

**Supplemental File 1:** Mascot Search Results of mass spectrometry identification for bands 1 and 17 (band 17 is rename band 4).

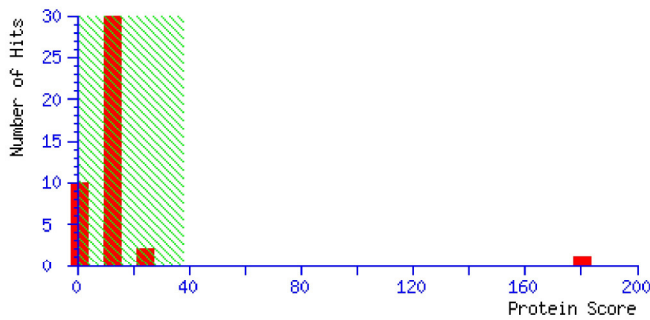
# **MASCOT** Mascot Search Results

**User** : Unidad Proteomica CACTI  
**Email** : proteomica@uvigo.es  
**Search title** : Banda 1 MSMS  
**MS data file** : DATA.TXT  
**Database** : NCBIInr 20070216 (4626804 sequences; 1596079197 residues)  
**Taxonomy** : Firmicutes (gram-positive bacteria) (320691 sequences)  
**Timestamp** : 24 Feb 2011 at 15:37:44 GMT  
**Protein hits** : [gi|452163](#) alpha-toxin [Clostridium septicum]  
[gi|89099867](#) Aminopeptidase N [Bacillus sp. NRRL B-14911]  
[gi|77683548](#) conserved hypothetical protein [Alkaliphilus metalliredigenes QYMF]  
[gi|30023346](#) uracil phosphoribosyltransferase [Bacillus cereus ATCC 14579]  
[gi|15616326](#) uracil phosphoribosyltransferase [Bacillus halodurans C-125]

	NCBIInr	Decoy	False discovery rate
Peptide matches above identity threshold	1	0	0.00 %
Peptide matches above homology or identity threshold	2	0	0.00 %

## Mascot Score Histogram

Ions score is  $-10 \cdot \log(P)$ , where P is the probability that the observed match is a random event.  
 Individual ions scores  $> 38$  indicate identity or extensive homology ( $p < 0.05$ ).  
 Protein scores are derived from ions scores as a non-probabilistic basis for ranking protein hits.



## Peptide Summary Report

Format As  [Help](#)  
 Significance threshold  $p <$   Max. number of hits   
 Standard scoring  MudPIT scoring  Ions score or expect cut-off  Show sub-sets   
 Show pop-ups  Suppress pop-ups  Sort unassigned  Require bold red

## Overview Table

Click on column header to jump to entry in results list.  
 Move mouse over any indicator to highlight identical peptides.  
 Click on an indicator to see details of individual match.  
 Use check boxes to select sub-set of queries for new search.

**Mouse over:**

Hit:	<a href="#">1</a>	<a href="#">2</a>	<a href="#">3</a>	<a href="#">4</a>	<a href="#">5</a>
<input checked="" type="checkbox"/> <a href="#">908.52</a> (1+)	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/> <a href="#">1026.48</a> (1+)	<input checked="" type="checkbox"/>				
<input checked="" type="checkbox"/> <a href="#">1130.62</a> (1+)	<input checked="" type="checkbox"/>		<input checked="" type="checkbox"/>		
<input checked="" type="checkbox"/> <a href="#">1326.63</a> (1+)	<input checked="" type="checkbox"/>				

[1416.63](#) (1+)

Select All Select None Search Selected  Error tolerant Archive Report

1. [gi|452163](#) Mass: 49926 Score: 180 Matches: 5(1) Sequences: 5(1)  
alpha-toxin [Clostridium septicum]

