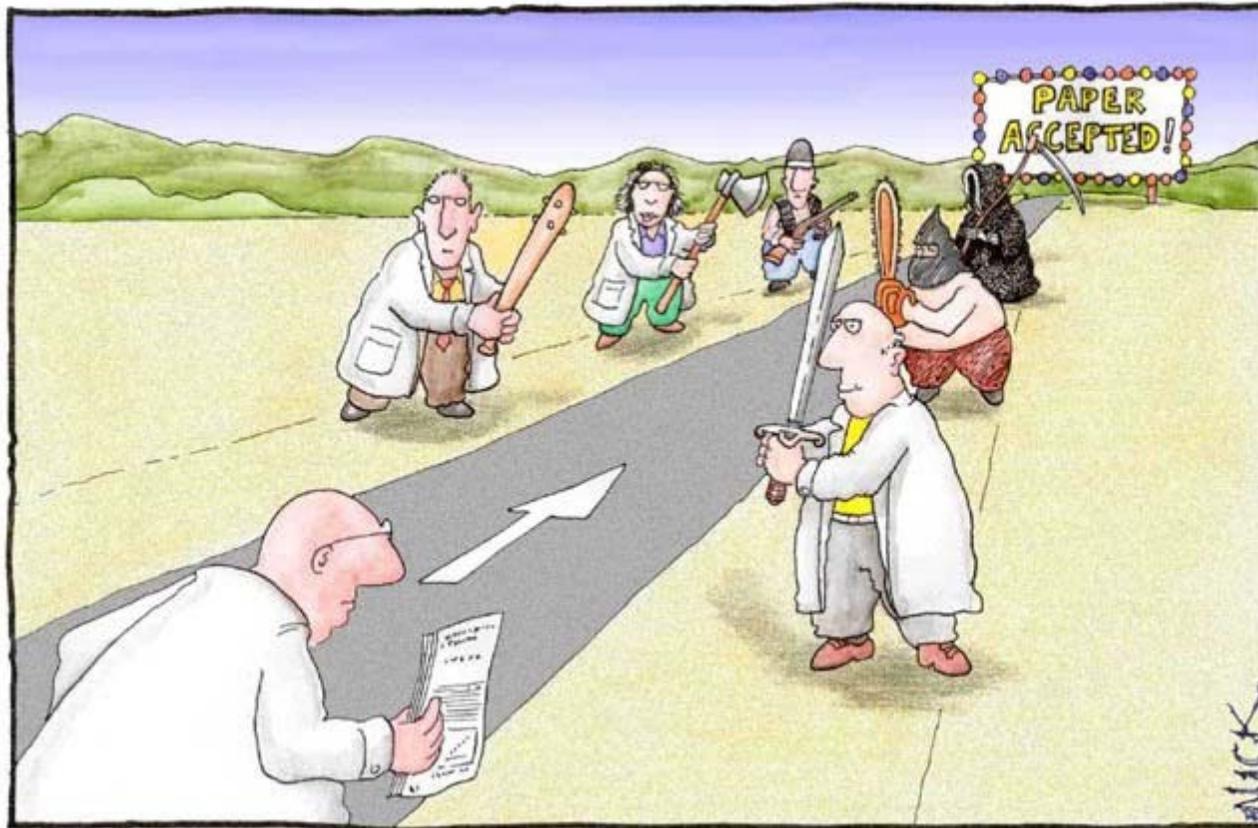


St. Louis - ASMS 2015



San Antonio - ASMS 2016

Why do we publish?



<https://computervisionblog.files.wordpress.com/2012/02/publication.jpg>

Dissemination

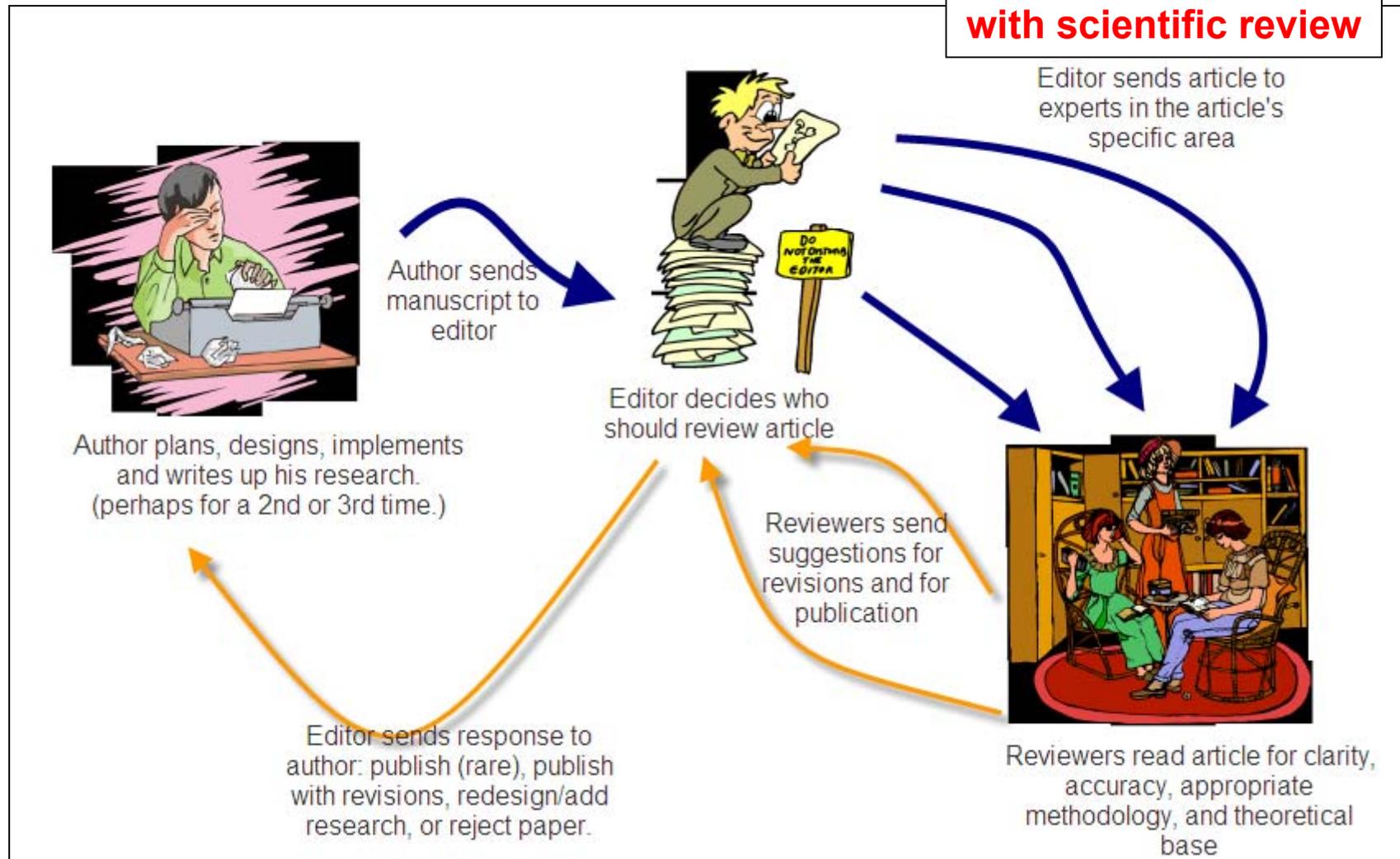
Education

Promotion/tenure/funding

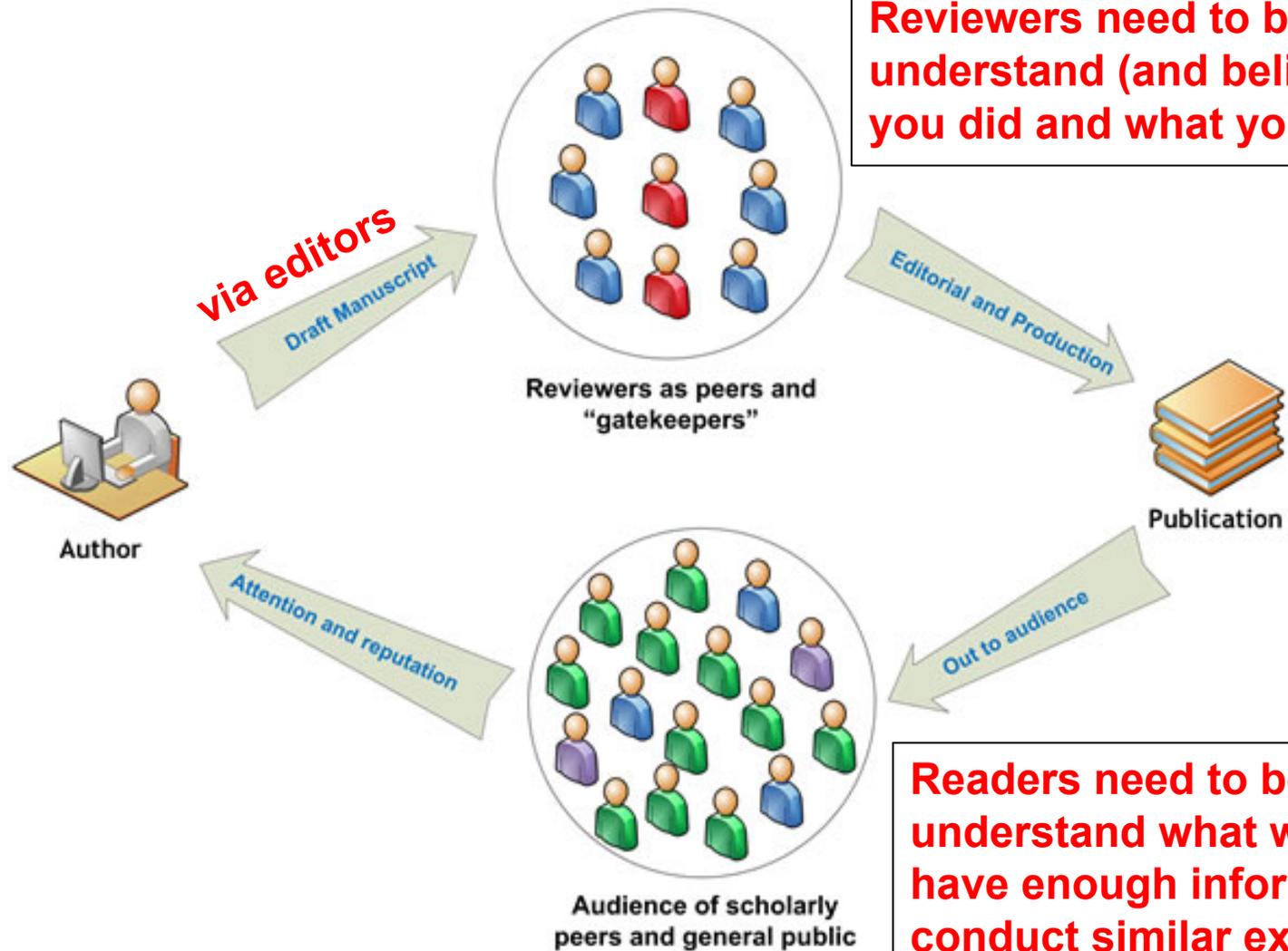
Masochism?

Who do we need to satisfy?

**“Technology” check
may be conducted
before or in parallel
with scientific review**



Peer Review Process



Reviewers need to be able understand (and believe) what you did and what you found.

Readers need to be able to understand what was done, have enough information to conduct similar experiments and mine the data.

Elements of a manuscript

For submission, be prepared

Provide a list of "pre-

Pick people who are
the area of t

Don't count
on you. The
less than s

Don't pick t
They most
review and
process.

Provide a list of people
will be biased against

Abstract

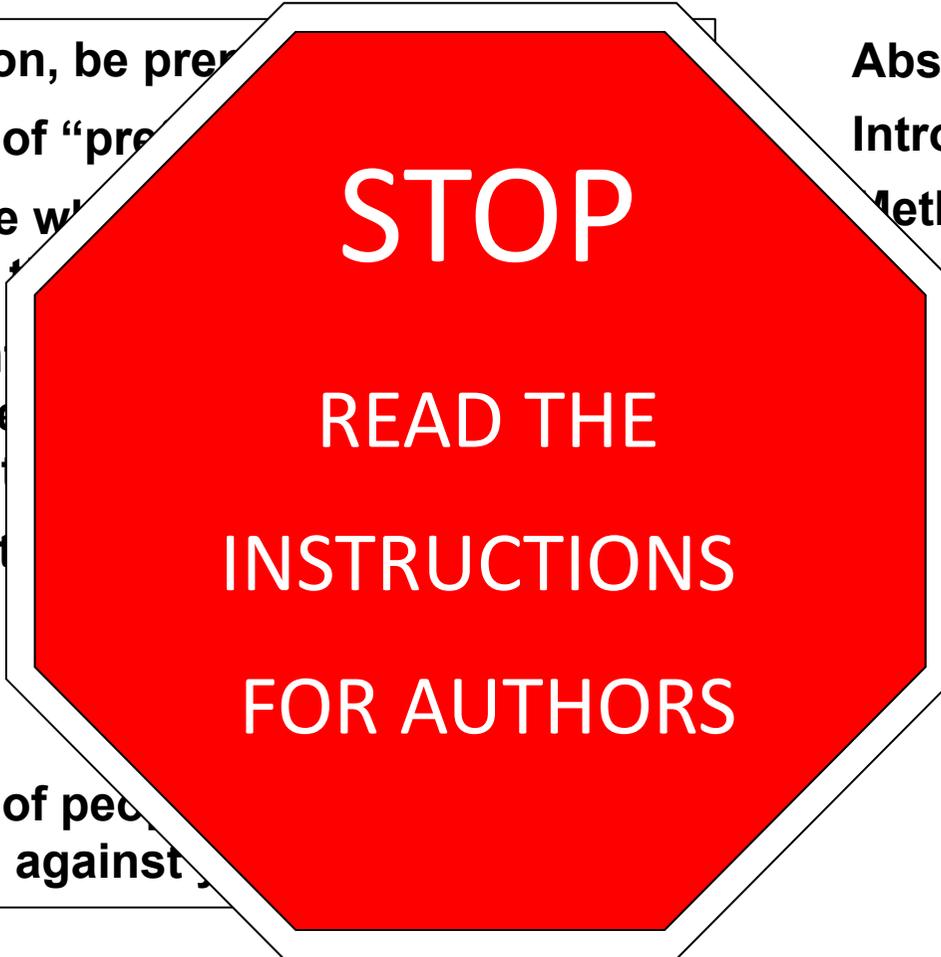
Introduction

Methods

Results and Discussion

Conclusions

Supporting information



Elements of a manuscript

For submission, be prepared to:

Provide a list of “preferred reviewers.”

Pick people who are knowledgeable in the area of the study.

Don’t count on your friends being easy on you. They don’t want you to publish a less than stellar paper.

Don’t pick the “top names” in the field. They most likely won’t have time for the review and it will delay the evaluation process.

Provide a list of people who you truly feel will be biased against your work.

Abstract

Introduction

Methods

Results and Discussion

Conclusions

Supporting information

Elements of a manuscript

Succintly describe your project and results.

This may be all that the editor reads before inviting reviewers.



Abstract

Introduction

Methods

Results and Discussion

Conclusions

Supporting information

Elements of a manuscript

Here's your chance to make the case for your study. Keep on topic. This isn't a review article.



Abstract

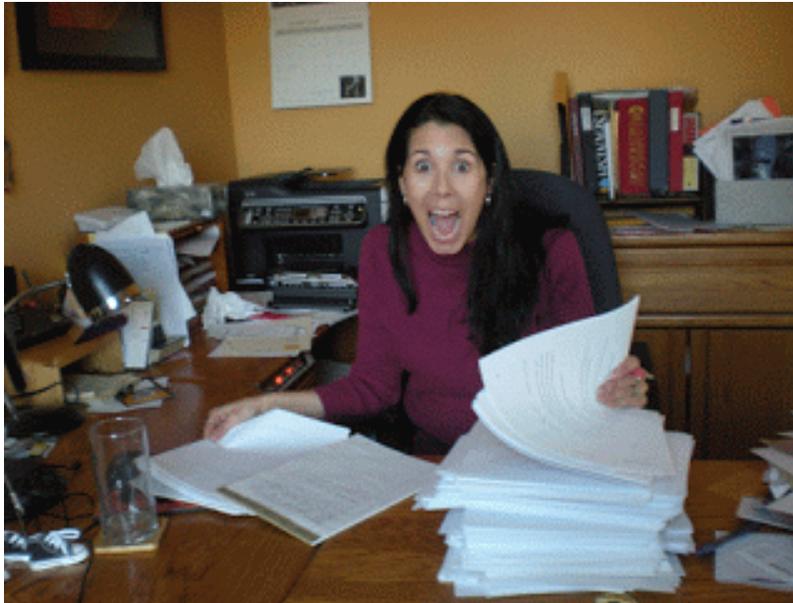
Introduction

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Supporting information



http://1.bp.blogspot.com/_9cOxMQ3Smgw/S53ZEN8FdPI/AAAAAAAAAXk/O16IPL1EM8/s320/DV-revision.gif

Elements of a manuscript

Now the details . . .
How much is enough?



Abstract

Introduction

Methods

Results and Discussion

Conclusions

Supporting information

Methods section

Protein analysis by mass spectrometry ... were separated by 1-D SDS-PAGE and the gel lanes were divided into fractions and then digested with trypsin. The digests were analyzed by HPLC-tandem mass spectrometry followed by data processing as previously described (21).

NOT ENOUGH

Methods section

Rodriguez KA, Osmulski PA, Pierce A, Weintraub ST, Gaczynska M, Buffenstein R. A cytosolic protein factor from the naked mole-rat activates proteasomes of other species and protects these from inhibition. *Biochim Biophys Acta*. 2014 Nov;1842(11):2060-72. doi: 10.1016/j.bbadis.2014.07.005

	NMR	MS	NMR	MS	
Cytosolic/Adh (VS)	125.0 ± 5.6*	5.56 ± 1.57*	80.6 ± 2.5*	16.2 ± 1.9*	analyzed by capillary HPLC electrospray ionization tandem mass spectrometry (HPLC-ESI-MS/MS) on a Thermo Fisher Orbitrap Velos mass spectrometer. The MS data were searched against the rodent subset of the NCBI nr protein database (NCBI nr_20130102; 316,972 sequences)
Cytosolic/MG132	122.0 ± 5.5*	8.22 ± 2.75*	71.4 ± 8.7*	14.6 ± 4.4*	
Cytosolic/LC					
Cytosolic/BZ					
Microsomal					
Nuclear/MG					

2.11. Protein identification by mass spectrometry

Proteins were separated by 1-D SDS-PAGE. Proteins in each gel lane were digested *in situ* with trypsin. The digests were analyzed by capillary HPLC electrospray ionization tandem mass spectrometry (HPLC-ESI-MS/MS) on a Thermo Fisher Orbitrap Velos mass spectrometer. The MS data were searched against the rodent subset of the NCBI nr protein database (NCBI nr_20130102; 316,972 sequences) by Mascot (Matrix Science). The Mascot results were subjected to a subset search in tandem followed by determination of probability assessment of the peptide assignments and protein identifications by Scaffold (Proteome Software).

THE BARE MINIMUM!

