

ORIGINAL ARTICLE

Allergens

Towards complete identification of allergens in Jack Jumper (*Myrmecia pilosula*) ant venom and their clinical relevance: An immunoproteomic approach

Troy Wanandy^{1,2,3,4}  | Richard Wilson⁵  | David Gell³ | Hayley E. Rose¹ | Nuri Gueven² | Noel W. Davies⁵ | Simon G. A. Brown^{1,3,6,7} | Michael D. Wiese^{1,8}

¹Jack Jumper Allergy Program, Royal Hobart Hospital, Hobart, TAS, Australia

²Division of Pharmacy, School of Medicine, University of Tasmania, Hobart, TAS, Australia

³School of Medicine, University of Tasmania, Hobart, TAS, Australia

⁴Department of Pharmacy, Royal Hobart Hospital, Hobart, TAS, Australia

⁵Central Science Laboratory, University of Tasmania, Hobart, TAS, Australia

⁶Ambulance Tasmania, Hobart, TAS, Australia

⁷Department of Emergency Medicine, Royal Hobart Hospital, Hobart, TAS, Australia

⁸School of Pharmacy and Medical Sciences, University of South Australia, Adelaide, SA, Australia

Correspondence:

Troy Wanandy, Jack Jumper Allergy Program, Royal Hobart Hospital, GPO Box 1061L, Hobart, Tasmania 7001, Australia.

Email: troy.wanandy@ths.tas.gov.au

Funding information

This work was funded by the Jack Jumper Allergy Program, Royal Hobart Hospital, Tasmania. TW was supported through an Australian Government Research Training Program Scholarship and The University of Tasmania ELITE Research Scholarship to conduct part of this study.

Summary

Background: The venomous stings of Jack Jumper ant (JJA; species of the *Myrmecia pilosula* taxonomic group) are a significant public health issue in parts of south-eastern and south-western Australia, causing anaphylaxis in approximately 3% of the population. Three allergenic peptides, Myr p 1, Myr p 2 and Myr p 3, and one histamine-releasing peptide, pilosulin 5, have been fully described, but there are at least 5 additional high molecular weight IgE-binding components that have not been identified.

Objective: To identify IgE-binding components in JJA venom (JJAV) and to relate the IgE recognition of these components to relevant clinical parameters.

Methods: Identification of IgE-binding components and determination of their sensitizing prevalence was performed using SDS-PAGE immunoblot assay and sera from 90 patients with confirmed allergy to JJAV. Tandem mass spectrometry was used for identification of novel JJAV components fractionated by size exclusion chromatography (SEC) and SDS-PAGE.

Results: Using SDS-PAGE immunoblot, 10 IgE-binding bands were identified in JJAV, two of which were recognized by 81% and 47% of the population studied. Mass spectrometry identified 17 novel JJAV proteins, including 2 glycoproteins, and confirmed the presence of 4 known Myr p and pilosulin peptides in JJAV. Most of the newly identified IgE-binding proteins were enzymes, including phospholipase A₂, hyaluronidase, arginine kinase and dipeptidyl peptidase IV. Correlations were found between recognition of certain IgE-binding bands with JJAV-specific IgE titre by ImmunoCAP, intradermal test threshold and treatment-related issues.

Conclusions and Clinical Relevance: This study has for the first time revealed the identity of various proteins with IgE-binding capacity in the venom of JJA and demonstrated their clinical relevance in the diagnosis and treatment of JJAV allergy.

KEYWORDS

allergen, Hymenoptera venom, immunoproteomics, *Myrmecia pilosula*

1 | INTRODUCTION

Jack Jumper ant (JJA) comprises six closely related species of the Australian *Myrmecia pilosula* taxonomic group.¹ They are stinging Hymenoptera of medical importance. Allergy to JJA venom affects approximately 3% of the population living in parts of south-eastern and south-western Australia,^{2–4} causing rapid onset and severe systemic allergic reactions and impaired quality of life in sensitized individuals. Fatal anaphylaxis following JJA sting has been documented,⁵ and the venom appears to be highly allergenic in comparison to other Hymenoptera venoms.^{2,6} Using standardized extracts suitable for venom immunotherapy,^{7–9} the efficacy and safety of JJA venom immunotherapy (JJA VIT) in reducing future risk of severe allergic reactions and preventing anaphylaxis have been prospectively demonstrated in 2 randomized controlled clinical trials.^{6,10} The ants studied here were all sourced from localities in lowland Tasmania, and can thus be confidently assigned to the Western Race of *Myrmecia pilosula* Fredrick Smith (R.W. Taylor *pers com.*). A diagnostic framework has also been established to identify appropriate candidates for JJA VIT.¹¹