Check to include this hit in error tolerant search or archive report

Query	Observed	Mr(expt)	Mr(calc)	ppm	Miss	Score	Expect	Rank	Unique	Peptide
<u>1</u>	908.52	907.51	907.51	1.13	0	27	0.93	1	U	K.VSYLLSAR.Y
<u>2</u>	1026.48	1025.48	1025.48	-0.04	0	29	0.43	1	U	K.NSYDALTSR.K
<u>3</u>	1130.62	1129.61	1129.61	0.51	0	38	0.081	1	U	K.IIQDPEFIR.N
<u>4</u>	1326.63	1325.63	1325.62	4.20	0	26	0.9	1	U	R.EDHTEDRPTVK.L
<u>5</u>	1416.63	1415.62	1415.61	6.47	0	61	0.00025	1	U	R.YNPNDPYASGYR.A

Proteins matching the same set of peptides:

- [gi|27531076](#) Mass: 49634 Score: 180 Matches: 5(1) Sequences: 5(1)  
alpha-toxin [Clostridium septicum]
- [gi|27531078](#) Mass: 49650 Score: 180 Matches: 5(1) Sequences: 5(1)  
alpha-toxin [Clostridium septicum]
- [gi|27531080](#) Mass: 49588 Score: 180 Matches: 5(1) Sequences: 5(1)  
alpha-toxin [Clostridium septicum]
- [gi|89257968](#) Mass: 49513 Score: 180 Matches: 5(1) Sequences: 5(1)  
alpha-toxin [Clostridium septicum]

2. [gi|89099867](#) Mass: 91440 Score: 25 Matches: 1(0) Sequences: 1(0)  
Aminopeptidase N [Bacillus sp. NRRL B-14911]

Check to include this hit in error tolerant search or archive report

Query	Observed	Mr(expt)	Mr(calc)	ppm	Miss	Score	Expect	Rank	Unique	Peptide
<u>1</u>	908.52	907.51	907.48	41.2	0	25	1.5	2	U	K.SVYIEAAR.A

3. [gi|77683548](#) Score: 20 Matches: 1(0) Sequences: 1(0)  
conserved hypothetical protein [Alkaliphilus metalliredigenes QYMF]

Check to include this hit in error tolerant search or archive report

Query	Observed	Mr(expt)	Mr(calc)	ppm	Miss	Score	Expect	Rank	Unique	Peptide
<u>3</u>	1130.62	1129.61	1129.61	4.09	1	20	4.8	2	U	R.LIRSEEDLR.D

4. [gi|30023346](#) Mass: 22943 Score: 18 Matches: 1(0) Sequences: 1(0)  
uracil phosphoribosyltransferase [Bacillus cereus ATCC 14579]

Check to include this hit in error tolerant search or archive report

Query	Observed	Mr(expt)	Mr(calc)	ppm	Miss	Score	Expect	Rank	Unique	Peptide
<u>1</u>	908.52	907.51	907.51	1.13	1	18	8.3	3	U	K.ITYIRDK.N

Proteins matching the same set of peptides:

- [gi|47570682](#) Mass: 8607 Score: 18 Matches: 1(0) Sequences: 1(0)  
uracil phosphoribosyltransferase [Bacillus cereus G9241]
- [gi|89203556](#) Score: 18 Matches: 1(0) Sequences: 1(0)
- [gi|89207647](#) Score: 18 Matches: 1(0) Sequences: 1(0)
- [gi|118480351](#) Score: 18 Matches: 1(0) Sequences: 1(0)

5. [gi|15616326](#) Score: 17 Matches: 1(0) Sequences: 1(0)  
uracil phosphoribosyltransferase [Bacillus halodurans C-125]

Check to include this hit in error tolerant search or archive report

Query	Observed	Mr(expt)	Mr(calc)	ppm	Miss	Score	Expect	Rank	Unique	Peptide
<u>1</u>	908.52	907.51	907.51	1.13	1	17	9.1	4	U	K.LTYIRDK.S