- = no data;
(methyl)-sulf
LC = lactacystin
* p > 0.05.

com/support
1 µg of anti-
or naked mole-rat
After an
protein A/G
beads were

Methods section - samples

Easy to provide

Source

Animals

Species

Strain/genetic background

Cells

Cell line name
designation

Source

Genetic alteration(s)

Labeling strategy (SILAC, iTRAQ/TMT, SILAM)

Number of biological and/or technical replicates

Methods section - sample preparation

Easy to provide

Protein isolation

Proteolytic digestion (if used)

Internal standards added (if used)

Chemical modification (if used), including labeling scheme

Off-line chromatography/cleanup

PTM-specific enrichment/isolation

Methods section - MS analysis

Easy to provide

HPLC

Instrument vendor/model

Column, mobile phases, flow rate, gradient, auxiliary detection details

Strategy for sample injection order

Mass spectrometry

Instrument vendor/model

Instrument parameters/scan strategy

HPLC-ESI-tandem-MS

Data-dependent analysis: MS1 mass resolution, MS1 scan range, charge-state screening parameters, mass window for precursor ion isolation, fragmentation mode, relative collision energy (or other parameter, as appropriate), mass analyzer for tandem-MS, MS2 mass resolution (where appropriate), number of product ion spectra per scan cycle, dynamic exclusion

Data-independent analysis: MS1 mass resolution, MS1 scan range(s), relative collision energy, mass analyzer for tandem-MS, MS2 mass resolution (where appropriate)

Methods section - data processing

Easy to provide

Software/method for peak list generation

Database searching

Software name(s), vendor(s) or literature citation, version

Databases

Name/source

Date/version

Taxonomy

Number of sequences

Search parameters

Precursor and product ion mass tolerances

Enzyme specificity

Charge states considered

Fixed and variable modifications

Other settings (e.g., ¹³C number in Mascot)

Quantitation method (where applicable)

Decoy search option

Do not say “using the default parameters”

Methods section - data processing

Getting harder

Criteria for acceptance of peptide assignments and protein identifications

Mascot ions scores/expect values

SEQUEST X_{corr} cutoffs

X! Tandem scores

Post-processing with additional software

PeptideProphet/ProteinProphet

Scaffold

Proteome Discoverer

In-house software (need to document)

False discovery rate (FDR) determination

Decoy database details

Method for FDR calculation

De novo sequencing

Approach (e.g., manual or computational)

Validation

Methods section - quantitative analysis

Getting even harder

Software name, vendor or literature citation, version

Quantitation parameters

Normalization

Methods section - quantitative analysis

Getting even harder

Considerations for acceptance of peptide values

SILAC/metabolic labeling

Variability of ratios across an EIC

Fraction of the EIC window

Agreement with predicted isotope pattern

Reporter ion-based methods

Variability assessment for reporter ion ratios of within-sample replicates

Spectral counting

Minimum number of assigned peptides/spectra

Spectrum designation

Total spectra, unique spectra, unique sequence

Intensity-based methods

Method for peak integration/intensity determination

Variability assessment for peptides assigned to a protein

Methods section - quantitative analysis

Getting even harder

Considerations for acceptance of peptide values

SILAC/metabolic labeling

Variability of ratios across an EIC

Fraction of the EIC window

Agreement with predicted isotope pattern

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Minimum number of assigned peptides/spectra

Spectrum designation

Total spectra, unique spectra, unique sequence

Intensity-based methods

Method for peak integration/intensity determination

Variability assessment for peptides assigned to a protein

Variability assessment of peptides assigned to a protein

Relative quantities of selected tRNA synthetases in *C. albicans* grown at different temperatures

tRNA synthetase	Accession	30 min			60 min			180 min		
		L/H	SD(geo)	#	L/H	SD(geo)	#	L/H	SD(geo)	#
Val	orf19.1295	3.13	2.60	89	26.93	4.81	62	7.92	1.19	47
Ile	orf19.2138	4.13	3.77	33	28.75	3.92	16	7.07	1.35	22
Leu	orf19.2560	5.09	2.08	5	22.93	1.83	3	18.73	2.12	5
Ala	orf19.5746	5.94	1.09	6	15.36	13.60	3	5.76	1.11	4
Asn	orf19.6702	7.18	1.76	24	29.64	1.81	4	8.33	1.23	7
Gln	orf19.7064	5.55	1.51	11	4.95	31.09	17	5.91	17.21	16

Values were obtained from Mascot Distiller processing of the MS data and search results as multi-file projects for each time-point. H/L, median ratio of peak areas of extracted ion chromatograms for peptides assigned above the homology threshold; SD(geo), geometric standard deviation of the assigned peptides; #, number of peptides used for relative quantification.

Methods section - statistics

May be really difficult

Software/program

Test(s) applied

Significance levels



“I can prove it or disprove it! What do you want me to do?”

Elements of a manuscript

What did you find?

How much documentation do you need to present - and where?

Abstract

Introduction

Methods

Results and Discussion

Conclusions

Supporting information

Provide a clear, succinct report of your results and insightful interpretations.

Highlight key findings. Do not cover every detail presented in the results tables and figures.

Focus on truly meaningful observations. Do you really need to discuss the biological significance of every protein you identified?

Results - tables of proteins

Table 3

Mass spectrometry of fractions 22 and 23 revealed the presence of several molecular chaperones. For a complete list please see Table S1.

Identified proteins (8/223)	Accession number	MW	fr.22	fr.23
Inducible heat shock protein 70 (HSP72) [<i>Heterocephalus glaber</i>]	gi 13242237 (+26)	71 kDa	28	27
Ubiquitin-like modifier-activating enzyme 1 [<i>Heterocephalus glaber</i>]	gi 351699501	119 kDa	20	12
78 kDa glucose-regulated protein [<i>Heterocephalus glaber</i>]	gi 351702099	72 kDa	10	5
Inducible heat shock protein 70 [<i>Mus musculus</i>]	gi 118490060 (+7)	70 kDa	8	6
Hsp90aa1 protein [<i>Mus musculus</i>]	gi 118142832 (+23)	66 kDa	8	7
Heat shock protein 90 beta [<i>Equus caballus</i>]	gi 12082134 (+17)	82 kDa	7	8
Protein disulfide-isomerase [<i>Heterocephalus glaber</i>]	gi 351706419	57 kDa	7	5
Stress-70 protein, mitochondrial [<i>Mus musculus</i>]	gi 162461907 (+9)	73 kDa	7	6

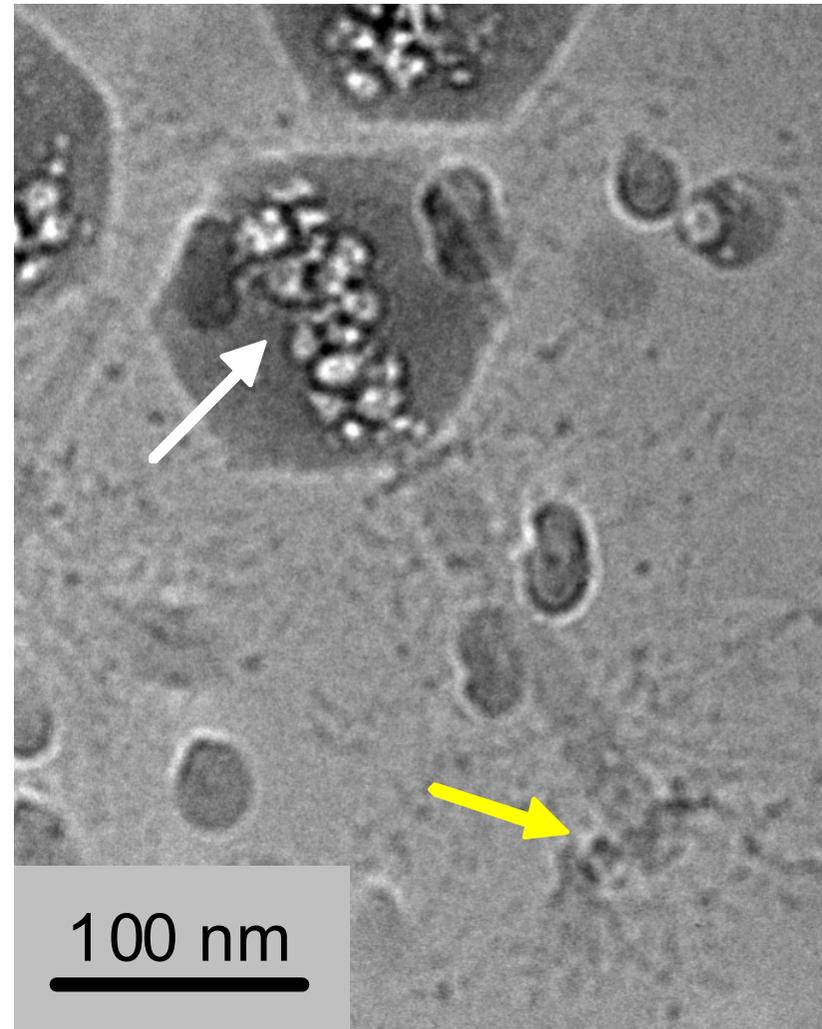
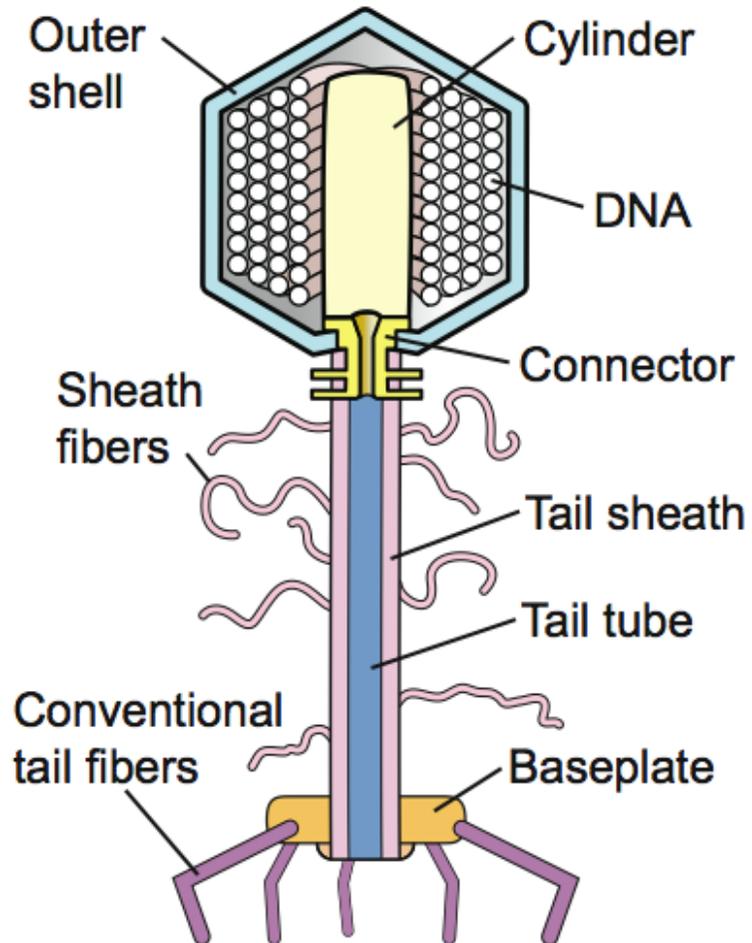
Spectral counts (quantitative value) determined by Scaffold (v3) are shown in the table under the columns labeled fr.22 and fr.23.

Will readers know what this is?

What were the criteria for acceptance of peptide assignments and protein identifications?

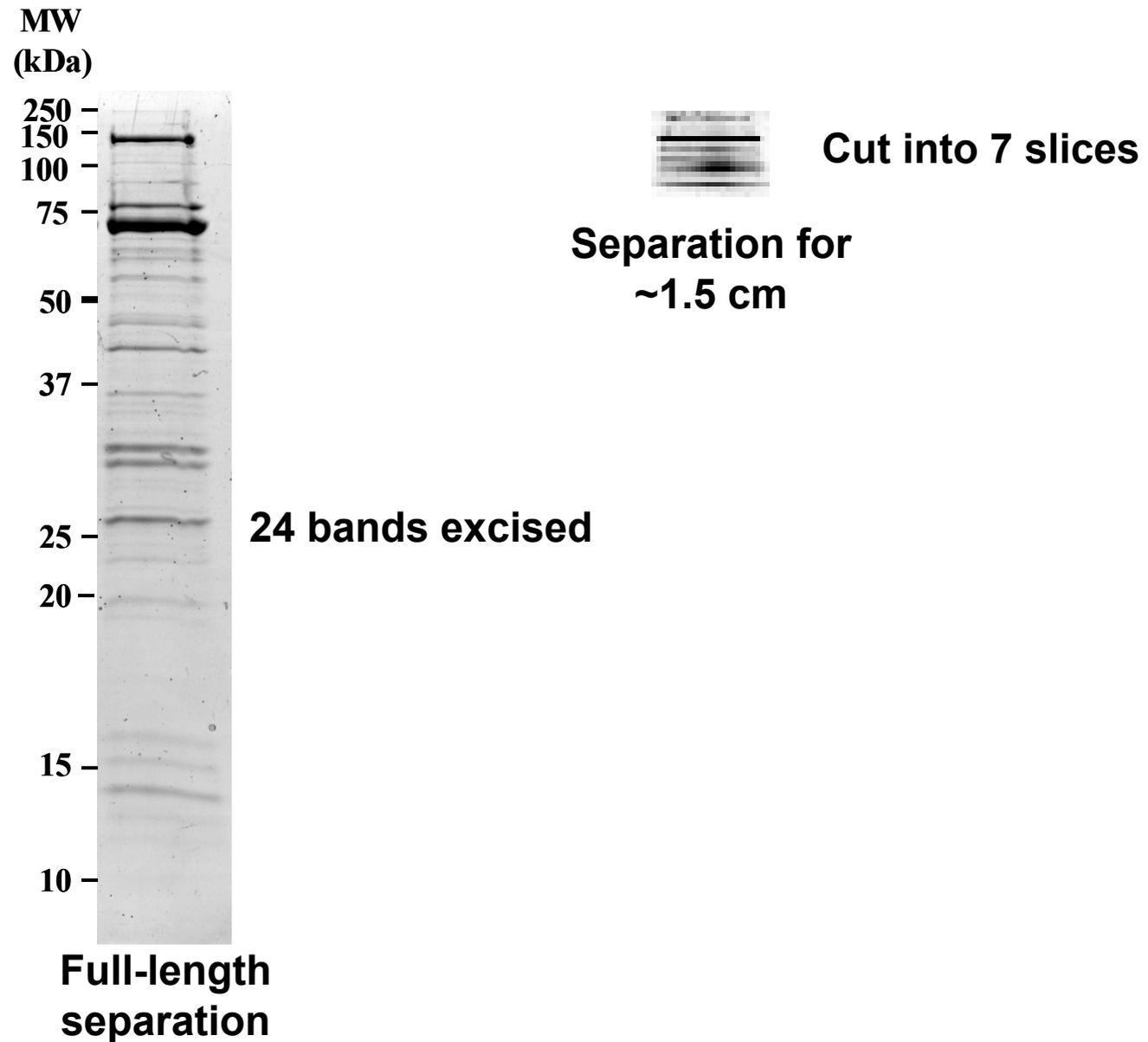
Was an FDR assessed? How was it used?

Bacteriophage 201 ϕ 2-1 structure and morphology

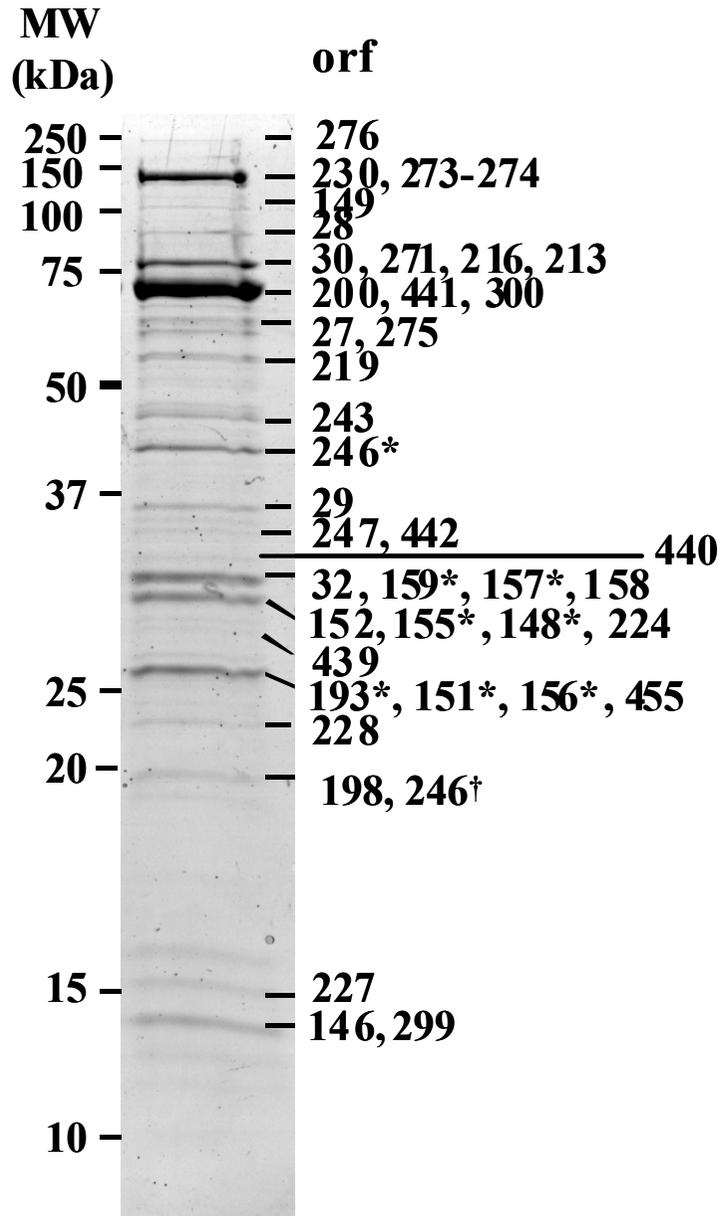


Cryoelectron micrograph

1-D SDS PAGE of phage 201 ϕ 2-1 structural proteins



1-D SDS PAGE of phage 201 ϕ 2-1 structural proteins



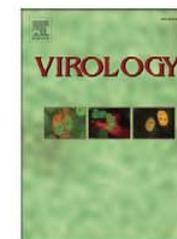
76 proteins identified
≥2 peptides/protein
Scaffold post-processing
95% confidence (peptides)
≥99.9% probability (protein)



Contents lists available at [ScienceDirect](http://www.sciencedirect.com)

Virology

journal homepage: www.elsevier.com/locate/yviro



Characterization of *Pseudomonas chlororaphis* myovirus 201 ϕ 2-1 via genomic sequencing, mass spectrometry, and electron microscopy

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^b Department of Chemistry and Biochemistry, Brigham Young University, Provo, Utah 84602, USA

ARTICLE INFO

Article history:

Received 13 December 2007

Returned to author for revision

28 January 2008

ABSTRACT

Pseudomonas chlororaphis phage 201 ϕ 2-1 is a relative of *Pseudomonas aeruginosa* myovirus ϕ KZ. Phage 201 ϕ 2-1 was examined by complete genomic sequencing (316,674 bp), by a comprehensive mass spectrometry survey of its virion proteins and by electron microscopy. Seventy-six proteins, of which at least 69

Table 1
MS data and homologues for the 201 ϕ 2-1 proteins identified by HPLC-ESI-MS/MS

gp	M _r (kDa)	Identification by MS ¹				Function, homologues, paralogues ²
		Unique peptides	Total spectra	Spectra/Mw	% coverage	
<i>A. Proteins of established virion function according to Fokine et al. (2007)</i>						
30 ³	77.5	22	355	4.6	44	major sheath protein, KZ ⁴ 29 (63% over 693); EL6 (21% over 707)
200 ⁵	82.4	22	696	8.4	38	major capsid protein, KZ120 (64% over 749); EL78 (20% over 325)
276 ⁵	251.8	23	34	0.1	10	cell-puncturing device, KZ181 (33% over 2387); KZ144 (45% over 187); EL183 (22% over 270)
<i>B. RNA polymerase-related virion proteins</i>						
139	49.6	8	34	0.7	24	RNA polymerase, beta' subunit, KZ80 (56% over 449); EL44 (23% over 447)
273/274	173.4	24	87	0.5	19	RNA polymerase, beta subunit, KZ178 (53% over 1548); EL186 (23% over 1142); EL187 (26% over 356)
275	62.7	8	27	0.4	15	RNA polymerase, beta subunit KZ180 (68% over 490); EL184 (32% over 491)

¹ All proteins had a protein identity probability of 100%, as determined by Scaffold (Proteome Software), with the exception of gp164 (99%) and gp229 (96%). Results displayed were obtained from a combined data set of the GeLCMS analysis, with the exception of gp276 which was only detected in analysis of an individual gel band (see text).

² Homologues were determined using Psi-Blast and BlastP (% identities over the homologous region are provided). The best matching ϕ KZ and EL homologue for each 201 ϕ 2-1 protein is listed. Parologue families are as follows: **parologue family a** refers to a domain found in 201 ϕ 2-1 gp216, 217, 218, 219, 220. A homologous domain exists in ϕ KZ gp131, 132, 133, 134 and 135 and EL gp113, 114 and 115; **parologue family b** refers to a domain found in 201 ϕ 2-1 gp155, 156, 157, 246, 247. Homologous domains exist in ϕ KZ gp93, 94, 95, 162 and 163; **parologue family c** refers to a domain found in 201 ϕ 2-1 gps 456 and 452. Homologous domains exist in ϕ KZ gp83 and EL gp155.

³ An N-terminal peptide lacking only the initiator methionine was identified using semi-tryptic analysis.