Analysis of the venom of JJA has so far identified four peptides—Myr p 1, Myr p 2 and Myr p 3—that have been recognized as allergens by the International Union of Immunology Societies,¹² and a histamine-releasing peptide called pilosulin 5. Myr p 1 is a 6067 Da monomer peptide (also called pilosulin 1); Myr p 2 is a 5608 Da heterodimer (also called pilosulin 3 and delta-Myrtoxin-Mp1a); Myr p 3 is a 8198 Da homodimer (also called pilosulin 4); pilosulin 5 is a 8546 Da homodimer; all four are highly basic.^{13–16} Multiple isoforms of these peptides have been identified by genetic analysis or mass spectrometry (reviewed in reference¹⁷), and the three-dimensional (3D) structure of Myr p 2 has been determined by NMR spectroscopy.¹⁶ A number of components of >20 kDa with IgE-binding capacity remain to be characterized.¹⁷

A goal in allergy research is to implement component-resolved diagnostics (CRD) and personalized treatment.^{18–22} This can only be achieved by the identification and characterization of a complete set of allergens in the allergenic source. It is therefore important to understand the composition and identity of these IgE-binding components in JJAV as proper characterization is expected to lead to significant improvement in the diagnosis and treatment of JJAV allergy.

Recently, we completed a randomized controlled clinical trial on JJA VIT with the objective to optimize the safety and delivery of the treatment (TasVIT II study, Australian New Zealand Clinical Trials Registry ID: ACTRN12606000333516). Utilizing an immunoproteomic approach and sera from patients who participated in this clinical trial, the present study was aimed at: (a) investigating IgE-binding components in JJAV, (b) identifying the unknown high MW venom components with IgE-binding capacity and (c) relating IgE recognition to these components to relevant clinical parameters.

2 | MATERIALS AND METHODS

2.1 | Materials

If not otherwise specified, all chemicals and reagents used in the experiments were as previously described⁹ or obtained from Sigma-Aldrich (St. Louis, MO, USA).

2.2 | Study population and determination of reactivity to JJAV allergens

2.2.1 | Individual serum samples

Sera from JJAV-allergic patients who were recruited in the TasVIT II trial were used in this study. All sera were obtained as part of the diagnostic work-up and prior to administration of any immunotherapy. Sensitivity to JJAV was shown based on positive clinical history of JJA sting anaphylaxis and detection of JJAV-specific IgE-mediated sensitization by intradermal test and/or ImmunoCAP.⁹ Severity of anaphylaxis (Grades 1–3) was classified according to the criteria of Brown.²³ Serum was isolated from whole blood (after incubating at room temperature for 30 minutes) by centrifugation at $2500 \times g$ for 10 minutes and stored at -80°C until used in the analysis. The TasVIT II trial and use of patient sera were approved by the Human Research Ethics Committee (Tasmanian) Network and the ethics approval is H0008934. Individual serum samples were used in immunoblotting experiments as indicated.

2.2.2 | Pooled sera

Sera from JJAV-allergic patients were pooled as previously described⁹ and used in selected immunoblotting experiments.

2.2.3 | Intradermal test

Intradermal test (IDT) for the assessment of sensitivity to JJAV was performed as previously described.^{6,10,24} The IDT result was considered positive if wheal growth was ≥ 2 mm and flare was ≥ 10 mm within 20 minutes.

2.2.4 | JJAV-specific IgE

Quantification of JJAV-specific serum IgE titre in individual serum samples ($n = 81$ of 90 patients included in this study) was performed using the ImmunoCAP system (ThermoFisher Scientific, Uppsala, Sweden; with JJAV sourced from Tasmania) at SA Pathology (Adelaide, SA, Australia) according to manufacturer's instruction.²⁵ Results were expressed in classes of positivity from 0 to 6, where class 0 corresponds to <0.35 kilo units (kU)/L, class 1: 0.35 to <0.7 kU/L, class 2: 0.7 to <3.5 kU/L, class 3: 3.5 to <17.5 kU/L, class 4: 17.5 to 50 kU/L, class 5: 51 to 99 kU/L and class 6: >99 kU/L.