## Proteins matching the same set of peptides:

<a href="#">gi 22096373</a>	Score: 17	Matches: 1 (0)	Sequences: 1 (0)
<a href="#">gi 23100439</a>	Score: 17	Matches: 1 (0)	Sequences: 1 (0)
<a href="#">gi 56421903</a>	Score: 17	Matches: 1 (0)	Sequences: 1 (0)

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## Search Parameters

Type of search : MS/MS Ion Search  
Enzyme : Trypsin  
Fixed modifications : [Carbamidomethyl \(C\)](#)  
Variable modifications : [Oxidation \(M\)](#)  
Mass values : Monoisotopic  
Protein Mass : Unrestricted  
Peptide Mass Tolerance :  $\pm$  100 ppm  
Fragment Mass Tolerance:  $\pm$  0.5 Da  
Max Missed Cleavages : 1  
Instrument type : MALDI-TOF-TOF  
Number of queries : 5

Mascot: <http://www.matrixscience.com/>

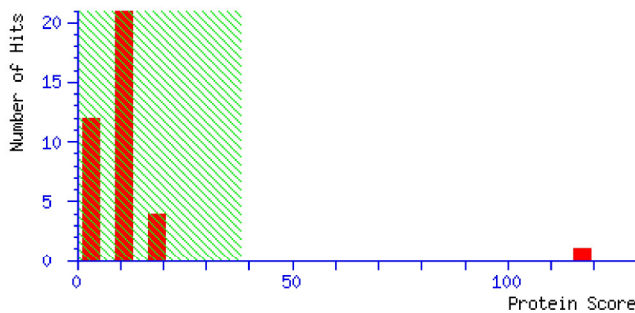
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**Taxonomy** : Firmicutes (gram-positive bacteria) (320691 sequences)  
**Timestamp** : 24 Feb 2011 at 16:20:48 GMT  
**Protein hits** : [gi|452163](#) alpha-toxin [Clostridium septicum]  
[gi|30023346](#) uracil phosphoribosyltransferase [Bacillus cereus ATCC 14579]  
[gi|15616326](#) uracil phosphoribosyltransferase [Bacillus halodurans C-125]  
[gi|77683548](#) conserved hypothetical protein [Alkaliphilus metalliredigenes QYMF]  
[gi|89099867](#) Aminopeptidase N [Bacillus sp. NRRL B-14911]

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Hit:	<a href="#">1</a>	<a href="#">2</a>	<a href="#">3</a>	<a href="#">4</a>	<a href="#">5</a>
<input checked="" type="checkbox"/> <a href="#">908.50</a> (1+)	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/> <a href="#">1026.46</a> (1+)	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
<input checked="" type="checkbox"/> <a href="#">1130.59</a> (1+)	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
<input checked="" type="checkbox"/> <a href="#">1326.60</a> (1+)	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

[1416.60](#) (1+)

**Error tolerant**

1. [gi|452163](#) **Mass:** 49926 **Score:** 117 **Matches:** 5(1) **Sequences:** 5(1)  
alpha-toxin [Clostridium septicum]

Check to include this hit in error tolerant search or archive report

Query	Observed	Mr(expt)	Mr(calc)	ppm	Miss	Score	Expect	Rank	Unique	Peptide
<u>1</u>	908.50	907.50	907.51	-17.57	0	17	9.7	1	U	K.VSYLLSAR.Y
<u>2</u>	1026.46	1025.46	1025.48	-21.50	0	18	4.2	1	U	K.NSYDALTSR.K
<u>3</u>	1130.59	1129.59	1129.61	-24.27	0	22	2.8	1	U	K.IIQDPEFIR.N
<u>4</u>	1326.60	1325.60	1325.62	-19.18	0	11	21	1	U	R.EDHTEDRPTVK.L
<u>5</u>	1416.60	1415.59	1415.61	-11.90	0	48	0.0037	1	U	R.YNPNDPYASGYR.A