⁴ KZ refers to ϕ KZ.

⁵ N-terminus is expected to be processed as the ϕ KZ homologue is processed. Although no semi-tryptic fragments were found to define the mature ends, there is also a lack of peptide coverage in the N-terminal region that would be consistent with processing.

⁶ A mature N-terminus containing the initiator methionine was confirmed by semi-tryptic analysis.

⁷ Gel analysis indicated that the protein is processed consistent with a lack of MS sequence coverage in the N-terminal region of these sequences, except for gp246N which lacks MS coverage of the C terminal region. The exact positions of the processed ends are unknown. The normalized spectrum count in parentheses was calculated using the apparent molecular weight of the processed form (Fig. 1).

⁸ Semi-tryptic analysis indicated removal of 63 and 60 N-terminal residues from gp238 and gp271, respectively.

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<i>B. RNA polymerase-related virion proteins</i>						
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²As related to ϕ KZ.

⁵N-terminus is expected to be processed as the ϕ KZ homologue is processed. Although no semi-tryptic fragments were found to define the mature ends, there is also a lack of peptide coverage in the N-terminal region that would be consistent with processing.

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Elements of a manuscript

Abstract

Introduction

Methods

Results and Discussion

Conclusions - not a repeat of the Results →

Conclusions

Supporting information

Elements of a manuscript

Abstract

Introduction

Methods

Results and Discussion

Conclusions

How much documentation do you need to provide? —————> Supporting information

Think about what you're including as supporting data.

Make sure the figures and tables are informative.

Use meaningful titles for the figures and tables.

Don't provide every spreadsheet you or the software generated as a part of the analysis.

Rearrange spreadsheet columns as needed so that the key information is easily found.

Supporting information

What needs to be documented?

There is no consensus about whether all identified proteins need to be listed or only those that exhibited significant differences in quantity among experimental groups or are of special interest to the study.

Identification by HPLC-ESI-tandem-MS

Protein level report - spreadsheet format, PLEASE

Columns

Protein name

Accession number

Molecular weight

Number of assigned spectra (total and unique)

Percent sequence coverage

Probability of protein inference (if determined during post-processing)

Clear/meaningful column heading names

Legend - at the top of long tables or on a separate worksheet

Explanations for abbreviated or non-standard column headings

Significance level cutoff of assigned peptides

Supporting information

MALDI-TOF-MS (peptide mass fingerprint, PMF)

Only suitable for low-complexity samples

Protein level report

Columns

Protein name

Accession number

Molecular weight

Number of spectra searched

Number of spectra assigned

Percent sequence coverage

Probability of protein inference

Clear/meaningful column heading names

Legend - at the top of long tables or on a separate worksheet

Explanations for abbreviated or non-standard column headings

Supporting information

MALDI-TOF/TOF

Protein level report

Columns

Protein name

Accession number

Molecular weight

Number of spectra searched for PMF

Number of spectra assigned for PMF

Number of tandem-mass spectra searched

Number of tandem-mass spectra assigned

Percent sequence coverage

Probability of protein inference

Clear/meaningful column heading names

Legend - at the top of long tables or on a separate worksheet

Explanations for abbreviated or non-standard column headings

Significance level cutoff of assigned peptides

Supporting information

Peptide level (grouped by protein)

For documentation of PTMs, sequence variations

Not usually necessary for manuscripts focusing on identification or relative quantification

Columns

Protein name

Peptide sequence - clearly showing modification(s)

Start/stop residue numbers

Observed *m/z*

Charge state

Mass error

Score/expect value for sequence assignment

Probability for localization of modification site (where appropriate)

Clear/meaningful column heading names

Legend - at the top of long tables or on a separate worksheet

Explanations for abbreviated or non-standard column headings

Significance level cutoff of assigned peptides

Supporting information

Annotated tandem mass spectra

There is no concensus about when annotated tandem mass spectra need to be provided.

Post-translational modifications

Do we need to see all spectra for a large phosphoproteomics study if acceptable parameters have been used for database searching and reasonable cutoffs have been applied to site localization probabilities? Unusual modifications or surprising findings that are the focus of the manuscript should be documented in the body of the manuscript.

Proteins identified by a single, high-confidence peptide assignment

Will examinng the annotated spectra influence confidence about the assignment? Will you really look at them?

Annotated tandem mass spectra - annotate the following for each

Peptide sequence

Observed m/z

Mass error

Charge state

Database search score

Probability/expect score

Site localization probability (where appropriate)

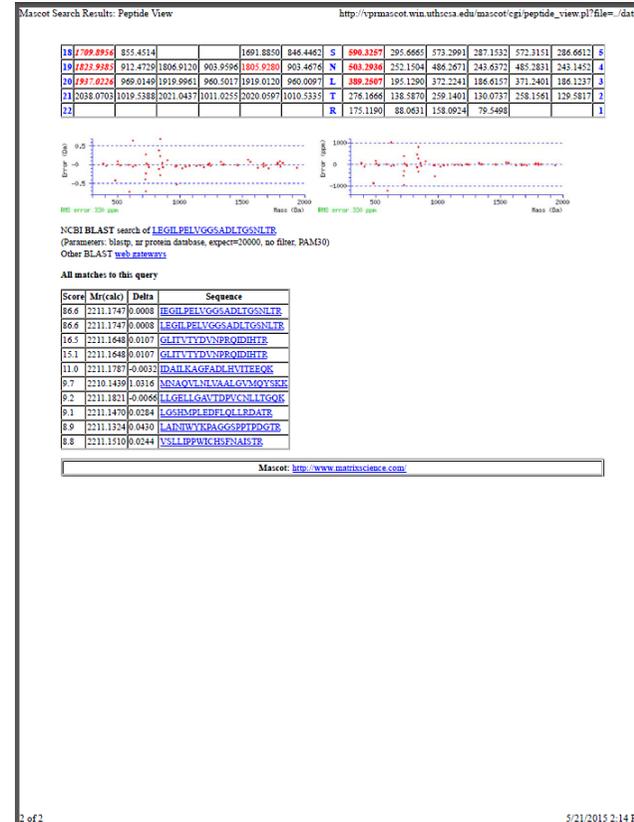
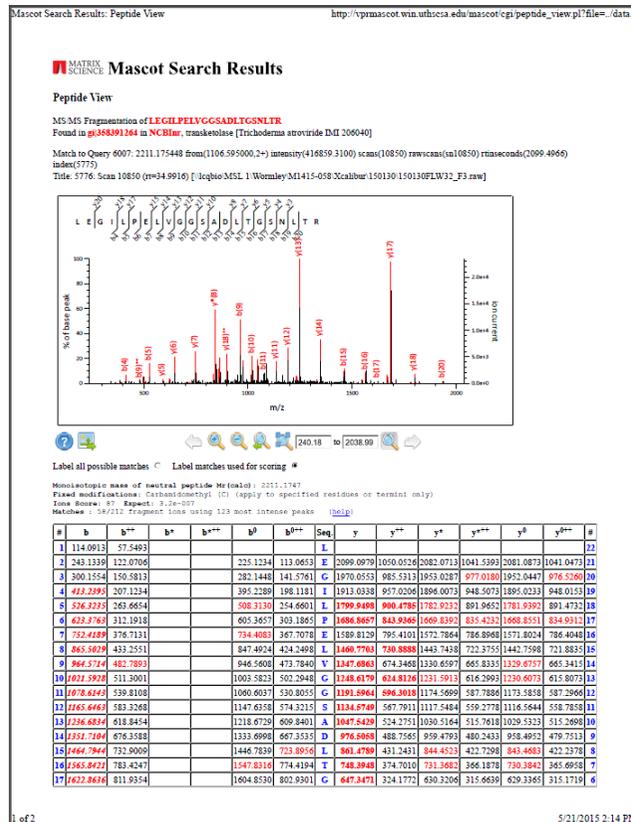
Supporting information

Annotated tandem mass spectra

Protein family 139

transketolase [Trichoderma atroviride IMI 206040]

Score, 106; matches, 2; match(sig), 2; sequences, 2; seq(sig), 2; eMPAI, 0.06



Print a PDF of the Mascot Peptide View

Peptide View

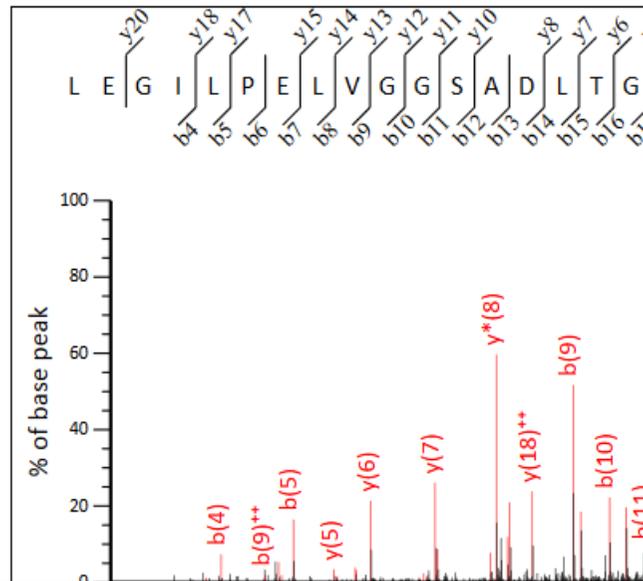
MS/MS Fragmentation of **LEGILPELVGGSADLTGSNLT^{TR}**

Found in [gi|358391264](#) in [NCBI nr](#), transketolase [Tricho

Match to Query 6007: 2211.175448 from(1106.595000,2+

Title: 5776: Scan 10850 (rt=34.9916) [\\lcqbio\MSL 1\Wo

All matches to this query



Modification(s), ions score, expect value, matches

Score	Mr(calc)	Delta	Sequence
86.6	2211.1747	0.0008	LEGILPELVGGSADLTGSNLTR
86.6	2211.1747	0.0008	LEGILPELVGGSADLTGSNLTR
16.5	2211.1648	0.0107	GLITVTYDVNPRQIDIHTR
15.1	2211.1648	0.0107	GLITVTYDVNPRQIDIHTR
11.0	2211.1787	-0.0032	IDAILKAGFADLHVITEEQK
9.7	2210.1439	1.0316	MNAQVLNLVAALGVMQYSKK
9.2	2211.1821	-0.0066	LLGELLGAVTDPVCNLLTGQK
9.1	2211.1470	0.0284	LGSHMPLEDFLQLLRDATR
8.9	2211.1324	0.0430	LAINIWYKPAGGSPPTPDGTR
8.8	2211.1510	0.0244	VSL LIPPWICH SFNAISTR



240.18

to

2038.99



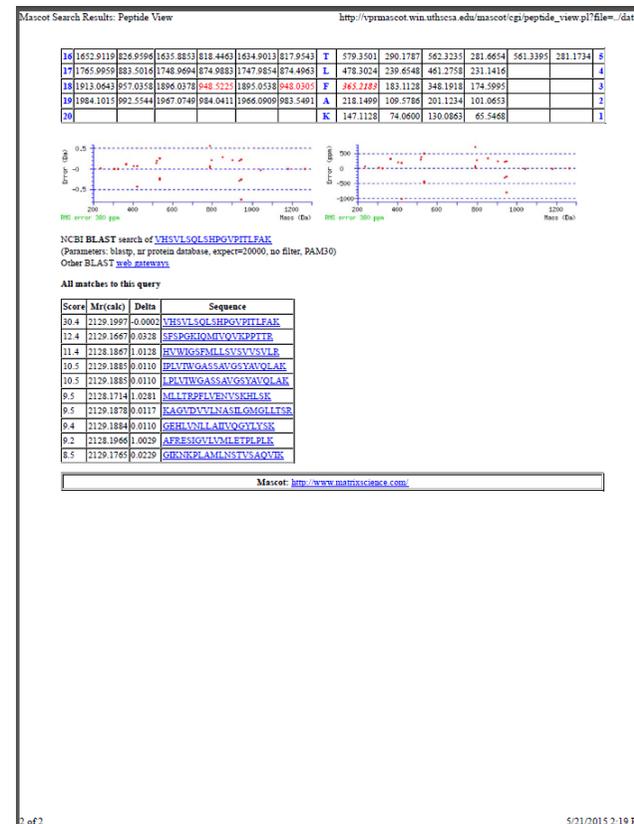
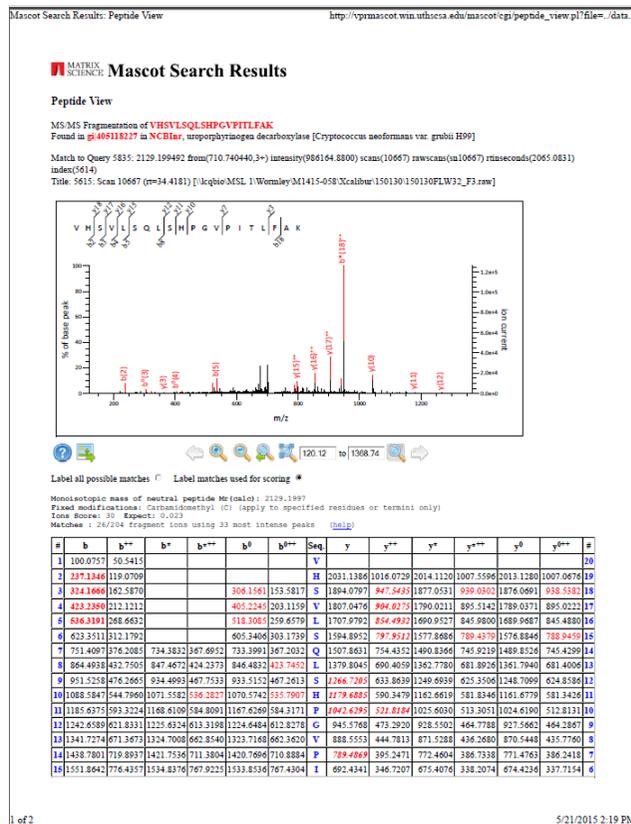
Monoisotopic mass of neutral peptide Mr(calc): 2211.1747
 Fixed modifications: Carbamidomethyl (C) (apply to specified residues or termini only)
 Ions Score: 87 Expect: 3.2e-007
 Matches : 58/212 fragment ions using 123 most intense peaks ([help](#))

Supporting information

Annotated tandem mass spectra

Protein family 376

uroporphyrinogen decarboxylase [Cryptococcus neoformans var. grubii H99]
 Score, 30; matches, 1; match(sig), 1; sequences, 1; seq(sig), 1; eMPAI, 0.07

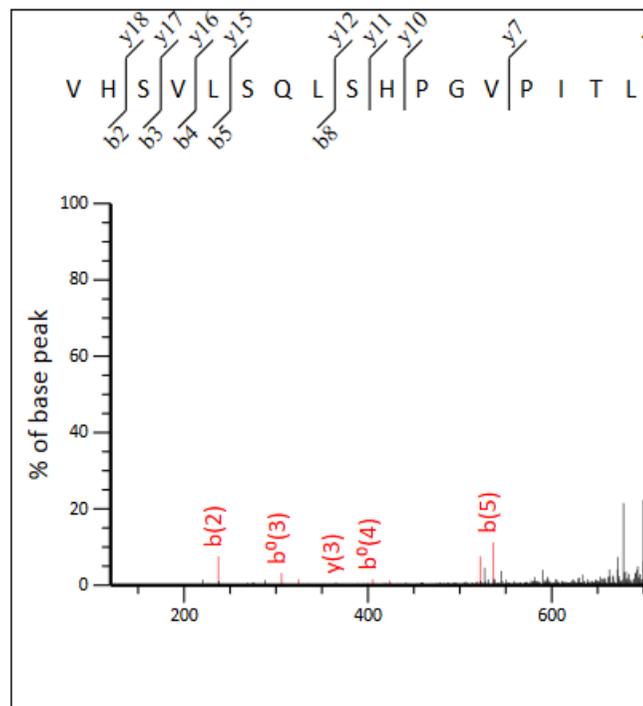


Peptide View

MS/MS Fragmentation of **VHSVLSQLSHPGVPITLFAK**
Found in [gi|405118227](#) in [NCBI](#), uroporphyrinogen dec

Match to Query 5835: 2129.199492 from(710.740440,3+)
Title: 5615: Scan 10667 (rt=34.4181) [\\lcqbio\MSL 1\Wo

All matches to this query



Score	Mr(calc)	Delta	Sequence
30.4	2129.1997	-0.0002	VHSVLSQLSHPGVPITLFAK
12.4	2129.1667	0.0328	SFSPGKIQMIVQVKPPTTR
11.4	2128.1867	1.0128	HVWIGSFMLLSVSVVSVLR
10.5	2129.1885	0.0110	IPLVIWGASSAVGSYAVQLAK
10.5	2129.1885	0.0110	LPLVIWGASSAVGSYAVQLAK
9.5	2128.1714	1.0281	MLLTRPFLVENVSKHLSK
9.5	2129.1878	0.0117	KAGVDVVLNASILGMGLLTSR
9.4	2129.1884	0.0110	GEHLVNLLAIIVQGYLYSK
9.2	2128.1966	1.0029	AFRESIGVLVMLETPLPLK
8.5	2129.1765	0.0229	GIKNKPLAMLNSTVSAQVIK



Monoisotopic mass of neutral peptide Mr(calc): 2129.1997
Fixed modifications: Carbamidomethyl (C) (apply to specified residues or termini only)
Ions Score: 30 **Expect:** 0.023
Matches : 26/204 fragment ions using 33 most intense peaks ([help](#))

Supporting information

Quantitative analysis

Protein level report

Documentation can be added to the ID report or in a separate table

Columns

Protein name

Accession number

Molecular weight

Number of assigned spectra (total and unique)

Percent sequence coverage

Probability of protein inference (if determined post-processing)

Number of peptides used for quantitative analysis

Variability of results for peptides assigned to a protein

Clear/meaningful column heading names

Legend - at the top of long tables or on a separate worksheet

Explanations for abbreviated or non-standard column headings

Significance level cutoff of assigned peptides

Supporting information

Quantitative analysis

Protein level report

Documentation can be added to the ID report or in a separate table

Columns

Protein name

Accession number

Molecular weight

Number of assigned spectra (total and unique)

Percent sequence coverage

Probability of protein inference (if determined post-processing)

Number of peptides used for quantitative analysis

Variability of results for peptides assigned to a protein

Clear/meaningful column heading names

Legend - at the top of long tables or on a separate worksheet

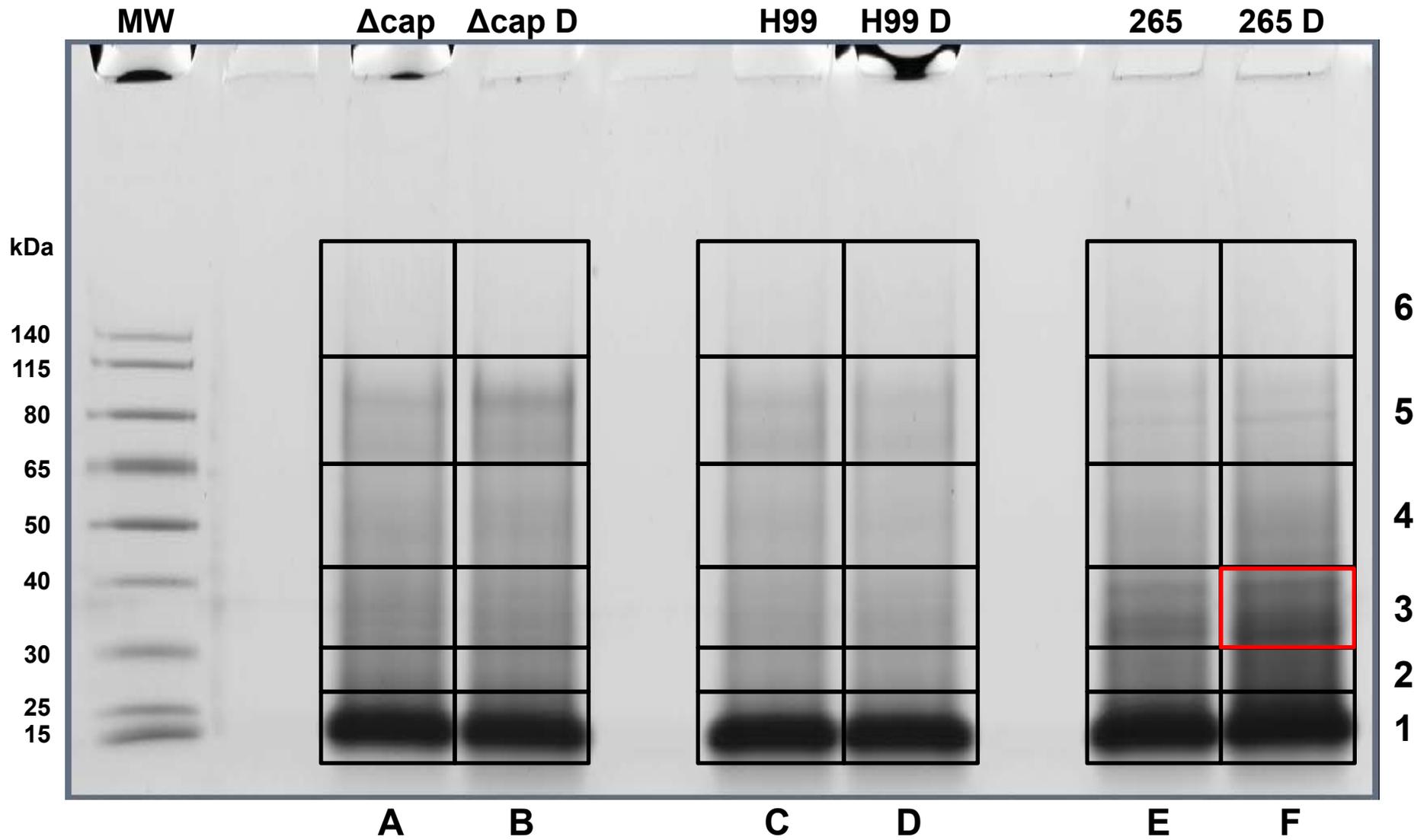
Explanations for abbreviated or non-standard column headings

Significance level cutoff of assigned peptides

Supporting information

You can generate the supplemental data tables needed for publication directly from Mascot by exporting a CSV file from the Mascot Results Report page.