2.3 | JJAV preparations

2.3.1 | JJA

Jack Jumper ant species used in the experiments were sourced from localities around Tasmania and had been examined by an entomologist from the University of Tasmania to be the Western Race of *Myrmecia pilosula* as delineated by Dr. R.W. Taylor (*sensu stricto*).¹

2.3.2 | JJAV extracts

Jack Jumper ant venom extracts used in these experiments were of the Active Pharmaceutical Ingredient grade, prepared and stored as previously described.⁹

2.3.3 | Reduction and alkylation of JJAV

Jack Jumper ant venom samples for the reduction/alkylation experiments were prepared immediately prior to use as previously described.²⁶

2.3.4 | Fractionation of JJAV components

Fractionation of non-reduced JJAV components was carried out using size exclusion chromatography (SEC) on a Superose[®] 12 column (GE Healthcare Life Sciences, Pittsburgh, PA, USA) with a bed volume of 24 mL, equilibrated in 50 mmol/L sodium phosphate, 150 mmol/L sodium chloride, pH = 7 at 0.5 mL/min flow rate. Injections consisted of 0.5 mL of non-reduced JJAV at a concentration of 1 mg/mL. Fraction volume was 0.5 mL and eluents were detected by absorbance at 235 nm. The column was calibrated for molecular weight (MW) determination by injecting standards containing a mixture of thyroglobulin (670 kDa), γ -globulin (158 kDa), ovalbumin (44 kDa), myoglobin (17 kDa) and vitamin B₁₂ (1.36 kDa) (Bio-Rad, Hercules, CA, USA). Column fractions were concentrated using Amicon Ultra 0.5 mL filters MWCO 3 kDa (Merck Millipore, Billerica, MA, USA) by centrifugation at 14 000 $\times$ g and 4°C for 45 minutes.

2.4 | Electrophoresis and immunoblotting analysis

2.4.1 | SDS-PAGE

Non-reduced, reduced/alkylated and fractionated JJAV were resolved using SDS-PAGE and visualized via silver stain or electro-transferred to PVDF membrane for immunoblotting as previously described.⁹

2.4.2 | Acid urea PAGE

Acid urea (AU)-PAGE gel was cast and non-reduced JJAV was resolved and either visualized via silver stain or electro-transferred to PVDF membrane for immunoblotting as previously described.⁹

2.4.3 | Two-Dimensional Electrophoresis (2-DE)

Jack Jumper ant venom (90 μ g) was dissolved in isoelectric focussing (IEF) sample buffer containing 20 mmol/L DTT, 8 mol/L urea, 2% CHAPS, 0.5% ampholytes, and 0.002% bromophenol blue, and 155 μ L was applied to a precast ZOOM IPG strip (7 cm, pH 3-11NL; ThermoFisher Scientific). The strip was rehydrated overnight at room temperature (RT), and then focussed using a gradient mode: 250 V for 15 minutes, 4000 V for 1 hour, 4000 V for a total of 10 000 Volt-hours, and 500 V for 15-20 hours in a Protean IEF Cell System (Bio-Rad). IPG strips were then incubated for 30 minutes in equilibration buffer containing NuPAGE LDS Sample Buffer and NuPAGE Sample Reducing Agent (ThermoFisher Scientific) at RT, and followed by 30-minute incubation in alkylation solution containing NuPAGE LDS Sample Buffer and 125 mmol/L iodoacetamide at RT. The strip was then positioned on top of a NuPAGE 4%-12% Bis-Tris ZOOM Protein gel, 1.0 mm (ThermoFisher Scientific) and fixed with 0.5% (w/v) low-melting point agarose. Five microlitre of Precision Plus Protein WesternC Standards (Bio-Rad) or non-reduced JJAV dissolved in NuPAGE LDS sample buffer was loaded in the marker well as appropriate. Electrophoresis was performed using MES buffer (ThermoFisher Scientific) at 40 V for 20 minutes for the initial migration and stacking step, and at 165 V for 40 minutes for the separation step. The second dimension gel was either stained with SYPRO Ruby Protein stain (ThermoFisher Scientific) and visualized using Amersham Imager 600 (GE Healthcare Bio-Sciences AB, Uppsala, Sweden) or electro-transferred to PVDF membrane for immunoblotting as previously described.⁹

2.5 | Glycoprotein detection

To visualize glycoproteins in JJAV, non-reduced JJAV (100 μ g) was separated by SDS-PAGE and stained with Pro-Q[®] Emerald 488 Glycoprotein stain (ThermoFisher Scientific) according to the manufacturer's instructions. Fluorescence intensity of the stained gel was imaged at 460 nm using Amersham Imager 600.