**Proteins matching the same set of peptides:**

- [gi|27531076](#) **Mass:** 49634 **Score:** 117 **Matches:** 5(1) **Sequences:** 5(1)  
alpha-toxin [Clostridium septicum]
- [gi|27531078](#) **Mass:** 49650 **Score:** 117 **Matches:** 5(1) **Sequences:** 5(1)  
alpha-toxin [Clostridium septicum]
- [gi|27531080](#) **Mass:** 49588 **Score:** 117 **Matches:** 5(1) **Sequences:** 5(1)  
alpha-toxin [Clostridium septicum]
- [gi|89257968](#) **Mass:** 49513 **Score:** 117 **Matches:** 5(1) **Sequences:** 5(1)  
alpha-toxin [Clostridium septicum]

2. [gi|30023346](#) **Mass:** 22943 **Score:** 16 **Matches:** 1(0) **Sequences:** 1(0)  
uracil phosphoribosyltransferase [Bacillus cereus ATCC 14579]

Check to include this hit in error tolerant search or archive report

Query	Observed	Mr(expt)	Mr(calc)	ppm	Miss	Score	Expect	Rank	Unique	Peptide
<u>1</u>	908.50	907.50	907.51	-17.57	1	16	13	2	U	K.ITYIRDK.N

**Proteins matching the same set of peptides:**

- [gi|47570682](#) **Mass:** 8607 **Score:** 16 **Matches:** 1(0) **Sequences:** 1(0)  
uracil phosphoribosyltransferase [Bacillus cereus G9241]
- [gi|89203556](#) **Score:** 16 **Matches:** 1(0) **Sequences:** 1(0)
- [gi|89207647](#) **Score:** 16 **Matches:** 1(0) **Sequences:** 1(0)
- [gi|118480351](#) **Score:** 16 **Matches:** 1(0) **Sequences:** 1(0)

3. [gi|15616326](#) **Score:** 16 **Matches:** 1(0) **Sequences:** 1(0)  
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Query	Observed	Mr(expt)	Mr(calc)	ppm	Miss	Score	Expect	Rank	Unique	Peptide
<u>1</u>	908.50	907.50	907.51	-17.57	1	16	14	3	U	K.LTYIRDK.S

**Proteins matching the same set of peptides:**

- [gi|22096373](#) **Score:** 16 **Matches:** 1(0) **Sequences:** 1(0)
- [gi|23100439](#) **Score:** 16 **Matches:** 1(0) **Sequences:** 1(0)
- [gi|56421903](#) **Score:** 16 **Matches:** 1(0) **Sequences:** 1(0)

4. [gi|77683548](#) **Score:** 15 **Matches:** 1(0) **Sequences:** 1(0)  
conserved hypothetical protein [Alkaliphilus metalliredigenes QYMF]

Check to include this hit in error tolerant search or archive report

Query	Observed	Mr(expt)	Mr(calc)	ppm	Miss	Score	Expect	Rank	Unique	Peptide
<u>3</u>	1130.59	1129.59	1129.61	-20.69	1	15	15	2	U	R.LIRSEEDLR.D

5. [gi|89099867](#) **Score:** 15 **Matches:** 1(0) **Sequences:** 1(0)  
Aminopeptidase N [Bacillus sp. NRRL B-14911]

Check to include this hit in error tolerant search or archive report

Query	Observed	Mr(expt)	Mr(calc)	ppm	Miss	Score	Expect	Rank	Unique	Peptide
<u>1</u>	908.50	907.50	907.48	22.5	0	15	16	4	U	K.SVYIEAAR.A

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## Search Parameters

Type of search : MS/MS Ion Search  
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Variable modifications : [Oxidation \(M\)](#)  
Mass values : Monoisotopic  
Protein Mass : Unrestricted  
Peptide Mass Tolerance :  $\pm 100$  ppm  
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Max Missed Cleavages : 1  
Instrument type : MALDI-TOF-TOF  
Number of queries : 5

Mascot: <http://www.matrixscience.com/>