1-D SDS PAGE - proteins of *Cryptococcus neoformans*



BioRad Criterion XT MOPS 12% SDS-PAGE reducing gel, blue silver stain

A.K. Chaturvedi and F.L. Wormley, Jr.

Mascot search results report

Mascot search engine | Protei... x Wormley Chaturvedi M1415-058 1... x +

vprmascot.win.uthscsa.edu/mascot/cgi/master_results_2.pl?file=.%2Fdata%2F20150515%2FF035682.dat;sessionID=weintraub_264016471540778

MATRIX SCIENCE **MASCOT Search Results**

User : stweintraub
E-mail : weintraub@uthscsa.edu
Search title : Wormley Chaturvedi M1415-058 150130FLW32_F3.raw (NCBINr_fungi; contam) trypsin-1 Ox(M) Carb(C) D(NQ) decoy (Wormley Chaturvedi M1415-058 265 D, slice F3, 5ul, D8)
Databases : **1:** contaminants 20120713 (247 sequences; 128,130 residues)
 2: NCBINr 20140522 (39,649,990 sequences; 14,178,194,136 residues)
Taxonomy : **1:** (none)
 2: Fungi (2,653,696 sequences)
Timestamp : 15 May 2015 at 19:07:55 GMT

Re-search All Non-significant Unassigned [\[help\]](#) Export As XML

Not what you expected? Try [the select summary](#).

- Search parameters
- Score distribution
- Modification statistics
- Legend

Protein Family Summary

Filter	Significance threshold p<	0.05	Max. number of families	AUTO	[help]
	Ions score or expect cut-off	0	Dendrograms cut at	0	
	Show Percolator scores	<input type="checkbox"/>			
	Preferred taxonomy	All entries			

Decoy search summary (reversed protein sequences)

Proteins (389) [Report Builder](#) [Unassigned \(5102\)](#) [S permalink](#)

Protein families 1-10 (out of 389)

10 per page 1 [2](#) [3](#) [4](#) [5](#) [6](#) ... [39](#) [Next](#) [Expand all](#) [Collapse all](#)

Accession contains Find

1 **2:gi|58261082** 1222 14-3-3 protein [Cryptococcus neoformans var. neoformans JEC21]
2:gi|521772018 500 hypothetical protein DC706234_020 [Plumaria graminis f. sp. tritici 06234]

Mascot search results report

Mascot search engine | Protei... x Wormley Chaturvedi M1415-058 1... x +

vprmascot.win.uthscsa.edu/mascot/cgi/master_results_2.pl?file=.%2Fdata%2F20150515%2F035682.dat;sessionID=weintraub_264016471540778

MATRIX SCIENCE **MASCOT Search Results**

User : stweintraub
E-mail : weintraub@uthscsa.edu
Search title : Wormley Chaturvedi M1415-058 150130FLW32_F3.raw (NCBINr_fungi; contam) trypsin-1 Ox(M) Carb(C) D(NQ) decoy (Wormley Chaturvedi M1415-058 265 D, slice F3, 5ul, D8)
Databases : **1**: contaminants 20120713 (247 sequences; 128,130 residues)
 2: NCBINr 20140522 (39,649,990 sequences; 14,178,194,136 residues)
Taxonomy : **1**: (none)
 2: Fungi (2,653,696 sequences)
Timestamp : 15 May 2015 at 19:07:55 GMT

Re-search All Non-significant Unassigned

Not what you expected? Try [the select summary](#).

- ▶ Search parameters
- ▶ Score distribution
- ▶ Modification statistics
- ▶ Legend

Protein Family Summary

Filter	Significance threshold p<	0.05
	Ions score or expect cut-off	0
	Show Percolator scores	<input type="checkbox"/>
	Preferred taxonomy	All entries

▶ Decoy search summary (reversed protein sequences)

Proteins (389) [Report Builder](#) [Unassigned](#) [S permalink](#)

Protein families 1-10 (out of 389)

10 per page 1 2 3 4 5 6 ... 39 N

Accession contains Find

▶ 1 2:gi|58261082 1222 14-3-3 protein [Cryptococcus neoformans var. neoformans JEC21]
2:gi|521772018 500 hypothetical protein DC706234.020 [Phycometia sorokinii f. sp. tritici 06234]

Mascot search results report

Mascot search engine | Protei... x Wormley Chaturvedi M1415-058 1... x +

vprmscot.win.uthscsa.edu/mascot/cgi/master_results_2.pl?file=.%2Fdata%2F20150515%2F035682.dat;sessionID=weintraub_264016471540778

MATRIX SCIENCE **MASCOT Search Results**

User : stweintraub
E-mail : weintraub@uthscsa.edu
Search title : Wormley Chaturvedi M1415-058 150130FLW32_F3.raw (NCBINr_fungi; contam) trypsin-1 Ox(M) Carb(C) D(NQ) decoy (Wormley Chaturvedi M1415-058 265 D, slice F3, 5ul, D8)
Databases : **1**: contaminants 20120713 (247 sequences; 128,130 residues)
 2: NCBINr 20140522 (39,649,990 sequences; 14,178,194,136 residues)
Taxonomy : **1**: (none)
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Timestamp : 15 May 2015 at 19:07:55 GMT

Re-search All Non-significant Unassigned [\[help\]](#) Export As XML

Not what you expected? Try [the select summary](#).

► Search parameters
► Score distribution

▼ Score distribution

Peptide score distribution. Ions score is $-10\log(P)$, where P is the probability that the observed match is a random event. There are **1,263** peptide matches above identity threshold and **1,808** matches above homology threshold for **8,057** queries. Histogram score range is (0, 120). On average, individual ions scores **> 48** (beyond green shading) indicate **identity or extensive homology** ($p < 0.05$).

[Deprecated] Protein score distribution. Score distribution for family members in the first 50 proteins. Protein scores are derived from ions scores as a non-probabilistic basis for ranking protein families.

Mascot search results report

Mascot search engine | Protei... x Wormley Chaturvedi M1415-058 1... x +

vpr Mascot: win.uthscsa.edu/mascot/cgi/master_results_2.pl?file=.%2Fdata%2F20150515%2F035682.dat;sessionID=weintraub_264016471540778

MATRIX SCIENCE **MASCOT Search Results**

User : stweintraub
E-mail : weintraub@uthscsa.edu
Search title : Wormley Chaturvedi M1415-058 150130FLW32_F3.raw (NCBINr_fungi; contam) trypsin-1 Ox(M) Carb(C) D(NQ) decoy (Wormley Chaturvedi M1415-058 265 D, slice F3, 5ul, D8)
Databases : **1:** contaminants 20120713 (247 sequences; 128,130 residues)
 2: NCBIInr 20140522 (39,649,990 sequences; 14,178,194,136 residues)
Taxonomy : **1:** (none)
 2: Fungi (2,653,696 sequences)
Timestamp : 15 May 2015 at 19:07:55 GMT

Re-search All Non-significant Unassigned [\[help\]](#) Export As XML

Not what you expected? Try [the select summary](#).

- ▶ Search parameters
- ▶ Score distribution
- ▶ Modification statistics

▼ **Modification statistics**

Modification	Site	Above thr.
Oxidation	M	322
Carbamidomethyl	C	207
Deamidated	N	130
Deamidated	Q	66

Proteins (389) [Report Builder](#) [Unassigned \(5102\)](#) [\[permalink\]](#)

Protein families 1-10 (out of 389)

10 per page 1 [2](#) [3](#) [4](#) [5](#) [6](#) ... [39](#) [Next](#) [Expand all](#) [Collapse all](#)

Accession contains Find

▶ 1 **2:gi|58261082** 1222 14-3-3 protein [Cryptococcus neoformans var. neoformans JEC21]
2:gi|521772018 500 hypothetical protein DC706234_020 [Phlebotomus perniciosus f. sp. tritici 06234]

Mascot search results report

Mascot search engine | Protei... x Wormley Chaturvedi M1415-058 1... x

vpmscot.win.uthscsa.edu/mascot/cgi/master_results_2.pl?file=.%2Fdata%2F20150515%2F035682.dat;sessionID=weintraub_264016471540778

MATRIX SCIENCE **MASCOT Search Results**

User : stweintraub
E-mail : weintraub@uthscsa.edu
Search title : Wormley Chaturvedi M1415-058 150130FLW32_F3.raw (NCBIInr_fungi; contam) trypsin-1 Ox(M) Carb(C) D(NQ) decoy (Wormley Chaturvedi M1415-058 265 D, slice F3, 5ul, D8)
Databases : **1**: contaminants 20120713 (247 sequences; 128,130 residues)
 2: NCBIInr 20140522 (39,649,990 sequences; 14,178,194,136 residues)
Taxonomy : **1**: (none)
 2: Fungi (2,653,696 sequences)
Timestamp : 15 May 2015 at 19:07:55 GMT

Re-search All Non-significant Unassigned [\[help\]](#) Export As XML

Not what you expected? Try [the select summary](#).

- Search parameters
- Score distribution
- Modification statistics
- Legend

Protein Family Summary

Protein Family Summary

Filter Significance threshold p< 0.05 Max. number of families AUTO [\[help\]](#)
Ions score or expect cut-off 0 Dendrograms cut at 0 [permalink](#)
Show Percolator scores
Preferred taxonomy All entries

Accession	Contam	Score	Protein
1		2::gi 58261082	1222 14-3-3 protein [Cryptococcus neoformans var. neoformans JEC21]
2		2::gi 521772018	500 hypothetical protein DC706234_020 [Plumaria graminis f. sp. tritici 06234]

Mascot search results report

Mascot search engine | Protei... x Wormley Chaturvedi M1415-058 1... x +

vprmscot.win.uthscsa.edu/mascot/cgi/master_results_2.pl?file=.%2Fdata%2F20150515%2FF035682.dat;sessionID=weintraub_264016471540778

MATRIX SCIENCE **MASCOT Search Results**

User : stweintraub
E-mail : weintraub@uthscsa.edu
Search title : Wormley Chaturvedi M1415-058 150130FLW32_F3.raw (NCBINr_fungi; contam) trypsin-1 Ox(M) Carb(C) D(NQ) decoy (Wormley Chaturvedi M1415-058 265 D, slice F3, 5ul, D8)
Databases : **1**: contaminants 20120713 (247 sequences; 128,130 residues)
 2: NCBINr 20140522 (39,649,990 sequences; 14,178,194,136 residues)
Taxonomy : **1**: (none)
 2: Fungi (2,653,696 sequences)
Timestamp : 15 May 2015 at 19:07:55 GMT

Re-search All Non-significant Unassigned [\[help\]](#) Export As XML

Not what you expected? Try [the select summary](#).

- ▶ Search parameters
- ▶ Score distribution
- ▶ Modification statistics
- ▶ Legend

Protein Family Summary

Filter Significance threshold p< 0.05 Max. number of families AUTO [\[help\]](#)
Ions score or expect cut-off 0 Dendrograms cut at 0
Show Percolator scores
Preferred taxonomy All entries

▶ Decoy search summary (reversed protein sequences)

▼ **Decoy search summary (reversed protein sequences)** [\[permalink\]](#)

Peptide matches	in target	in Decoy	FDR
- above identity threshold	1263	26	2.06%
- above identity or homology threshold	1808	76	4.20%

Adjust to 1%

Decoy results are available in [the decoy report](#).

Mascot search results report

Mascot search engine | Protei... x Wormley Chaturvedi M1415-058 1... x

vprmascot.win.uthscsa.edu/mascot/cgi/master_results_2.pl?file=.%2Fdata%2F20150515%2FF035682.dat;sessionID=weintraub_264016471540778

MATRIX SCIENCE MASCOT Search Results

User : stweintraub
E-mail : weintraub@uthscsa.edu
Search title : Wormley Chaturvedi M1415-058 150130FLW32_F3.raw (NCBINr_fungi; contam) trypsin-1 Ox(M) Carb(C) D(NQ) decoy (Wormley Chaturvedi M1415-058 265 D, slice F3, 5ul, D8)
Databases : **1:** contaminants 20120713 (247 sequences; 128,130 residues)
 2: NCBINr 20140522 (39,649,990 sequences; 14,178,194,136 residues)
Taxonomy : **1:** (none)
 2: Fungi (2,653,696 sequences)
Timestamp : 15 May 2015 at 19:07:55 GMT

Re-search All Non-significant Unassigned [\[help\]](#) Export As XML

Not what you expected? Try [the select summary](#).

- ▶ Search parameters
- ▶ Score distribution
- ▶ Modification statistics
- ▶ Legend

Protein Family Summary

Filter Significance threshold p< 0.05 Max. number of families AUTO [\[help\]](#)
Ions score or expect cut-off 0 Dendrograms cut at 0
Show Percolator scores
Preferred taxonomy All entries

▶ Decoy search summary (reversed protein sequences)

Proteins (389) [Report Builder](#) [Unassigned \(5102\)](#) [\[permalink\]](#)

Protein families 1-10 (out of 389)

10 per page 1 2 3 4 5 6 ... 39 Next Expand all Collapse all

Accession contains Find

▶ 1 2:gi|58261082 1222 14-3-3 protein [Cryptococcus neoformans var. neoformans JEC21]
2:gi|521772018 500 hypothetical protein BC706234.020 [Plasmodium falciparum strain FAL0234]

Select "Report Builder"

Mascot search results report

Mascot search engine | Protei... x Wormley Chaturvedi M1415-058 1... x

vpvmascot.win.utmsca.edu/mascot/cgi/master_results_2.pl?file=.%2Fdata%2F20150515%2F035682.dat;_ignoreionsscorebelow=0;_prefertaxonomy=0;_sigthreshold=0.05;percolate=0;pr.show=reportbuilder; Search

Most Visited Getting Started Weather Forecast Sa... Examsoft Dental Austin-San Antonio R... Patient Portal Intellicast - San Anto... The University of Tex... Mascot_vprmscot

► **Modification statistics**

► **Legend**

Protein Family Summary

Filter Significance threshold p< 0.05 Max. number of families AUTO [help]
 Ions score or expect cut-off 0 Dendrograms cut at 0
 Show Percolator scores
 Preferred taxonomy All entries

▼ **Decoy search summary (reversed protein sequences)**

Peptide matches **in target in Decoy FDR**
 - above identity threshold 1263 26 2.06%
 - above identity or homology threshold 1808 76 4.20% 1%

Decoy results are available in [the decoy report](#).

[Proteins \(389\)](#) [Unassigned \(5102\)](#) [§ permalink](#)

Protein hits (464 proteins)

► **Columns: Standard (12 out of 16)**

► **Filters: (none)**

Family	M	DB	Accession	Score	Mass	Matches	Match(sia)	Sequences	Seq(sia)	emPAI	Description
1	1	NCBIInr	2::gj 58261082	1222	29090	112	61	27	18	64.29	14-3-3 protein [Cryptococcus neoformans var. neoformans JEC21]
1	2	NCBIInr	2::gj 62420901	629	28911	72	33	17	10	12.65	14-3-3 1 protein [Phanerochaete chrysosporium]
1	3	NCBIInr	2::gj 521773918	500	30146	50	29	10	8	9.60	hypothetical protein BGT96224_929 [Blumeria graminis f. sp. tritici 96224]
1	4	NCBIInr	2::gj 254567754	161	29122	36	17	10	6	4.64	hypothetical protein [Komagataella pastoris GS115]
1	5	NCBIInr	2::gj 1040756	132	30471	22	9	7	5	2.00	rad24 [Schizosaccharomyces pombe]
1	6	NCBIInr	2::gj 50546823	61	31318	12	3	4	3	0.49	YALI0B14377p [Yarrowia lipolytica]
2	1	NCBIInr	2::gj 321265283	688	85793	45	28	31	20	1.96	heat shock protein [Cryptococcus gattii WM276]
2	2	NCBIInr	2::gj 405123671	488	85923	36	20	24	14	1.09	heat shock 70kDa protein 4 [Cryptococcus neoformans var. grubii H99]
2	3	NCBIInr	2::gj 597927424	178	85983	8	5	5	4	0.22	hypothetical protein SERLADRAFT_355892 [Serpula lacrymans var. lacrymans]

Mascot search results report

Mascot search engine | Protei... x Wormley Chaturvedi M1415-058 1... x

vpr Mascot: win.uthscsa.edu/mascot/cgi/master_results_2.pl?file=.%2Fdata%2F20150515%2F035682.dat;_ignoreionsscorebelow=0;_prefertaxonomy=0;_sigthreshold=0.05;percolate=0;pr.show=reportbuilder; Search

MATRIX SCIENCE MASCOT Search Results

User : stweintraub
E-mail : weintraub@uthscsa.edu
Search title : Wormley Chaturvedi M1415-058 150130FLW32_F3.raw (NCBIInr_fungi; contam) trypsin-1 Ox(M) Carb(C) D(NQ) decoy (Wormley Chaturvedi M1415-058 265 D, slice F3, Sul, D8)
Databases : **1**: contaminants 20120713 (247 sequences; 128,130 residues)
2: NCBIInr 20140522 (39,649,990 sequences; 14,178,194,136 residues)
Taxonomy : **1**: (none)
2: Fungi (2,653,696 sequences)
Timestamp : 15 May 2015 at 19:07:55 GMT

Re-search All Non-significant Unassigned [help] Export As XML

Not what you expected? Try [the select summary](#).