2.6 | Identification of IgE-binding and non-IgE-binding components by mass spectrometry

IgE-binding and non-IgE-binding bands from the fractionated JJAV were identified by silver staining and immunoblotting. Matched bands in the SDS-PAGE gel were excised using a scalpel and transferred to Protein LoBind microcentrifuge tubes (Eppendorf AG, Hamburg, Germany). Silver stain was removed using 30 mmol/L potassium ferricyanide and 100 mmol/L sodium thiosulfate (1:1 mix) and gel pieces were dried by vacuum centrifugation. In-gel trypsin digestion was performed using proteomic grade trypsin (Sigma) as previously described.²⁷ Digested samples were analysed using a LTQ-Orbitrap tandem mass spectrometer and Ultimate 3000 RSLCnano (ThermoFisher Scientific) using a 20 mm $\times$ 75 mm PepMap 100 column for sample trapping and a 150 mm $\times$ 75 mm PepMap 100 column for separation over a 1 hour gradient from

98% mobile phase A (0.1% formic acid in water) to 50% mobile phase B (0.08% formic acid in 80% acetonitrile and 20% water) at 300 nL/min. The LTQ-Orbitrap was controlled using Xcalibur 2.1 software in data-dependent mode and MS/MS spectra were acquired using a Top8 method with 30-second dynamic exclusion of fragmented peptides, as previously described.²⁸ RAW data files were imported into PEAKS studio v7.5 software (Bioinformatics Solutions, Inc., Waterloo, ON, Canada) and MS/MS spectra were searched against the National Centre for Biotechnology Information (NCBI) protein database comprising the *Formicidae* family (taxonomy ID 36668; 602 573 entries). Search parameters specified mass error tolerances of 5 ppm and 0.5 Da for precursor and fragment ions, respectively, a maximum of three missed trypsin cleavages and variable methionine oxidation. The *P* values assigned to peptide spectrum matches are based on linear discriminative function scores for the number of matching fragment ion peaks, where a more significant match produces a higher $-\log_{10} P$ value.²⁹ Proteins identified on the basis of a minimum of one unique peptide and $-\log_{10} P$ values of >20 were considered significant. Peptide spectrum match thresholds were manually set, based on the minimum PEAKS score that retained a 0% FDR. The PEAKS output for each statistical analysis, including the filtering parameters, number of peptide-spectrum matches and complete set of protein identifications is included in Data S1.

2.7 | Statistical and graphical analysis

GraphPad Prism v5.03 (GraphPad Software Inc., San Diego, CA, USA) was used for statistical analysis and Spearman's rank correlation. ImageJ v1.46r (Wayne Rasband, HIH, Baltimore, MD, USA) and ImageQuant TL v8.1 (GE Healthcare Bio-Sciences AB) software was used for gel image analysis. Data analysis of immunoblots was performed using ImageQuant TL v8.1. software, which calculated the MW of SDS-PAGE resolved IgE-binding bands using Precision Plus Protein WesternC Standards as the MW reference standard and provided densitometry data with band detection set at median filter: 8. Correlations in the data were detected using Hierarchical Clustering analysis with Spearman's rank correlation (Multi Experiment Viewer v4.8.1, TM Software Suite, Boston, MA, USA). *P* values <0.05 were considered significant.

3 | RESULTS

3.1 | Clinical and serological characteristics

Demographic and clinical details of the 90 patients with JJA sting allergy included in this study are shown in Table 1. In total, 58% of the patients were male, the median age was 59 years, and 96% of the patients had either Grade II or Grade III as their worst anaphylactic reaction. Ninety-eight per cent of the patient population was assessed for JJAV-specific IgE using IDT; 68% had a positive reaction to JJAV at 0.01 µg/mL and an equal proportion of the remainder were reactive to 0.1 and 1 µg/mL. A total of 90% of the patient population was serologically tested for JJAV-specific IgE titre using

ImmunoCAP; the median JJAV-specific IgE titre was 2 kU/L (interquartile range: 0.5–15 kU/L). Fourteen patients (17%) had no measurable JJAV-specific IgE despite positive histories of JJA sting allergy and/or positive IDT results. Levels of JJAV-specific IgE ImmunoCAP and IDT threshold correlated significantly (Spearman's rank $r = -0.625$, $P < 0.0001$). Half of the study population (45/90) responded to JJA VIT without experiencing notable adverse reactions during treatment and sting challenge, and the remaining patients developed various types of adverse reactions to JJA VIT or JJA sting challenge as described in Table 1.

