

**Supplemental File 2:** Mascot Search Results of mass spectrometry identification for purified electroeluted protein.

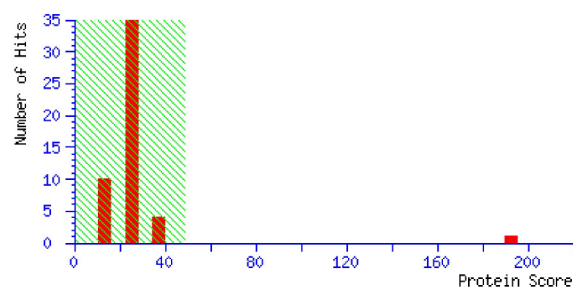
**MATRIX SCIENCE Mascot Search Results**

User : Unidad Proteomica CACTI  
 Email : proteomica@uvigo.es  
 Search title : Banda 1 COOMASSIE\_MSMS  
 MS data file : DATA.TXT  
 Database : NCBIInr 20130503 (25052984 sequences; 8638475353 residues)  
 Taxonomy : Firmicutes (gram-positive bacteria) (3326529 sequences)  
 Timestamp : 7 May 2013 at 14:14:18 GMT  
 Protein hits : [gi|452163](#) alpha-toxin [Clostridium septicum]

|  | NCBIInr | Decoy | False discovery rate |
|--|---------|-------|----------------------|
| Peptide matches above identity threshold             | 2       | 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 > 49 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

Preferred taxonomy

**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:   | 1                     |
|--|-----------------------|
| <input checked="" type="checkbox"/> <a href="#">774.4174</a> (1+)  | <input type="radio"/> |
| <input checked="" type="checkbox"/> <a href="#">908.5189</a> (1+)  | <input type="radio"/> |
| <input checked="" type="checkbox"/> <a href="#">1130.6171</a> (1+) | <input type="radio"/> |
| <input checked="" type="checkbox"/> <a href="#">1267.7096</a> (1+) | <input type="radio"/> |
| <input checked="" type="checkbox"/> <a href="#">1416.6077</a> (1+) | <input type="radio"/> |
| <input checked="" type="checkbox"/> <a href="#">1759.9419</a> (1+) | <input type="radio"/> |

Select All  Select None  Search Selected   Error tolerant

1. [gi|452163](#) Mass: 49926 Score: 193 Matches: 4 (2) Sequences: 4 (2)  
 alpha-toxin [Clostridium septicum]

Check to include this hit in error tolerant search

Query Observed Mr (expt) Mr (calc) ppm Miss Score Expect Rank Unique Peptide

|          |           |           |           |       |   |    |         |   |   |                  |
|----------|-----------|-----------|-----------|-------|---|----|---------|---|---|------------------|
| <u>1</u> | 774.4174  | 773.4101  | 773.4112  | -1.38 | 0 | 29 | 11      | 4 | U | K.FGYLFK.N       |
| <u>2</u> | 908.5189  | 907.5116  | 907.5127  | -1.22 | 0 | 16 | 1.2e+02 | 1 | U | K.VSYLLSAR.Y     |
| <u>3</u> | 1130.6171 | 1129.6098 | 1129.6131 | -2.94 | 0 | 56 | 0.012   | 1 | U | K.IIQDPEFIR.N    |
| <u>5</u> | 1416.6077 | 1415.6004 | 1415.6106 | -7.16 | 0 | 92 | 1.7e-06 | 1 | U | R.YNPNDPYASGYR.A |

Proteins matching the same set of peptides:

|                                    |             |            |                |                  |
|------------------------------------|-------------|------------|----------------|------------------|
| <a href="#">gi 27531076</a>        | Mass: 49634 | Score: 193 | Matches: 4 (2) | Sequences: 4 (2) |
| alpha-toxin [Clostridium septicum] |             |            |                |                  |
| <a href="#">gi 27531078</a>        | Mass: 49650 | Score: 193 | Matches: 4 (2) | Sequences: 4 (2) |
| alpha-toxin [Clostridium septicum] |             |            |                |                  |
| <a href="#">gi 27531080</a>        | Mass: 49588 | Score: 193 | Matches: 4 (2) | Sequences: 4 (2) |
| alpha-toxin [Clostridium septicum] |             |            |                |                  |
| <a href="#">gi 89257968</a>        | Mass: 49513 | Score: 193 | Matches: 4 (2) | Sequences: 4 (2) |
| alpha-toxin [Clostridium septicum] |             |            |                |                  |
| <a href="#">gi 169639783</a>       | Mass: 49997 | Score: 193 | Matches: 4 (2) | Sequences: 4 (2) |
| alpha-toxin [Clostridium septicum] |             |            |                |                  |
| <a href="#">gi 169639785</a>       | Mass: 49997 | Score: 193 | Matches: 4 (2) | Sequences: 4 (2) |
| alpha-toxin [Clostridium septicum] |             |            |                |                  |
| <a href="#">gi 169639787</a>       | Mass: 49990 | Score: 193 | Matches: 4 (2) | Sequences: 4 (2) |
| alpha-toxin [Clostridium septicum] |             |            |                |                  |
| <a href="#">gi 169639791</a>       | Mass: 49994 | Score: 193 | Matches: 4 (2) | Sequences: 4 (2) |
| alpha-toxin [Clostridium septicum] |             |            |                |                  |
| <a href="#">gi 169639793</a>       | Mass: 50029 | Score: 193 | Matches: 4 (2) | Sequences: 4 (2) |
| alpha-toxin [Clostridium septicum] |             |            |                |                  |
| <a href="#">gi 169639797</a>       | Mass: 49924 | Score: 193 | Matches: 4 (2) | Sequences: 4 (2) |
| alpha-toxin [Clostridium septicum] |             |            |                |                  |
| <a href="#">gi 169639799</a>       | Mass: 49897 | Score: 193 | Matches: 4 (2) | Sequences: 4 (2) |
| alpha-toxin [Clostridium septicum] |             |            |                |                  |
| <a href="#">gi 169639801</a>       | Mass: 49925 | Score: 193 | Matches: 4 (2) | Sequences: 4 (2) |
| alpha-toxin [Clostridium septicum] |             |            |                |                  |
| <a href="#">gi 313585702</a>       | Mass: 49575 | Score: 193 | Matches: 4 (2) | Sequences: 4 (2) |
| alpha-toxin [Clostridium septicum] |             |            |                |                  |

Peptide matches not assigned to protein hits: (no details means no match)

| Query  | Observed  | Mr(expt)  | Mr(calc)  | ppm  | Miss | Score | Expect  | Rank | Unique | Peptide                    |
|--|-----------|-----------|-----------|------|------|-------|---------|------|--------|----------------------------|
| <input checked="" type="checkbox"/> <u>1</u> | 774.4174  | 773.4101  | 773.3782  | 41.3 | 0    | 31    | 5.5     | 1    |        | MGYIFK + Oxidation (M)     |
| <input checked="" type="checkbox"/> <u>4</u> | 1267.7096 | 1266.7023 | 1266.6642 | 30.1 | 1    | 27    | 8.5     | 1    |        | YGEMLKELIR + Oxidation (M) |
| <input checked="" type="checkbox"/> <u>6</u> | 1759.9419 | 1758.9346 | 1758.8900 | 25.3 | 1    | 13    | 1.6e+02 | 1    |        | ASYITGTTYNIAGGKSR          |

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 : ± 100 ppm  
 Fragment Mass Tolerance : ± 0.5 Da  
 Max Missed Cleavages : 1  
 Instrument type : MALDI-TOF-TOF  
 Number of queries : 6

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