Search parameters
Score distribution
Modification statistics
Legend

Protein Family Summary

Filter Significance threshold Ions score or expect Show Percolator scores Preferred taxonomy

Protein Family Summary

Filter Significance threshold p < 0.05 Max. number of families AUTO [help]
Ions score or expect cut-off 0 Dendrograms cut at 0
Show Percolator scores
Preferred taxonomy All entries

Decoy search summary (reversed protein sequences)

Peptide matches	in target	in Decoy	FDR
- above identity threshold	1263	26	2.06%
- above identity or homology threshold	1808	76	4.20%

Adjust to 1%

Proteins (389) Report Builder

Protein hits (464 protein)

Columns: Standard (12 out of 16)
Filters: (none)

Mascot search results report - ions score cutoff 0, no FDR adjustment

Rank	Accession	Protein Name	Score	Length	Ion Score	Ion Count	Ion Type	Ion Charge	Ion Mass	Protein Description		
29	1	NCBIInr	378	35869	23	15	13	9	3.08	inorganic diphosphatase [Cryptococcus gattii WM276]		
29	2	NCBIInr	248	35443	20	14	11	9	2.69	inorganic pyrophosphatase [Cryptococcus neoformans var. grubii H99]		
30	1	NCBIInr	370	58177	32	19	20	13	1.76	ATP synthase alpha chain, mitochondrial precursor [Cryptococcus gattii WM276]		
31	1	NCBIInr	365	39278	27	16	17	11	3.02	hypothetical protein CGB_D4230W [Cryptococcus gattii WM276]		
31	2	NCBIInr	294	39332	14	10	8	6	1.35	hypothetical protein CNBD4520 [Cryptococcus neoformans var. neoformans B-265825]		
32	1	NCBIInr	363	34764	21	12	10	7	1.97	hypothetical protein CGB_C5340C [Cryptococcus gattii WM276]		
32	2	NCBIInr	58	34698	9	3	6	3	0.44	aldose reductase [Cryptococcus neoformans var. grubii H99]		
33	1	NCBIInr	349	48772	34	20	11	9	2.08	cellulase [Cryptococcus gattii WM276]		
34	1	NCBIInr	319	39890	36	16	16	11	2.55	6-phosphogluconolactonase [Cryptococcus gattii WM276]		
34	2	NCBIInr	301	34650	25	13	13	9	2.36	6-phosphogluconolactonase [Cryptococcus neoformans var. grubii H99]		
35	1	NCBIInr	303	69578	36	16	25	14	1.64	heat shock protein 70 [Cryptococcus gattii WM276]		
35	2	NCBIInr	260	69578	25	15	24	12	1.24	heat shock protein 70 [Cryptococcus neoformans var. neoformans JEC21]		
35	3	NCBIInr	321	321257093	23	15	13	9	3.08	gattii WM276]		
35	4	NCBIInr	121	121568	23	15	13	9	3.08	gulated protein homolog; Short=GRP-78; Al		
35	5	NCBIInr	321	321265704	23	15	13	9	3.08	ccus gattii WM276]		
35	6	NCBIInr	255	255712457	23	15	13	9	3.08	otolerans]		
35	7	NCBIInr	134	134106591	23	15	13	9	3.08	ryptococcus neoformans var. neoformans B-		
35	8	NCBIInr	599	599407270	23	15	13	9	3.08	_265825 [Phanerochaete carnosae HHB-1011		
36	1	NCBIInr	321	321260961	23	15	13	9	3.08	ccus gattii WM276]		
37	1	NCBIInr	259	259120714	23	15	13	9	3.08	276]		
38	1	NCBIInr	321	321254947	23	15	13	9	3.08	ans]		
38	2	NCBIInr	109	109156571	23	15	13	9	3.08	[Cryptococcus gattii WM276]		
39	1	NCBIInr	321	321265355	23	15	13	9	3.08	s var. grubii H99]		
39	2	NCBIInr	405	405123684	23	15	13	9	3.08	rotein [Cryptococcus gattii WM276]		
40	1	NCBIInr	321	321257249	23	15	13	9	3.08	ococcus gattii WM276]		
41	1	NCBIInr	321	321252988	23	15	13	9	3.08	[Cryptococcus gattii WM276]		
42	1	NCBIInr	321	321253782	23	15	13	9	3.08	[Cryptococcus gattii WM276]		
43	1	NCBIInr	321	321261545	23	15	13	9	3.08	[Cryptococcus gattii WM276]		
43	2	NCBIInr	134	134113809	23	15	13	9	3.08	ryptococcus neoformans var. neoformans B-		
44	1	NCBIInr	582	58258849	23	15	13	9	3.08	ococcus neoformans var. neoformans JEC21]		
45	1	NCBIInr	302	302907708	219	28241	16	7	6	4	1.44	predicted protein [Nectria haematococca mpVI 77-13-4]
45	2	NCBIInr	61	615413004	189	25535	10	5	5	3	0.93	putative deoxyribose-phosphate aldolase protein [Neofusicoccum parvum UCR]
46	1	NCBIInr	321	321264171	219	31471	14	9	10	7	1.90	hypothetical protein CGB_K3180C [Cryptococcus gattii WM276]
47	1	NCBIInr	321	321254861	218	52235	23	11	16	8	1.07	aminotransferase [Cryptococcus gattii WM276]
47	2	NCBIInr	405	405119067	193	52462	16	9	13	7	0.90	4-aminobutyrate transaminase [Cryptococcus neoformans var. grubii H99]
48	1	NCBIInr	582	58258141	217	26155	20	8	9	5	1.61	hypothetical protein CNA00560 [Cryptococcus neoformans var. neoformans JEC21]

Protein family 37
hexokinase 2 [Cryptococcus gattii WM276]

Score 256
 Matches 23
 Match(sig) 13
 Sequences 13
 Seq(sig) 7
 eMPAI 0.87

Mascot search results report - ions score cutoff 0, no FDR adjustment

Protein sequence coverage: 35%  **35% coverage**

Matched peptides shown in **bold red**.

1 MNFFDIRK**QI EPYFVLNDEK LVDIVKHFRK** EMEEGLANYG **KDMAMIPTFV**
 51 **TGVPDGTTEEG VFLALDLGGT NLRVCLIVLQ GNNQFKIEQQ** KYKVSEELKT
 101 GQARVLFYDI AESVDNFLT E VENHSDVAIP VTSEPLHLGF TFSFPVEQTA
 151 IDAGKLLTWT KGFNTKNAIG HDVVRLQDA **FDRKHMHVRC SALVNDTVGT**
 201 **LLSRYSQSGP ALIGAIFCTG TNGAYIDKSR** TISKLGKEKI **EAEKGGEGA**
 251 **GKYMVNTEW GAFDNKRLCL PVSFLDNKLD** RESINPRQM **FEKMGVSMYL**
 301 **GEITRNILLY** LIDSSLLFEG HSSEVLNTHY GFDTSFVSGI EGITSPEEVT
 351 QLIIEKELVD PKHITDKCPE IVQWTVRMVA DRACKLAACA IAAIVLHTGN
 401 DKAPEGEKDK GVDVGVDSV AQFLPMFNER VMAGLKALIG ERGAAR**VNIG**
 451 **LAKD**GGSGVA ALTALQAKKA LDQRSDRSTP YVPGKRAP

Unformatted sequence string: [488 residues](#) (for pasting into other applications).

Sort peptides by Residue Number Increasing Mass Decreasing Mass

Show predicted peptides also

Query	Start - End	Observed	Mr(expt)	Mr(calc)	ppm	M	Score	Expect	Rank	U	Peptide
5902	9 - 26	721.3964	2161.1673	2161.1671	0.13	1	37	0.0068	1	U	K.QIEPYFVLNDEKLV DI VK.H
7636	42 - 73	1123.5515	3367.6327	3367.6316	0.31	0	39	0.0079	1	U	K.DMAMIP TFVTGVPDGT TEEGVFLALDLGGT NLR.V + 2 Oxidation (M)
7637	42 - 73	1123.8851	3368.6335	3367.6316	297	0	41	0.0077	1	U	K.DMAMIP TFVTGVPDGT TEEGVFLALDLGGT NLR.V + 2 Oxidation (M)
4184	74 - 86	766.9161	1531.8175	1531.8181	-0.35	0	66	0.00093	1	U	R.VCLIVLQ GNNQ FK.I
4185	74 - 86	511.6135	1531.8186	1531.8181	0.36	0	40	0.46	1	U	R.VCLIVLQ GNNQ FK.I
1885	176 - 183	489.2554	976.4963	976.4978	-1.54	0	41	0.15	1	U	R.LLQDA FDR.K
2551	176 - 184	369.2042	1104.5908	1104.5927	-1.76	1	27	0.98	1	U	R.LLQDA FDRK.H
4467	190 - 204	803.4171	1604.8195	1604.8192	0.21	0	100	1.8e-007	1	U	R.CSALVND TVG TLLSR.S
4468	190 - 204	535.9474	1604.8204	1604.8192	0.72	0	45	0.12	1	U	R.CSALVND TVG TLLSR.S
6396	205 - 228	801.4020	2401.1841	2401.1801	1.64	0	59	0.008	1	U	R.SYQSGP ALIGAIFCTG TNGAYIDK.S + Deamidated (NQ)

Score	Expect	Rank	U	Peptide
37	0.0068	1	U	K.QIEPYFVLNDEKLV DI VK.H
39	0.0079	1	U	K.DMAMIP TFVTGVPDGT TEEGVFLALDLGGT NLR.V + 2 Oxidation (M)
41	0.0077	1	U	K.DMAMIP TFVTGVPDGT TEEGVFLALDLGGT NLR.V + 2 Oxidation (M)
66	0.00093	1	U	R.VCLIVLQ GNNQ FK.I
40	0.46	1	U	R.VCLIVLQ GNNQ FK.I
41	0.15	1	U	R.LLQDA FDR.K
27	0.98	1	U	R.LLQDA FDRK.H
100	1.8e-007	1	U	R.CSALVND TVG TLLSR.S

MATRIX SCIENCE MASCOT Search Results

User : stweintraub
E-mail : weintraub@uthscsa.edu
Search title : Wormley Chaturvedi M1415-058 150130FLW32_F3.raw (NCBIInr_fungi; contam) trypsin-1 Ox(M) Carb(C) D(NQ) decoy (Wormley Chaturvedi M1415-058 265 D, slice F3, Sul, D8)
Databases : **1**: contaminants 20120713 (247 sequences; 128,130 residues)
2: NCBIInr 20140522 (39,649,990 sequences; 14,178,194,136 residues)
Taxonomy : **1**: (none)
2: Fungi (2,653,696 sequences)
Timestamp : 15 May 2015 at 19:07:55 GMT

Re-search All Non-significant Unassigned [help] Export As XML

Not what you expected? Try the select summary.

- ▶ Search parameters
- ▶ Score distribution
- ▶ Modification statistics
- ▶ Legend

Protein Family Summary

- Filter
- Significance threshd
- Ions score or expec
- Show Percolator sco
- Preferred taxonomy

▼ **Decoy search summary (reversed protein sequences)**

- Peptide matches
- above identity threshold
- above identity or homology t

Decoy results are available in the d

Proteins (380) Report Builder

Protein hits (454 proteins)

▶ Columns: Standard (12 out of 16)

▶ Filters: (none)

Protein Family Summary

Filter Significance threshold p< 0.05 Max. number of families AUTO [help]
 Ions score or expect cut-off 0.05 Dendrograms cut at 0
 Show Percolator scores
 Preferred taxonomy All entries

▼ **Decoy search summary (reversed protein sequences)**

Peptide matches	in target	in Decoy	FDR
- above identity threshold	1263	26	2.06%
- above identity or homology threshold	1808	76	4.20%

Adjust to 1%

Mascot search results report

Rank	Accession	Protein Name	Score	Length	Identified	Missed	Score	Length	Identified	Missed	Protein Name
29	1	NCBIInr	2::gi 321258651	378	35869	23	15	13	9	3.08	inorganic diphosphatase [Cryptococcus gattii WM276]
29	2	NCBIInr	2::gi 540383854	248	35443	20	14	11	9	2.69	inorganic pyrophosphatase [Cryptococcus neoformans var. grubii H99]
30	1	NCBIInr	2::gi 321260106	370	58177	32	19	20	13	1.76	ATP synthase alpha chain, mitochondrial precursor [Cryptococcus gattii WM276]
31	1	NCBIInr	2::gi 321257325	365	39278	27	16	17	11	3.02	hypothetical protein CGB_D4230W [Cryptococcus gattii WM276]
31	2	NCBIInr	2::gi 134111162	294	39332	14	10	8	6	1.35	hypothetical protein CNBD4520 [Cryptococcus neoformans var. neoformans B-2699]
32	1	NCBIInr	2::gi 321253911	363	34764	21	12	10	7	1.97	hypothetical protein CGB_C5340C [Cryptococcus gattii WM276]
32	2	NCBIInr	2::gi 405119194	58	34698	9	3	6	3	0.44	aldose reductase [Cryptococcus neoformans var. grubii H99]
33	1	NCBIInr	2::gi 321259223	349	48772	34	20	11	9	2.08	cellulase [Cryptococcus gattii WM276]
34	1	NCBIInr	2::gi 321259373	319	39890	36	16	16	11	2.55	6-phosphogluconolactonase [Cryptococcus gattii WM276]
34	2	NCBIInr	2::gi 405120916	301	34650	25	13	13	9	2.36	6-phosphogluconolactonase [Cryptococcus neoformans var. grubii H99]
35	1	NCBIInr	2::gi 321253449	303	69578	36	16	25	14	1.64	heat shock protein 70 [Cryptococcus gattii WM276]
35	2	NCBIInr	2::gi 58264706	269	69538	35	15	24	13	1.34	heat shock protein 70 [Cryptococcus neoformans var. neoformans JEC21]
35	3	NCBIInr	2::gi 321257093	231	71915	11	6	10	5	0.34	heat shock protein [Cryptococcus gattii WM276]
35	4	NCBIInr	2::gi 121568	91	74459	4	3	3	2	0.12	RecName: Full=78 kDa glucose-regulated protein homolog; Short=GRP-78; Ali
35	5	NCBIInr	2::gi 321265704	85	82556	6	4	6	4	0.23	kar2 karyogamy protein [Cryptococcus gattii WM276]
35	6	NCBIInr	2::gi 255712457	69	70557	6	2	4	2	0.13	KLTH0C06556p [Lachancea thermotolerans]
35	7	NCBIInr	2::gi 134106591	64	72135	6	5	4	4	0.26	hypothetical protein CNBA3060 [Cryptococcus neoformans var. neoformans B-2699]
35	8	NCBIInr	2::gi 599407270	56	67308	6	5	4	4	0.29	hypothetical protein PHACADRAFT_265825 [Phanerochaete carnosae HHB-1011]
36	1	NCBIInr	2::gi 321260961	301	34696	22	11	12	7	1.63	L-malate dehydrogenase [Cryptococcus gattii WM276]
37	1	NCBIInr	2::gi 259120714	256	54004	23	13	13	7	0.87	hexokinase 2 [Cryptococcus gattii]
38	1	NCBIInr	2::gi 321254947	254	80372	48	18	28	15	1.32	catalase A [Cryptococcus gattii WM276]
38	2	NCBIInr	2::gi 109156571	131	80456	34	10	16	7	0.44	catalase 1 [Cryptococcus neoformans]
39	1	NCBIInr	2::gi 321265355	244	26827	21	15	7	6	3.07	hypothetical protein CGB_M3280C [Cryptococcus gattii WM276]
39	2	NCBIInr	2::gi 405123684	138	26927	17	9	5	4	1.17	allergen [Cryptococcus neoformans var. grubii H99]
40	1	NCBIInr	2::gi 321257249	235	33267	23	12	13	7	2.53	fatty acid beta-oxidation-related protein [Cryptococcus gattii WM276]
41	1	NCBIInr	2::gi 321252988	230	38587	20	8	13	5	0.92	zinc-binding dehydrogenase [Cryptococcus gattii WM276]
42	1	NCBIInr	2::gi 321253782	229	64153	13	8	9	5	0.69	hypothetical protein CGB_C5160W [Cryptococcus gattii WM276]
43	1	NCBIInr	2::gi 321261545	228	37514	10	7	6	5	1.19	hypothetical protein CGB_G1660W [Cryptococcus gattii WM276]
43	2	NCBIInr	2::gi 134113809	212	36778	9	6	6	5	0.99	hypothetical protein CNBG1350 [Cryptococcus neoformans var. neoformans B-2699]
44	1	NCBIInr	2::gi 58258849	226	40775	12	7	7	3	0.51	isocitrate dehydrogenase [Cryptococcus neoformans var. neoformans JEC21]
45	1	NCBIInr	2::gi 302907708	219	28241	16	7	6	4	1.44	predicted protein [Nectria haematococca mpVI 77-13-4]
45	2	NCBIInr	2::gi 615413004	189	25535	10	5	5	3	0.93	putative deoxyribose-phosphate aldolase protein [Neofusicoccum parvum UCR]
46	1	NCBIInr	2::gi 321264171	219	31471	14	9	10	7	1.90	hypothetical protein CGB_K3180C [Cryptococcus gattii WM276]
47	1	NCBIInr	2::gi 321254861	218	52235	23	11	16	8	1.07	aminotransferase [Cryptococcus gattii WM276]
47	2	NCBIInr	2::gi 405119067	193	52462	16	9	13	7	0.90	4-aminobutyrate transaminase [Cryptococcus neoformans var. grubii H99]
48	1	NCBIInr	2::gi 58258141	217	26155	20	8	9	5	1.61	hypothetical protein CNA00560 [Cryptococcus neoformans var. neoformans B-2699]

Mascot search results report - ions score cutoff 0.05, no FDR adjustment

Protein sequence coverage: 25% **25% coverage**
 Matched peptides shown in **bold red**.

1 MNFFDIRK**QI EPYFVLNDEK LVDIVK**HFRK EMEEGLANYG **KDMAMIP**TFV
 51 **TGVPD**GTEEG **VFLALDLGGT NLRVCLIVLQ GNNQFK**IEQQ KYKVSEELKT
 101 GQARVLFDYI AESVDN**FLTE VENHSDVAIP VTSEPLHLGF TFSFP**VEQTA
 151 IDAGKLLTWT KGFN**TKNAIG HDVVRLQDA FDRKHM**HVRC **SALVND**TVGT
 201 **LLSR**SYQSGP **ALIGAI**FGTG **TNGAYID**KSR TISKLGKEKI EEAERKGEHA
 251 GKYMVNT**EW GAFDNKRLCL PVS**LFDNKLD RESINPRQM FEK**MVSG**MYL
 301 **GEIT**RNILLY LIDSSLLFEG HSSEVLN**THY GFDTS**FSVSGI EGITSPEEVT
 351 QLI**IKEL**KVD PKHITDK**CE IVQ**WTVRMVA DRACKLAACA IAAIVLHTGN
 401 DKA**PEGE**KDK GVDVGV**DGSV AQ**FLPMFNER VMAGLKAILG ERGAARVNI
 451 LAKDGS**GVGA ALTALQAKKA LDQR**SDRSTP YVPGKRAP

Unformatted sequence string: [488 residues](#) (for pasting into other applications).

Sort peptides by Residue Number Increasing Mass Decreasing Mass

Show predicted peptides also

Query	Start - End	Observed	Mr (expt)	Mr (calc)	ppm	M	Score	Expect	Rank	U	Peptide
5902	9 - 26	721.3964	2161.1673	2161.1671	0.13	1	37	0.0068	1	U	K.QIEPYFVLNDEKLVDIVK.H
7636	42 - 73	1123.5515	3367.6327	3367.6316	0.31	0	39	0.0079	1	U	K.DMAMIPFVTGVPDGT EEGVFLALDLGGT NLR.V + 2 Oxidation (M)
7637	42 - 73	1123.8851	3368.6335	3367.6316	297	0	41	0.0077	1	U	K.DMAMIPFVTGVPDGT EEGVFLALDLGGT NLR.V + 2 Oxidation (M)
4184	74 - 86	766.9161	1531.8175	1531.8181	-0.35	0	66	0.00093	1	U	R.VCLIVLQ GNNQFK.I
4467	190 - 204	803.4171	1604.8195	1604.8192	0.21	0	100	1.8e-007	1	U	R.CSALVND TVGTLLSR.S
6396	205 - 228	801.4020	2401.1841	2401.1801	1.64	0	59	0.008	1	U	R.SYQSGPALIGAI FGTG TNGAYIDK.S + Deamidated (NQ)
6397	205 - 228	1201.6023	2401.1900	2401.1801	4.12	0	96	1.3e-006	1	U	R.SYQSGPALIGAI FGTG TNGAYIDK.S + Deamidated (NQ)
6398	205 - 228	801.4061	2401.1965	2401.1801	6.81	0	57	0.00016	1	U	R.SYQSGPALIGAI FGTG TNGAYIDK.S + Deamidated (NQ)
3395	268 - 278	653.3463	1304.6781	1304.6799	-1.35	0	55	0.022	1	U	R.LCLPV SLFDNK.L
3654	294 - 305	686.8336	1371.6526	1371.6526	-0.059	0	53	0.026	1	U	K.MVSGMYL GEITR.N + Oxidation (M)
3655	294 - 305	686.8346	1371.6547	1371.6526	1.50	0	71	0.00037	1	U	K.MVSGMYL GEITR.N + Oxidation (M)
3712	294 - 305	694.8292	1387.6439	1387.6476	-2.67	0	39	0.031	1	U	K.MVSGMYL GEITR.N + 2 Oxidation (M)
3713	294 - 305	694.8306	1387.6467	1387.6476	-0.63	0	50	0.041	1	U	K.MVSGMYL GEITR.N + 2 Oxidation (M)

Protein family 37
 hexokinase 2 [Cryptococcus gattii WM276]

Score 256
 Matches 13
 Match(sig) 13
 Sequences 7
 Seq(sig) 7
 eMPAI 0.87

Score	Expect	Rank	U	Peptide
37	0.0068	1	U	K.QIEPYFVLNDEKLVDIVK.H
39	0.0079	1	U	K.DMAMIPFVTGVPDGT EEGVFLALDLGGT NLR.V + 2 Oxidation (M)
41	0.0077	1	U	K.DMAMIPFVTGVPDGT EEGVFLALDLGGT NLR.V + 2 Oxidation (M)
66	0.00093	1	U	R.VCLIVLQ GNNQFK.I
100	1.8e-007	1	U	R.CSALVND TVGTLLSR.S
59	0.008	1	U	R.SYQSGPALIGAI FGTG TNGAYIDK.S + Deamidated (NQ)
96	1.3e-006	1	U	R.SYQSGPALIGAI FGTG TNGAYIDK.S + Deamidated (NQ)
57	0.00016	1	U	R.SYQSGPALIGAI FGTG TNGAYIDK.S + Deamidated (NQ)

Mascot search results report - FDR adjustment

MATRIX SCIENCE MASCOT Search Results

User : stweintraub
E-mail : weintraub@uthscsa.edu
Search title : Wormley Chaturvedi M1415-058 150130FLW32_F3.raw (NCBIInr_fungi; contam) trypsin-1 Ox(M) Carb(C) D(NQ) decoy (Wormley Chaturvedi M1415-058 265 D, slice F3, Sul, D8)
Databases : **1:** contaminants 20120713 (247 sequences; 128,130 residues)
2: NCBIInr 20140522 (39,649,990 sequences; 14,178,194,136 residues)
Taxonomy : **1:** (none)
2: Fungi (2,653,696 sequences)
Timestamp : 15 May 2015 at 19:07:55 GMT

Re-search | All | Non-significant | Unassigned | [help] | Export As XML

Not what you expected? Try [the select summary](#).