3.2 | Resolution of high molecular weight proteins and abundant low molecular weight peptides in JJAV by gel electrophoresis

Analysis of non-reduced JJAV proteins by SDS-PAGE showed diffuse and highly stained bands below 20 kDa (Figure 1, lanes 1 and 2),

TABLE 1 Demographic and clinical data from study participants

Median age (n = 90)	59 (range: 18–84)
Males	58.0%
Previous worst reaction grade ^a (n = 90)	
Grade 1	4.4%
Grade 2	57.8%
Grade 3	37.8%
Intradermal test positive threshold (n = 88)	
0.01 µg/mL	67.8%
0.1 µg/mL	16.1%
1 µg/mL	16.1%
JJAV IgE ImmunoCAP ^b (n = 81)	
Class 0	17.3%
Class 1	13.6%
Class 2	25.9%
Class 3	22.2%
Class 4	11.1%
Class 5	4.9%
Class 6	4.9%
Reaction score (n = 90)	
(0) No notable reaction during treatment and sting challenge	50.0%
(1) Frequent reactions during initiation phase	9.0%
(2) Frequent reactions during maintenance phase	10.0%
(3) Frequent reactions during initiation and maintenance phases	11.1%
(4) Reacted during sting challenge	14.4%
(5) Reacted to VIT post-sting challenge	2.2%
(6) Reacted during field sting	3.3%

^aAccording to Brown anaphylaxis severity grading system.²³

^bPerformed using the Phadia ImmunoCAP system.