Search parameters
Score distribution
Modification statistics
Legend

Protein Family Summary

Filter | Significance threshold p< 0.05 | Max. number of families AUTO | [help]
Ions score or expect cut-off 0 | Dendrograms cut at 0
Show Percolator scores
Preferred taxonomy All entries

Decoy search summary (reversed protein sequences)

Peptide matches	in target	in Decoy	FDR
- above identity threshold	1263	26	2.06%
- above identity or homology threshold	1808	76	4.20%

Adjust to 1%

Adjust FDR to 1% (or other desired value)

Mascot search results report - FDR adjustment

MASCOT Search Results

User : stweintraub
E-mail : weintraub@uthscsa.edu
Search title : Wormley Chaturvedi M1415-058 15013
Databases : 1: contaminants 20120713 (247 sequences)
2: NCBIInr 20140522 (39,649,990 sequences)
Taxonomy : 1: (none)
2: Fungi (2,653,696 sequences)
Timestamp : 15 May 2015 at 19:07:55 GMT

Significance threshold altered by Mascot to value needed to achieve 1% FDR

Filter

Significance threshold p < 0.0122

Ions score or expect cut-off 0

Show Percolator scores

Preferred taxonomy All entries

Decoy search summary (reversed protein sequences)

Peptide matches	in target	in Decoy	FDR
- above identity threshold	961	6	0.62%
- above identity or homology threshold	1384	13	0.94%

Adjust to 1% *

Protein hits (377 protein)

Columns: Standard (12 out of 16)

Filters: (none)

Mascot search results report - FDR adjustment

MATRIX SCIENCE MASCOT Search Results

User : stweintraub
E-mail : weintraub@uthscsa.edu
Search title : Wormley Chaturvedi M1415-058 1...
Databases : 1: contaminants
2: NCBInr 20140...
Taxonomy : 1: (none)
2: Fungi (2,653,3...
Timestamp : 15 May 2015 at 10:00:00 AM (GMT-05:00) (Wormley Chaturvedi M1415-058 265 D, slice F3, Sul, D8)

Re-search All Non-significant Unassigned [help] Export As XML

Not what you expected? Try [the select summary](#).

Search parameters
Score distribution
Modification statistics
Legend

Protein Family Summary

Filter Significance threshold p< 0.0122 Max. number of families AUTO [help]
Ions score or expect cut-off 0 Dendrograms cut at 0
Show Percolator scores
Preferred taxonomy All entries

Decoy search summary (reversed protein sequences)

Peptide matches	in target	in Decoy	FDR
- above identity threshold	961	6	0.62%
- above identity or homology threshold	1384	13	0.94%

Adjust to 1% *

Protein hits (377 protein...)
Columns: Standard (12 out of 16)
Filters: (none)

Mascot search results report - FDR adjustment

MASCOT Search Results

User : stweintraub
E-mail : weintraub@uthscsa.edu
Search title : Wormley Chaturvedi M1415-058 1...
Databases : 1: contaminants
2: NCBInr 20140101
Taxonomy : 1: (none)
2: Fungi (2,653,100)
Timestamp : 15 May 2015 at 10:00:00 AM (GMT-5:00) (slice F3, Sul, D8)

Re-search All Non-significant Unassigned [help] Export As XML

Not what you expected? Try [the select summary](#).

Protein Family Summary

Filter Significance threshold p< 0.0122 Max. number of families AUTO [help]
Ions score or expect cut-off 0.05 Dendrograms cut at 0
Show Percolator scores
Preferred taxonomy All entries

Decoy search summary (reversed protein sequences)

Peptide matches	in target	in Decoy	FDR
- above identity threshold	961	6	0.62%
- above identity or homology threshold	1384	13	0.94%

Adjust to 1% *

Protein hits (377 proteins)
Columns: Standard (12 out of 16)
Filters: (none)

Influence of Mascot significance and FDR settings

Hexokinase 2 [Cryptococcus gattii] gi|259120714

Significance Threshold	ions score cutoff	FDR (%)	Score	Matches	Significant Matches	Significant Sequences	Significant Sequences
0.05	0	(4.2)	256	23	13	13	7
0.05	0.05	(4.2)	256	13	13	7	7
0.0122	0	0.94	194	23	9	13	6
0.0122	0.05	0.94	194	13	9	7	6

Mascot results spreadsheet generation

Search parameters

Score distribution

Modification statistics

Legend

Protein Family Summary

Filter Significance threshold p < 0.0122 Max. number of families AUTO [help]

Ions score or expect cut-off 0.05 Dendrograms cut at 0

Show Percolator scores

Preferred taxonomy All entries

Decoy search summary (reversed protein sequences)

Peptide matches	in target	in Decoy	FDR
- above identity threshold	961	6	0.62%
- above identity or homology threshold	1384	13	0.94%

Adjust to 1%

Protein hits (377 proteins)

Columns: Standard (12 out of 16)

Filters: (none)

Export as CSV

Family	M	DB	Accession	Score	Mass	Matches	Match(sig)	Sequences	Seq(sig)	emPAI	Description
1	1	NCBIInr	2:::gj 58261082	899	29090	58	46	17	14	22.81	14-3-3 protein [Cryptococcus neoformans var. neoformans JEC21]
1	2	NCBIInr	2:::gj 62420901	460	28911	30	26	9	9	7.83	14-3-3 1 protein [Phanerochaete chrysosporium]
1	3	NCBIInr	2:::gj 521773918	350	30146	27	21	7	6	4.29	hypothetical protein BGT96224_929 [Blumeria graminis f. sp. tritici 96224]
1	4	NCBIInr	2:::gj 1040756	92	30471	8	6	4	3	0.99	rad24 [Schizosaccharomyces pombe]
2	1	NCBIInr	2:::gj 321265283	533	85793	28	25	20	19	1.82	heat shock protein [Cryptococcus gattii WM276]
2	2	NCBIInr	2:::gj 405123671	381	85923	20	17	14	13	0.99	heat shock 70kDa protein 4 [Cryptococcus neoformans var. grubii H99]
2	3	NCBIInr	2:::gj 597927424	156	85983	5	4	4	4	0.22	hypothetical protein SERLADRAFT_355892 [Serpula lacrymans var. lacrymans S...]

Mascot results spreadsheet generation

Mascot search engine | Protei... x Wormley Chaturvedi M1415-058 1... x

vprmascot.win.uthtcsa.edu/mascot/cgi/master_results_2.pl?file=.%2Fdata%2F20150515%2F035682.dat;_ignoreionsscorebelow=0.05;_prefertaxonomy=0;_sigthreshold=0.012201;percolate=0;pr.show=repor

Proteins (318) | Report Builder | Unassigned (6321) | [s permalink](#)

Protein hits (377 proteins)

▼Columns: Standard (12 out of 16)

Arrangement: <custom>

Enabled

- Family
- Member
- Database
- Accession
- Score
- Mass
- Num. of matches
- Num. of significant matches
- Num. of sequences
- Num. of significant sequences
- emPAI
- Description

Available

Protein hits

- Num. of unique sequences
- Num. of significant unique sequences
- Sequence coverage
- pl

►Filters: (none)

Family	M	DB	Accession	Score	Mass	Matches	Match(sig)	Sequences	Seq(sig)	emPAI	Description
1	1	NCBIInr	2:::gj 58261082	899	29090	58	46	17	14	22.81	14-3-3 protein [Cryptococcus neoformans var. neoformans JEC21]
1	2	NCBIInr	2:::gj 62420901	460	28911	30	26	9	9	7.83	14-3-3 1 protein [Phanerochaete chrysosporium]
1	3	NCBIInr	2:::gj 521773918	350	30146	27	21	7	6	4.29	hypothetical protein BGT96224_929 [Blumeria graminis f. sp. tritici 96224]
1	4	NCBIInr	2:::gj 1040756	92	30471	8	6	4	3	0.99	rad24 [Schizosaccharomyces pombe]
2	1	NCBIInr	2:::gj 321265283	533	85793	28	25	20	19	1.82	heat shock protein [Cryptococcus gattii WM276]
2	2	NCBIInr	2:::gj 405123671	381	85923	20	17	14	13	0.99	heat shock 70kDa protein 4 [Cryptococcus neoformans var. grubii H99]

Select "<custom>"

Enable/disable columns for report

Mascot results spreadsheet generation

▼ **Columns: Standard (12 out of 16)**

Arrangement: <custom>

Enabled

Family
Member
Database
Accession
Score
Mass
Num. of matches
Num. of significant matches
Num. of sequences
Num. of significant sequences
emPAI
Description

Available

Protein hits
Num. of unique sequences
Num. of significant unique sequences
Sequence coverage
pI

Enable/disable columns for report

▼ **Filters: (none)**

Family	M	DB									
1	1	NCBIr									
1	2	NCBIr									
1	3	NCBIr									
1	4	NCBIr									
2	1	NCBIr	2::gi 321265283	533	85793	28	25	20	19	1.82	heat shock protein [Cryptococcus gattii WM276]
2	2	NCBIr	2::gi 405123671	381	85923	20	17	14	13	0.99	heat shock 70kDa protein 4 [Cryptococcus neoformans var. grubii H99]

Mascot results spreadsheet generation

▼ **Columns (15 out of 16)**

Arrangement: <custom>

Enabled

- Family
- Member
- Database
- Accession
- Score
- Mass
- Num. of matches
- Num. of significant matches
- Num. of sequences
- Num. of significant sequences
- Num. of unique sequences
- Num. of significant unique sequences
- Sequence coverage
- emPAI
- Description

Available

Protein hits

pl

Filters: (none)

Family	M	DB	Length	Score	Mass	Num. of matches	Num. of significant matches	Num. of sequences	Num. of significant sequences	Num. of unique sequences	Num. of significant unique sequences	Sequence coverage	emPAI	Description
1	1	NCBI	1040756	92	30471	8	6	4	3	1	1	0.18	0.99	rad24 [Schizosaccharomyces pombe]

Export as CSV

Mascot results spreadsheet

Move search parameter list to a separate worksheet.

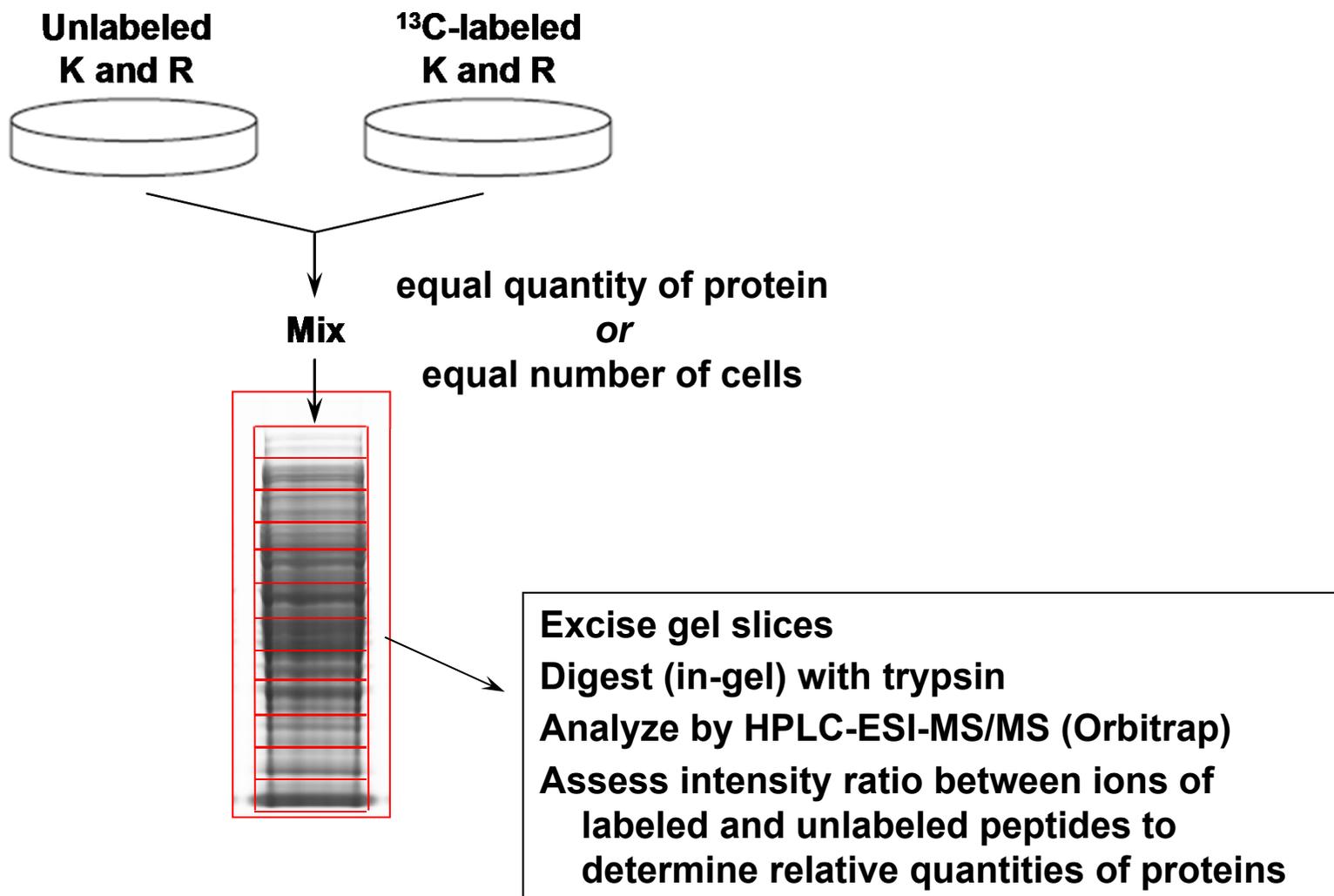
**Adjust column width as needed.
Re-format/abbreviate column headings for readability.
Use appropriate numbers of decimal points.**

Family	Member	Database	Accession	Score	Mass	Num. of r	Num. of s	Num. of s	Num. of s	Num. of u	Num. of s	Sequence	emPAI	Description
1	1	NCBI	gi1582610	899	29090	58	46	17	14	6	4	0.66	22.81	14-3-3 protein [Cryptococcus neoformans var. neoformans JEC21]
1	2	NCBI	gi1624209	460	28911	30	26	9	9	1	1	0.38	7.83	14-3-3 1 protein [Phanerochaete chrysosporium]
1	3	NCBI	gi1521773	350	30146	27	21	7	6	1	1	0.26	4.29	hypothetical protein BGT96224_929 [Blumeria graminis f. sp. tritici 96224]
1	4	NCBI	gi1104075	92	30471	8	6	4	3	1	1	0.18	0.99	rad24 [Schizosaccharomyces pombe]
2	1	NCBI	gi1321265	533	85793	28	25	20	19	7	7	0.43	1.82	heat shock protein [Cryptococcus gattii WM276]
2	2	NCBI	gi1405123	381	85923	20	17	14	13	1	1	0.25	0.99	heat shock 70kDa protein 4 [Cryptococcus neoformans var. grubii H99]
2	3	NCBI	gi1597927	156	85983	5	4	4	4	1	1	0.05	0.22	hypothetical protein SERLADRAFT_355892 [Serpula lacrymans var. lacrymans S7.9]
2	4	NCBI	gi1401889	118	104205	2	2	2	2	1	1	0.03	0.08	heat shock protein [Trichosporon asahii var. asahii CBS 2479]
3	1	NCBI	gi1582644	485	47854	20	17	13	11	13	11	0.4	1.88	phosphopyruvate hydratase [Cryptococcus neoformans var. neoformans JEC21]
3	4	NCBI	gi1321260	483	58664	24	20	18	15	2	2	0.51	2.65	ATP synthase beta chain, mitochondrial precursor [Cryptococcus gattii WM276]
4	2	NCBI	gi1589285	481	58967	23	19	17	14	1	1	0.49	2.38	hypothetical protein TREMEDRAFT_41300 [Tremella mesenterica DSM 1558]
4	4	NCBI	gi1911781	178	35771	6	6	5	5	1	1	0.22	1.02	mitochondrial F-ATPase beta subunit, partial [Candida rugosa]

Give worksheets informative names.

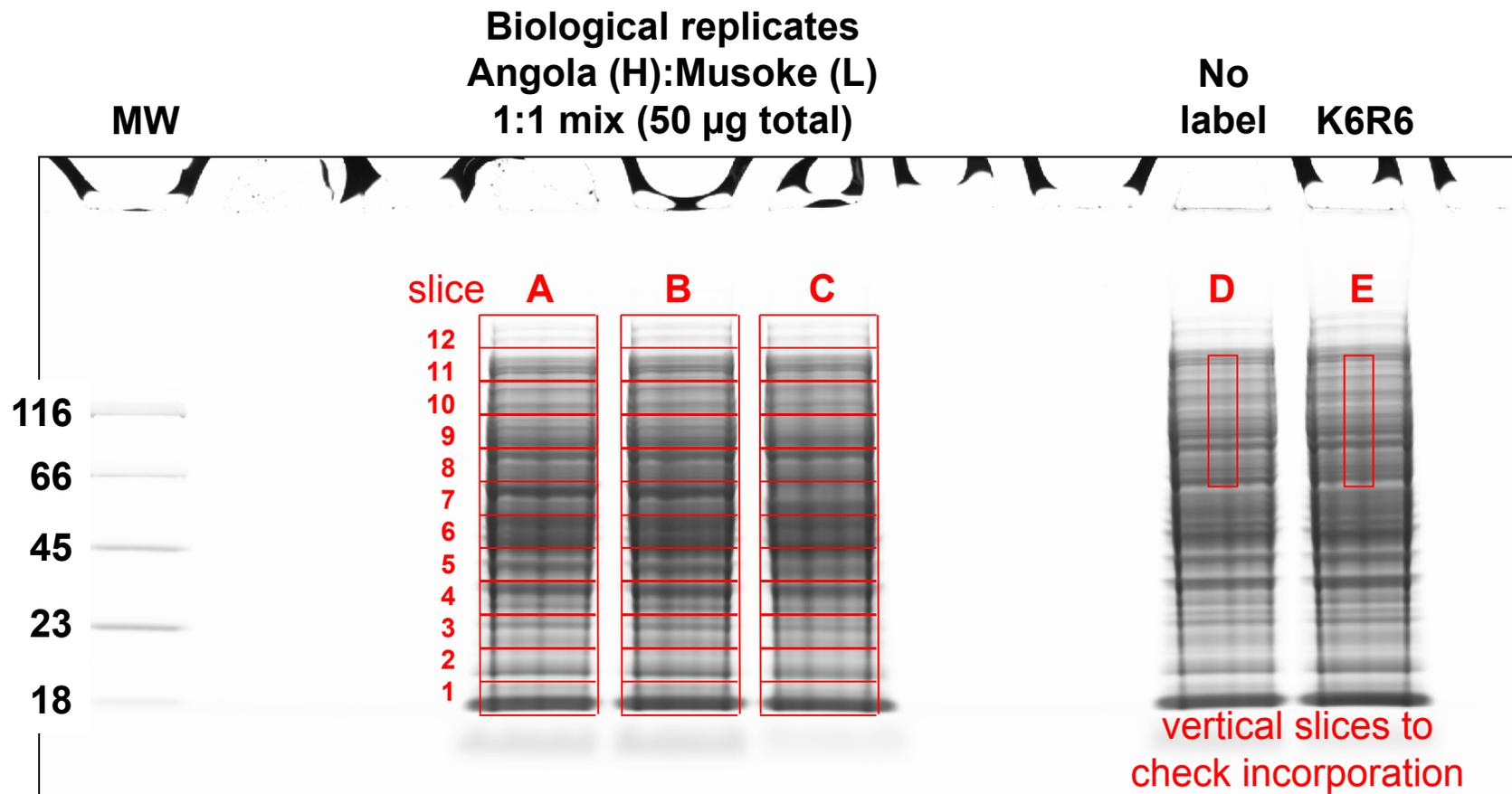
Database column can be deleted if only one database was used.

Differential expression analysis using SILAC (Stable Isotope Labeling with Amino Acids in Cell Culture)



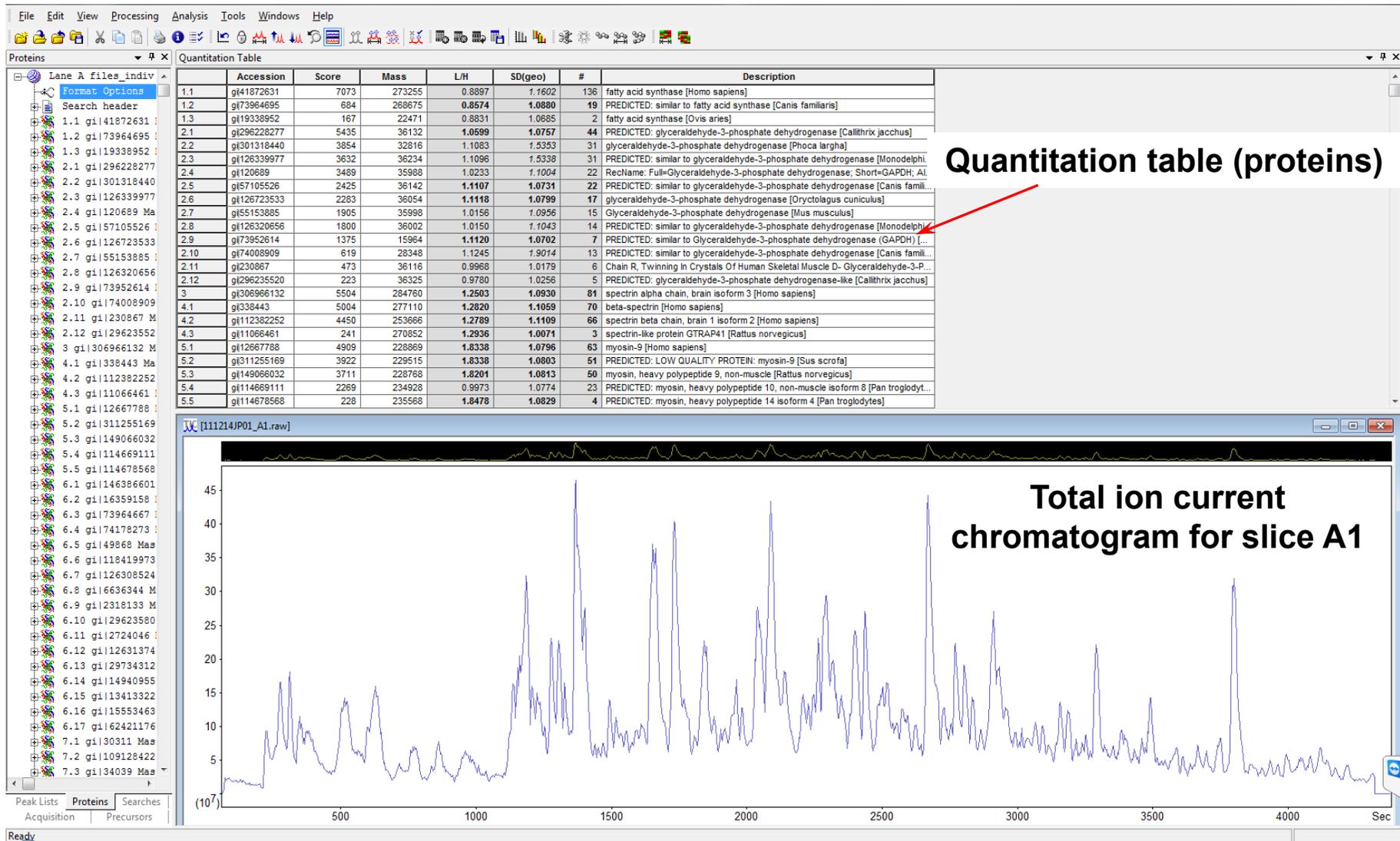
Assessment of differences in protein expression of human cells infected with Marburg viruses using SILAC

Lethality: Marburg virus-Angola (MARV-Ang) > Marburg virus-Musoke (MARV-Mus)



BioRad Criterion XT MOPS 12% SDS-PAGE reducing gel, “blue silver” stain

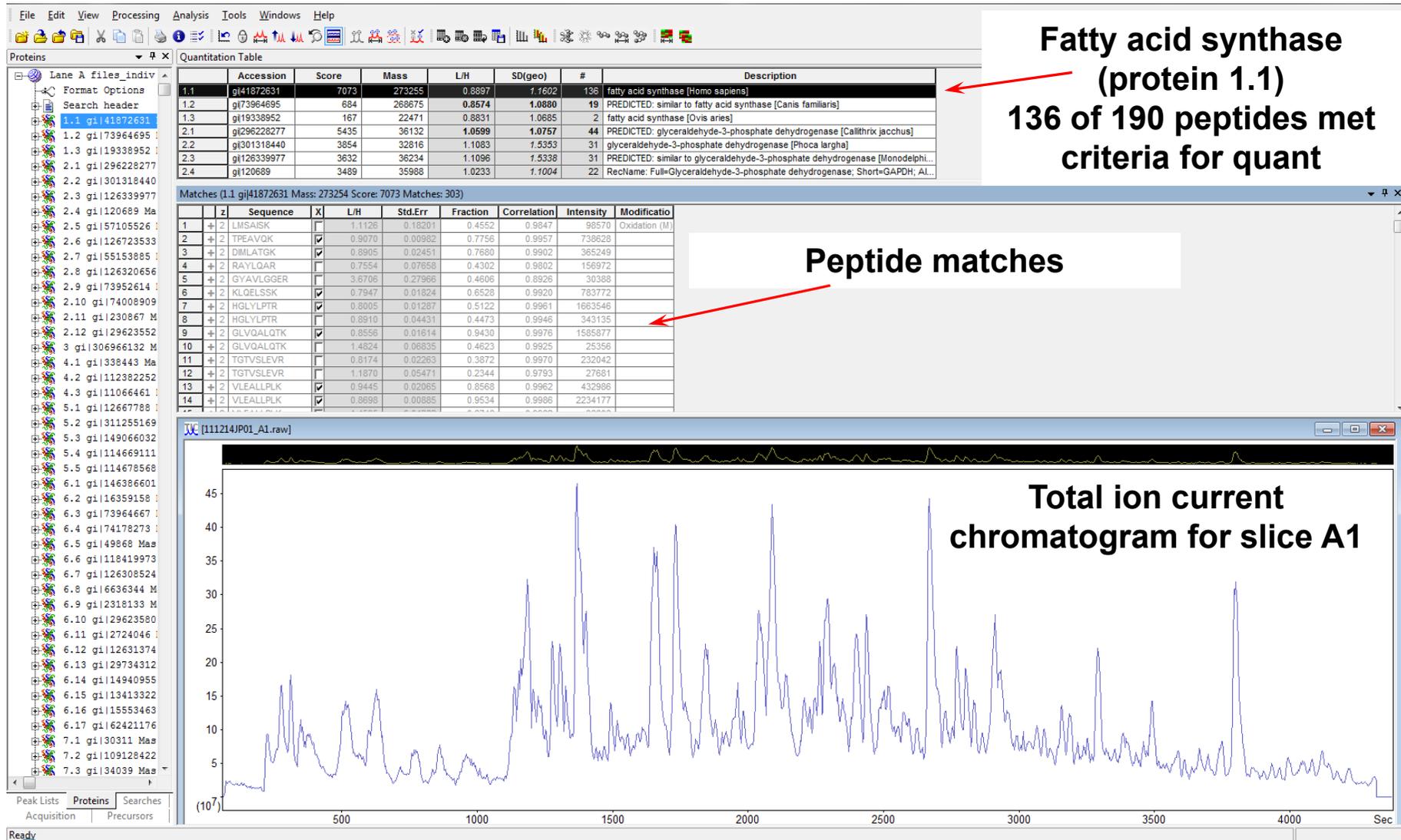
Mascot Distiller results



Quantitation table (proteins)

	L/H	SD(geo)	#	Description
1.1	0.8897	1.1602	136	fatty acid synthase [Homo sapiens]
1.2	0.8574	1.0880	19	PREDICTED: similar to fatty acid synthase [Canis familiaris]
1.3	0.8831	1.0685	2	fatty acid synthase [Ovis aries]
2.1	1.0599	1.0757	44	PREDICTED: glyceraldehyde-3-phosphate dehydrogenase [Callithrix jacchus]
2.2	1.1083	1.5353	31	glyceraldehyde-3-phosphate dehydrogenase [Phoca largha]
2.3	1.1096	1.5338	31	PREDICTED: similar to glyceraldehyde-3-phosphate dehydrogenase [Monodelphi...
2.4	1.0233	1.1004	22	RecName: Full=Glyceraldehyde-3-phosphate dehydrogenase; Short=GAPDH; Al...
2.5	1.1107	1.0731	22	PREDICTED: similar to glyceraldehyde-3-phosphate dehydrogenase [Canis famili...
2.6	1.1118	1.0799	17	glyceraldehyde-3-phosphate dehydrogenase [Oryctolagus cuniculus]
2.7	1.0156	1.0956	15	Glyceraldehyde-3-phosphate dehydrogenase [Mus musculus]
2.8	1.0150	1.1043	14	PREDICTED: similar to glyceraldehyde-3-phosphate dehydrogenase [Monodelphi...
2.9	1.1120	1.0702	7	PREDICTED: similar to Glyceraldehyde-3-phosphate dehydrogenase (GAPDH) [...
2.10	1.1245	1.9014	13	PREDICTED: similar to glyceraldehyde-3-phosphate dehydrogenase [Canis famili...
2.11	0.9968	1.0179	6	Chain R, Twinning In Crystals Of Human Skeletal Muscle D- Glyceraldehyde-3-P...
2.12	0.9780	1.0256	5	PREDICTED: glyceraldehyde-3-phosphate dehydrogenase-like [Callithrix jacchus]
3	1.2503	1.0930	81	spectrin alpha chain, brain isoform 3 [Homo sapiens]
4.1	1.2820	1.1059	70	beta-spectrin [Homo sapiens]
4.2	1.2789	1.1109	66	spectrin beta chain, brain 1 isoform 2 [Homo sapiens]
4.3	1.2936	1.0071	3	spectrin-like protein GTRAP41 [Rattus norvegicus]
5.1	1.8338	1.0796	63	myosin-9 [Homo sapiens]
5.2	1.8338	1.0803	51	PREDICTED: LOW QUALITY PROTEIN: myosin-9 [Sus scrofa]
5.3	1.8201	1.0813	50	myosin, heavy polypeptide 9, non-muscle [Rattus norvegicus]
5.4	0.9973	1.0774	23	PREDICTED: myosin, heavy polypeptide 10, non-muscle isoform 8 [Pan troglodyt...
5.5	1.8478	1.0829	4	PREDICTED: myosin, heavy polypeptide 14 isoform 4 [Pan troglodytes]

Mascot Distiller results



**Fatty acid synthase
(protein 1.1)
136 of 190 peptides met
criteria for quant**

Peptide matches

**Total ion current
chromatogram for slice A1**

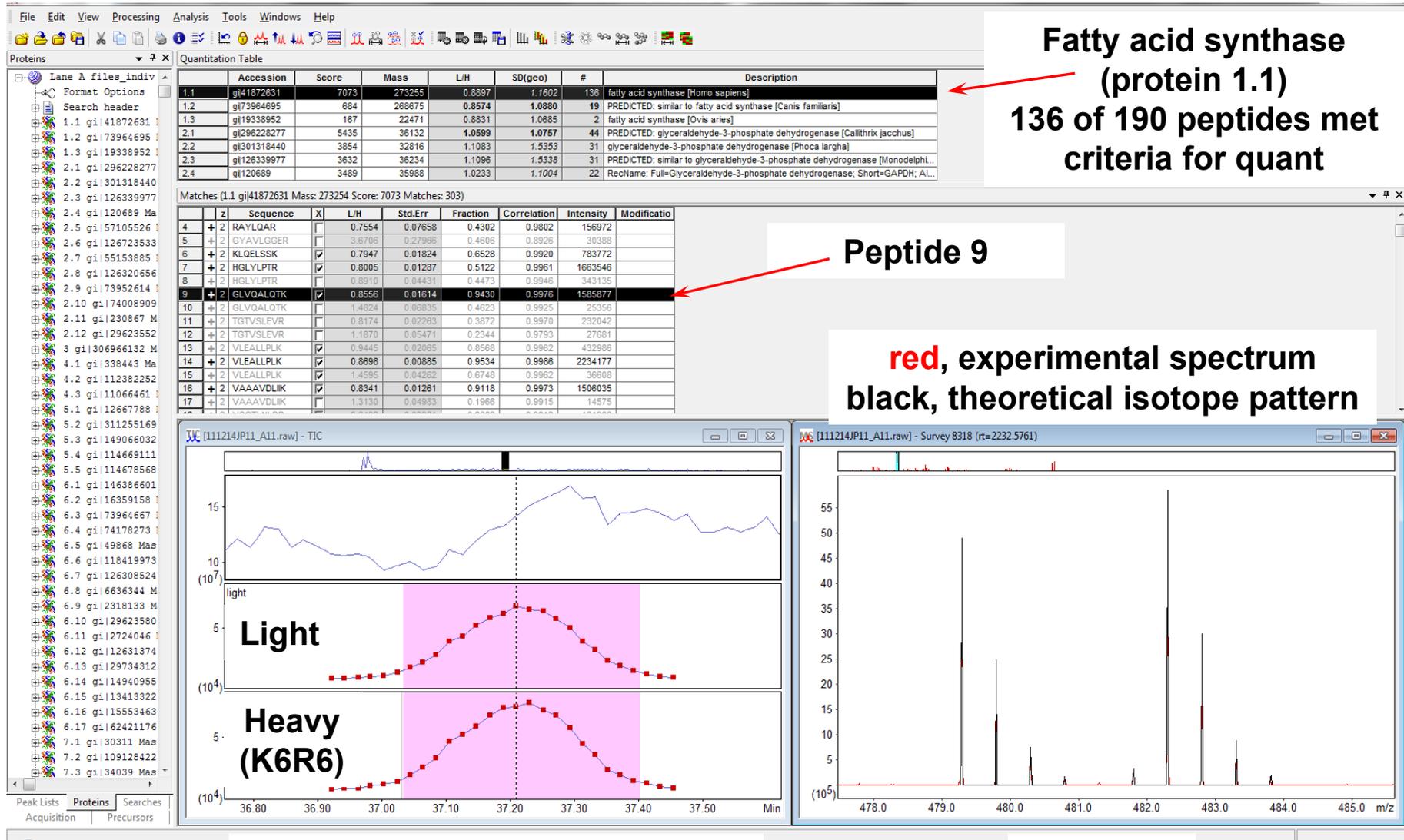
Peptide matches: fatty acid synthase (protein 1.1)

		z	Sequence	X	L/H	Std.Err	Fraction	Correlation	Intensity	Modification
1	+	2	LMSAISK	<input type="checkbox"/>	1.1126	0.18201	0.4552	0.9847	98570	Oxidation (M)
2	+	2	TPEAVQK	<input checked="" type="checkbox"/>	0.9070	0.00982	0.7756	0.9957	738628	
3	+	2	DIMLATGK	<input checked="" type="checkbox"/>	0.8905	0.02451	0.7680	0.9902	365249	
4	+	2	RAYLQAR	<input type="checkbox"/>	0.7554	0.07658	0.4302	0.9802	156972	
5	+	2	GYAVLGGER	<input type="checkbox"/>	3.6706	0.27966	0.4606	0.8926	30388	
6	+	2	KLQELSSK	<input checked="" type="checkbox"/>	0.7947	0.01824	0.6528	0.9920	783772	
7	+	2	HGLYLPTR	<input checked="" type="checkbox"/>	0.8005	0.01287	0.5122	0.9961	1663546	
8	+	2	HGLYLPTR	<input type="checkbox"/>	0.8910	0.04431	0.4473	0.9946	343135	
9	+	2	GLVQALQTK	<input checked="" type="checkbox"/>	0.8556	0.01614	0.9430	0.9976	1585877	
10	+	2	GLVQALQTK	<input type="checkbox"/>	1.4824	0.06835	0.4623	0.9925	25356	
11	+	2	TGTVSLEVR	<input type="checkbox"/>	0.8174	0.02263	0.3872	0.9970	232042	
12	+	2	TGTVSLEVR	<input type="checkbox"/>	1.1870	0.05471	0.2344	0.9793	27681	
13	+	2	VLEALLPLK	<input checked="" type="checkbox"/>	0.9445	0.02065	0.8568	0.9962	432986	
14	+	2	VLEALLPLK	<input checked="" type="checkbox"/>	0.8698	0.00885	0.9534	0.9986	2234177	
15	+	2	VLEALLPLK	<input type="checkbox"/>	1.1555	0.01888	0.8718	0.9988	88888	

Peptide matches: fatty acid synthase (protein 1.1)

		z	Sequence	X	L/H	Std.Err	Fraction	Correlation	Intensity	Modificatio
4	+	2	RAYLQAR	<input type="checkbox"/>	0.7554	0.07658	0.4302	0.9802	156972	
5	+	2	GYAVLGGER	<input type="checkbox"/>	3.6706	0.27966	0.4606	0.8926	30388	
6	+	2	KLQELSSK	<input checked="" type="checkbox"/>	0.7947	0.01824	0.6528	0.9920	783772	
7	+	2	HGLYLPTK	<input checked="" type="checkbox"/>	0.8005	0.01287	0.5122	0.9961	1663546	
8	+	2	HGLYLPTK	<input type="checkbox"/>	0.8910	0.04431	0.4473	0.9946	343135	
9	+	2	GLVQALQTK	<input checked="" type="checkbox"/>	0.8556	0.01614	0.9430	0.9976	1585877	
10	+	2	GLVQALQTK	<input type="checkbox"/>	1.4824	0.06835	0.4623	0.9925	25356	
11	+	2	TGTVSLEVR	<input type="checkbox"/>	0.8174	0.02263	0.3872	0.9970	232042	
12	+	2	TGTVSLEVR	<input type="checkbox"/>	1.1870	0.05471	0.2344	0.9793	27681	
13	+	2	VLEALLPLK	<input checked="" type="checkbox"/>	0.9445	0.02065	0.8568	0.9962	432986	
14	+	2	VLEALLPLK	<input checked="" type="checkbox"/>	0.8698	0.00885	0.9534	0.9986	2234177	
15	+	2	VLEALLPLK	<input checked="" type="checkbox"/>	1.4595	0.04262	0.6748	0.9962	36608	
16	+	2	VAAAVDLIK	<input checked="" type="checkbox"/>	0.8341	0.01261	0.9118	0.9973	1506035	
17	+	2	VAAAVDLIK	<input type="checkbox"/>	1.3130	0.04983	0.1966	0.9915	14575	
18	+	2	VAAAVDLIK	<input type="checkbox"/>	0.8100	0.02000	0.8000	0.9910	101000	

Mascot Distiller results



Mascot Distiller results

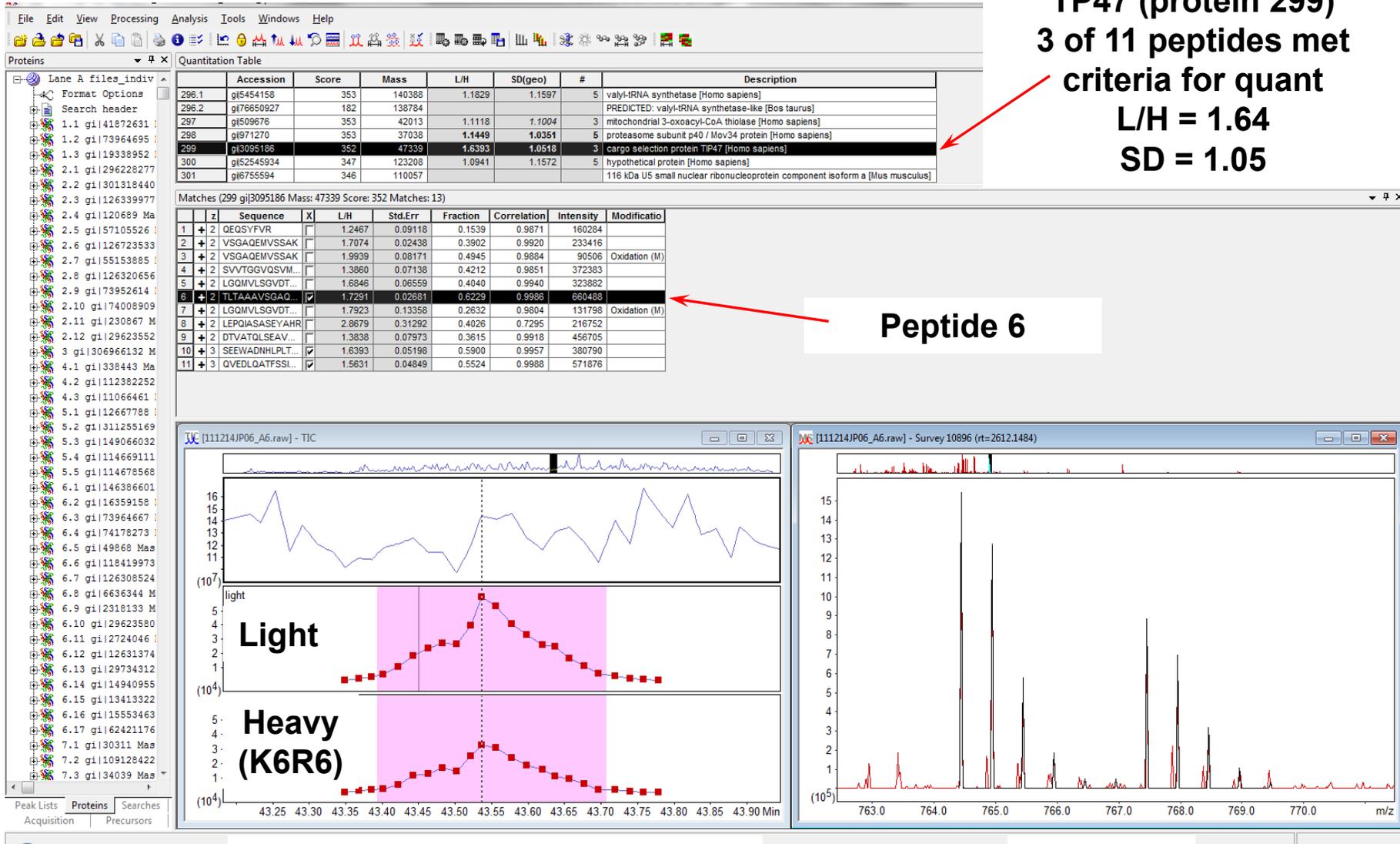
Cargo selection protein
TP47 (protein 299)

3 of 11 peptides met

criteria for quant

L/H = 1.64

SD = 1.05



Extracted ion chromatograms

[M+2H]²⁺

Mascot Distiller results

Cargo selection protein
TP47 (protein 299)

3 of 11 peptides met

criteria for quant

L/H = 1.64

SD = 1.05

The screenshot shows the Mascot Distiller interface. The top window displays a list of proteins with columns for Accession, Score, Mass, L/H, SD(geo), #, and Description. Protein 299, 'cargo selection protein TP47 [Homo sapiens]', is highlighted. Below this, a 'Matches' window shows a list of 11 peptides with columns for z, Sequence, X, L/H, Std.Err, Fraction, Correlation, Intensity, and Modification. Peptides 6, 10, and 11 are highlighted in red in the summary table, corresponding to the L/H values of 1.73, 1.64, and 1.56 respectively.

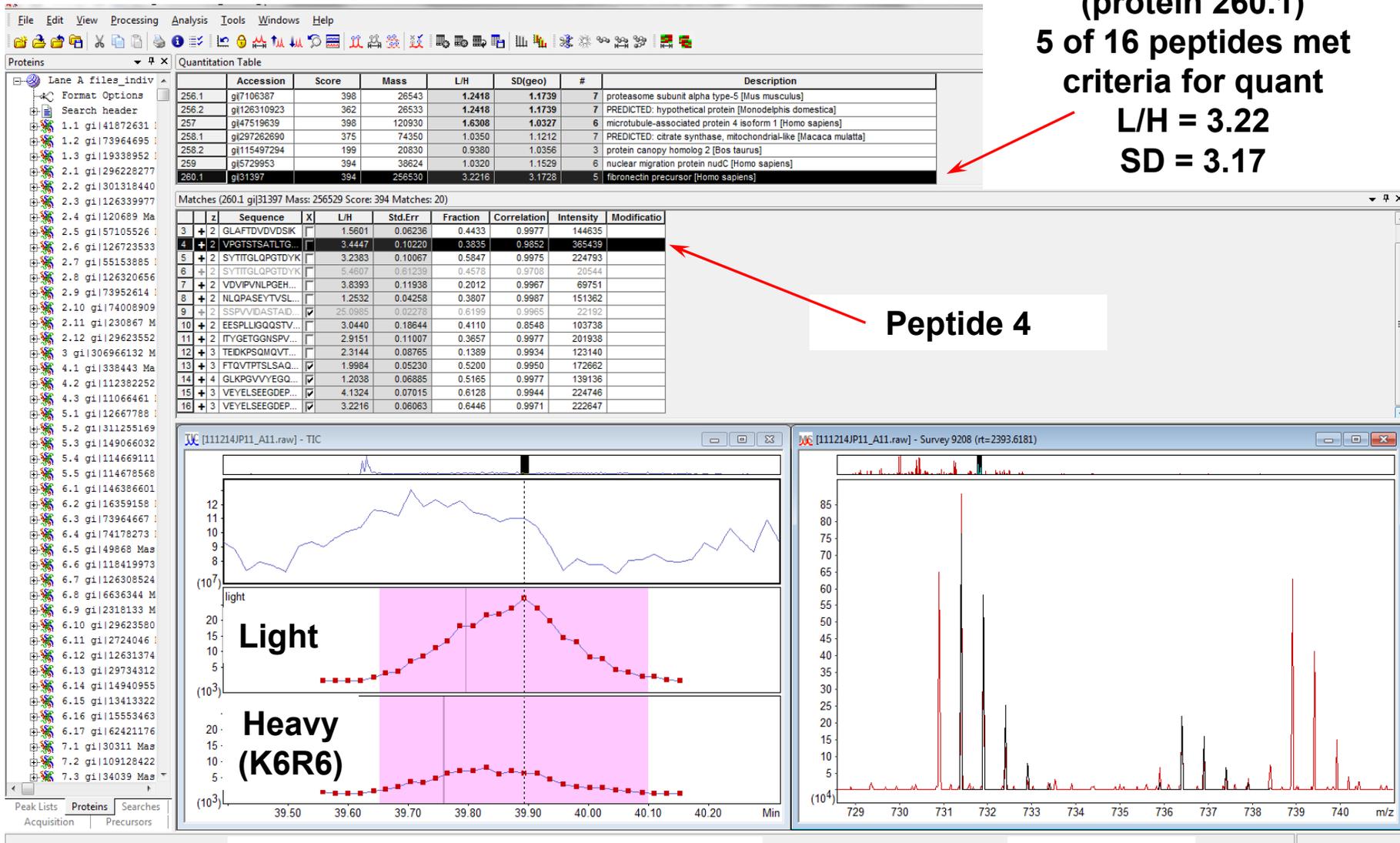
Accession	Score	Mass	L/H	SD(geo)	#	Description
296.1 gi 5454158	353	140388	1.1829	1.1597	5	valyl-tRNA synthetase [Homo sapiens]
296.2 gi 76650927	182	138784				PREDICTED: valyl-tRNA synthetase-like [Bos taurus]
297 gi 509676	353	42013	1.1118	1.1004	3	mitochondrial 3-oxoacyl-CoA thiolase [Homo sapiens]
298 gi 971270	353	37038	1.1449	1.0351	5	proteasome subunit p40 / Mov34 protein [Homo sapiens]
299 gi 3095186	352	47339	1.6393	1.0518	3	cargo selection protein TP47 [Homo sapiens]
300 gi 52545934	347	123208	1.0941	1.1572	5	hypothetical protein [Homo sapiens]
301 gi 6755594	346	110057				116 kDa U5 small nuclear ribonucleoprotein component isoform a [Mus musculus]

z	Sequence	X	L/H	Std.Err	Fraction	Correlation	Intensity	Modification
1	+2 QEQSYFVR		1.2467	0.09118	0.1539	0.9871	160284	
2	+2 VSGAQEMVSSAK		1.7074	0.02438	0.3902	0.9920	233416	
3	+2 VSGAQEMVSSAK		1.9939	0.08171	0.4945	0.9884	90506	Oxidation (M)
4	+2 SVVTGGVQSVML		1.3860	0.07138	0.4212	0.9851	372383	
5	+2 LGQMVLGVDL...		1.6846	0.06559	0.4040	0.9940	323882	
6	+2 TLTAADVSGAQ...		1.7291	0.02681	0.6229	0.9988	680488	
7	+2 LGQMVLGVDL...		1.7923	0.13358	0.2832	0.9804	131798	Oxidation (M)
8	+2 LEPQIASASEYADR		2.8679	0.31292	0.4026	0.7295	216752	
9	+2 DTVATQLSEAV...		1.3838	0.07973	0.3615	0.9918	456705	
10	+3 SEEWADNHLPLT...		1.6393	0.05198	0.5900	0.9957	380790	
11	+3 QVEDLQATFSSL...		1.5631	0.04849	0.5524	0.9988	571876	

Peptide	L/H
1	1.25
2	1.71
3	1.99
4	1.39
5	1.68
6	1.73
7	1.79
8	2.87
9	1.38
10	1.64
11	1.56

Mascot Distiller results

**Fibronectin
(protein 260.1)**
**5 of 16 peptides met
criteria for quant**
L/H = 3.22
SD = 3.17



Extracted ion chromatograms

[M+2H]²⁺

Mascot Distiller results

Fibronectin
(protein 260.1)
5 of 16 peptides met
criteria for quant
L/H = 3.22
SD = 3.17

Proteins

Accession	Score	Mass	L/H	SD(geo)	#	Description
256.1	398	26543	1.2418	1.1739	7	proteasome subunit alpha type-5 [Mus musculus]
256.2	362	26533	1.2418	1.1739	7	PREDICTED: hypothetical protein [Monodelphis domestica]
257	398	120930	1.6308	1.0327	6	microtubule-associated protein 4 isoform 1 [Homo sapiens]
258.1	375	74350	1.0350	1.1212	7	PREDICTED: citrate synthase, mitochondrial-like [Macaca mulatta]
258.2	199	20830	0.9380	1.0356	3	protein canopy homolog 2 [Bos taurus]
259	394	38624	1.0320	1.1529	6	nuclear migration protein nudC [Homo sapiens]
260.1	394	256530	3.2216	3.1728	5	fibronectin precursor [Homo sapiens]

Matches (260.1 gij31397 Mass: 256529 Score: 394 Matches: 20)

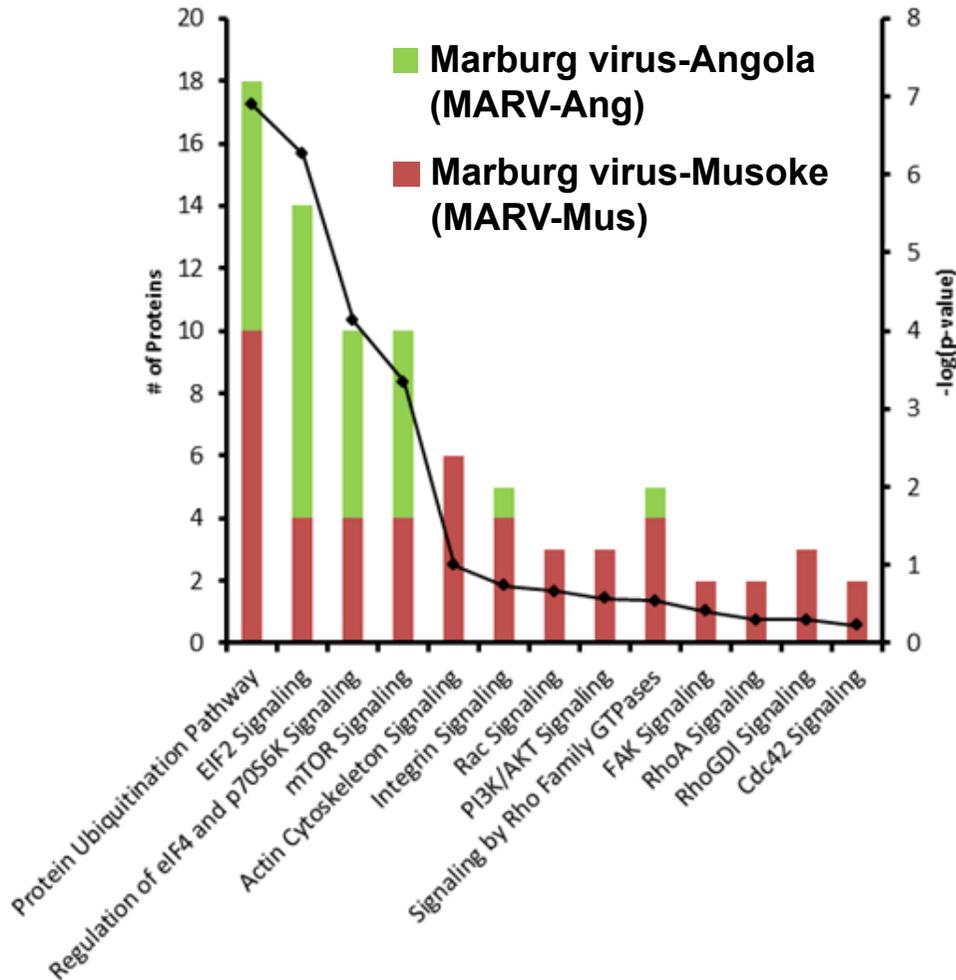
z	Sequence	L/H	Std.Err	Fraction	Correlation	Intensity	Modificatio
3	GLAFTD...VDSIK	1.5601	0.06236	0.4433	0.9977	144635	
4	VPGTST...ATLGTG	3.4447	0.10220	0.3835	0.9852	365439	
5	SYTTGL...QPGTDYK	3.2383	0.10067	0.5847	0.9975	224793	
6	SYTTGL...QPGTDYK	5.4607	0.61239	0.4578	0.9708	20544	
7	VDVIVP...VNLPGEH...	3.8393	0.11938	0.2012	0.9967	69751	
8	NLQPA...SEYTVSL...	1.2532	0.04258	0.3807	0.9987	151362	
9	SSPVV...IDASTAD...	25.0985	0.02276	0.6199	0.9965	22192	
10	EESPLL...GQSTV...	3.0440	0.18644	0.4110	0.8548	103738	
11	ITYGET...GGNSPV...	2.9151	0.11007	0.3657	0.9977	201938	
12	TEIDKP...SQMGVT...	2.3144	0.08765	0.1389	0.9934	123140	
13	FTQVTP...PTSLSAQ...	1.9984	0.05230	0.5200	0.9950	172662	
14	GLKPG...VYVEGQ...	1.2038	0.06885	0.5165	0.9977	139136	
15	VEYEL...SEEGDEP...	4.1324	0.07015	0.6128	0.9944	224746	
16	VEYEL...SEEGDEP...	3.2216	0.06063	0.6446	0.9971	222647	

Peptide	L/H
1	16.98
2	0.71
3	1.56
4	3.44
5	3.24
6	5.46
7	3.84
8	1.25
9	25.10
10	3.04
11	2.92
12	2.31
13	2.00
14	1.20
15	4.13
16	3.22

Differences in protein expression of human cells infected with Marburg viruses

1.12	Medlan		
L/H	SD(geo)	#	Description
0.21	1.13	21	NAD(P)H dehydrogenase [quinone] 1 Isoform a [Homo sapiens]
0.59	1.11	21	unnamed protein product [Homo sapiens]
0.59	1.16	10	ornithine aminotransferase, OAT
0.64	1.11	15	transketolase [Homo sapiens]
0.70	1.19	47	pyruvate carboxylase, mitochondrial precursor [Homo sapiens]
0.73	1.11	23	protein disulfide-isomerase A4 precursor [Homo sapiens]
0.77	1.21	10	microsomal triglyceride transfer protein [Homo sapiens]
0.78	1.17	10	estradiol 17-beta-dehydrogenase 12 [Homo sapiens]
0.79	1.08	12	chaperonin 10 [Homo sapiens]
0.79	1.08	77	60 kDa heat shock protein, mitochondrial [Homo sapiens]
1.59	1.33	10	drebrin E2 [Homo sapiens]
1.59	1.14	17	human rab GDI [Homo sapiens]
1.61	1.12	11	microtubule-associated protein RP/EB family member 1 [Homo sapiens]
1.63	1.11	11	cargo selection protein TIP47 [Homo sapiens]
1.63	1.11	18	microtubule-associated protein 1B [Homo sapiens]
1.63	1.09	23	vinculin isoform VCL [Homo sapiens]
1.65	1.09	18	microtubule-associated protein 4 isoform 1 [Homo sapiens]
1.69	1.09	14	peptidyl-prolyl cis-trans isomerase FKBP4 [Homo sapiens]
1.83	1.10	128	myosin-9 [Homo sapiens]
2.73	1.09	42	nestin, isoform CRA_c [Homo sapiens]

Pathway analysis of differential expression of proteins in human cells infected with Marburg viruses (SILAC data)



Lethality
MARV-Ang > MARV-Mus

Bars indicate the total number of proteins (y-axis left) involved in the indicated pathway; green, upregulated in MARV-Ang ; red, upregulated in MARV-Mus. The line graph indicates the assigned $-\log(p\text{-value})$ ratios (y-axis right) assessed via IPA for each respective pathway.

Differences in protein expression of human cells infected with Marburg viruses

1.12	Medlan		
L/H	SD(geo)	#	Description
0.09	6.00	11	VP30 [Lake Victoria marburgvirus - Angola2005]
0.39	328.10	20	RecName: Full=Matrix protein VP40
0.70	4.99	11	RecName: Full=Envelope glycoprotein
1.00	1.12	29	RecName: Full=Nucleoprotein
1.11	5.09	16	RecName: Full=Polymerase cofactor VP35
2.95	10.12	4	VP24 [Lake Victoria marburgvirus]
93.21	1.53	6	alpha-1B-glycoprotein precursor [Bos taurus]
97.45	7.10	131	PREDICTED: apolipoprotein B [Bos taurus]
100.50	9.57	4	PREDICTED: similar to complement component 4A [Bos taurus]
124.70	1.13	3	PREDICTED: pregnancy-zone protein-like [Bos taurus]
125.30	1.67	5	apolipoprotein A-I precursor [Bos taurus]
151.50	10.50	35	alpha-1-antitrypsin precursor [Bos taurus]
176.50	3.66	35	serotransferrin precursor [Bos taurus]
185.50	8.91	26	alpha-2-HS-glycoprotein precursor [Bos taurus]
253.20	4.06	6	transferrin precursor [Bos taurus]
309.50	3.43	19	alpha-1-acid glycoprotein precursor [Bos taurus]

Differences in protein expression of human cells infected with lethal viruses using spectral counting and SILAC

Protein	Total spectra			
	Control	Ebola	Angola	Musoke
fatty acid synthase	47	26	21	23
beta-actin	29	32	42	42
glyceraldehyde-3-phosphate dehydrogenase	13	14	19	20

Significant differences were found for each protein by ANOVA (Scaffold)

Protein	SILAC L/H (SD geom.)		
	A	B	C
Median	1.12	1.01	1.23
fatty acid synthase	0.89 (1.41)	0.79 (1.51)	0.97 (1.16)
beta-actin	1.27 (1.11)	1.14 (1.60)	1.40 (1.13)
glyceraldehyde-3-phosphate dehydrogenase	1.06 (1.30)	0.91 (1.09)	1.13 (1.43)