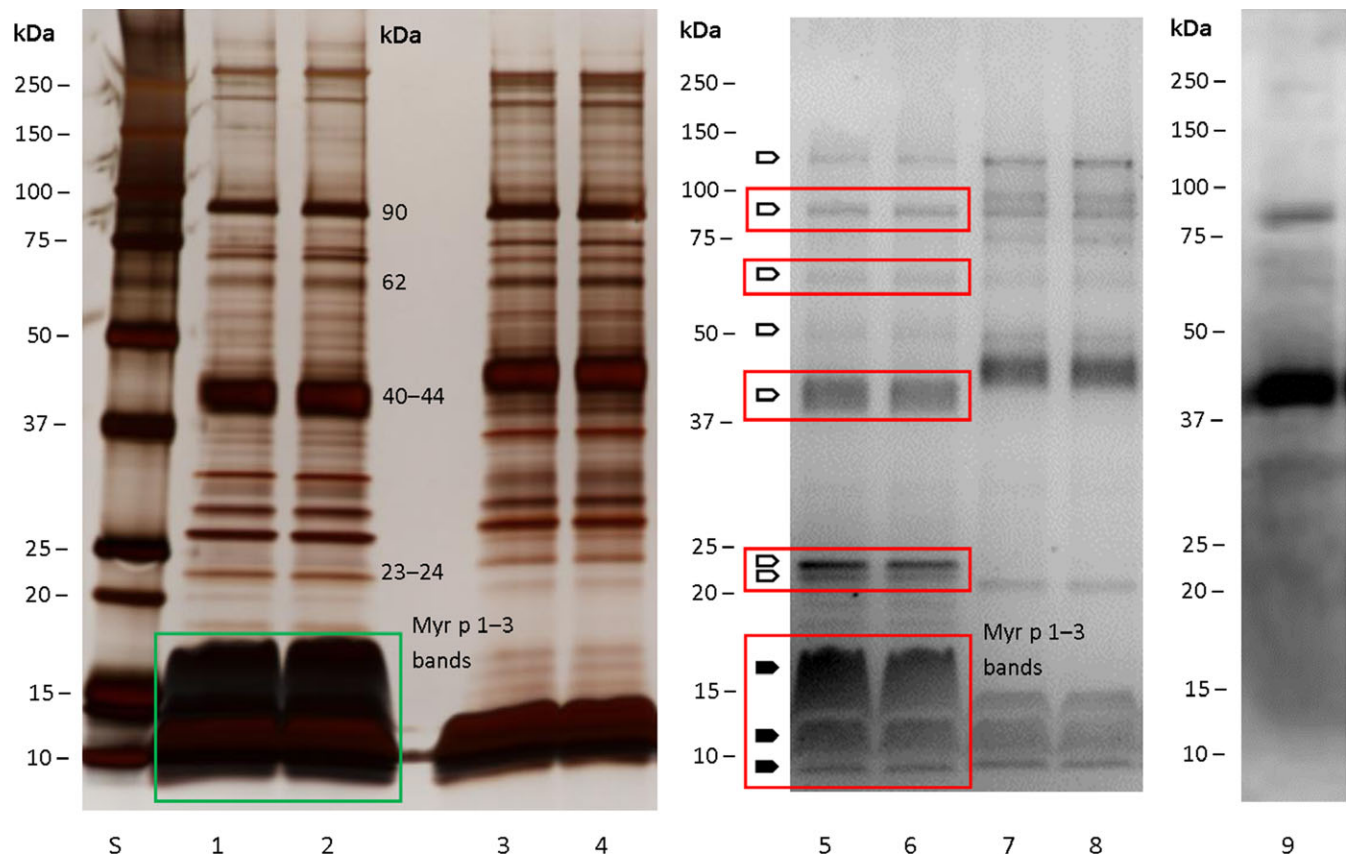


FIGURE 1 Representative results of JJAV components resolved on 10%-20% Tris-Glycine SDS-PAGE. Lane S, Precision Plus WesternC Standards; Lane 1 and 2, Non-reduced JJAV stained with silver; Lanes 3 and 4, Reduced and alkylated JJAV stained with silver; Lanes 5 and 6, Non-reduced JJAV immunoblotted with JJAV-sensitive pooled sera (arrows indicate IgE-binding bands); Lanes 7 and 8, Reduced and alkylated JJAV immunoblotted with JJAV-sensitive pooled sera; Lane 9, Non-reduced JJAV stained with glycoprotein stain Pro-Q Emerald 488. Green lined rectangular box indicates location of Myr p 1-3 bands. Red lined rectangular boxes indicate IgE-binding bands used in frequency analysis of Figure 3

previously identified as Myr p 1-3¹⁴; these peptides ran slower than would be expected based purely on their molecular weight, presumably due to large number of lysine residues, and were poorly resolved on SDS-PAGE. Another highly stained diffuse band migrated between 40 and 44 kDa, and at least 15 sharp bands were visible between 20 kDa and >250 kDa with variable staining intensities, defined herein as “high MW”. In contrast, separation of JJAV by AU-PAGE (Figure 2A, JJAV), which separates peptides on the basis of both size and charge and is particularly suited to the analysis of basic peptides, resolved the highly abundant low MW Myr p 1-3 peptides, and two lightly stained bands above the Myr p 2 band previously determined to be an oxidized form of Myr p 2.¹⁴ A comparison of JJAV immunoblots from AU-PAGE (Figure 2A) or SDS-PAGE (Figure 2B) separations, probed with serum from individual patients that each recognizes a subset of the Myr p bands, showed that Myr p 1 ran slightly ahead of Myr p 2 and Myr p 3 on SDS-PAGE, allowing patient immunoreaction to these two groups to be scored based on SDS-PAGE analysis (see below). Staining of JJAV for the presence of glycoproteins using Pro-Q[®] Emerald 488 glycoprotein stain indicated that protein components of 40-44 and 90 kDa were glycosylated (Figure 1, lane 9).

Reduction followed by alkylation of JJAV caused a shift in the heavily stained low MW smear to an apparent MW ≤ 15 kDa, due to reduction of the Myr p 2 and Myr p 3 disulfide linked dimers (Figure 1, lanes 3 and 4). The reduction and alkylation of JJAV proteins also resulted in an apparent upshift in MW distribution for most proteins in the 20-90 kDa range (Figure 1, lanes 3 and 4). Separation of reduced and alkylated JJAV by 2-DE revealed approximately 25 high MW (>20 kDa) spots with *pI* values between 3 and 9 and MW of 20-120 kDa (Figure S1, panel A). The low MW components separated into 6 diffuse bands with *pI* between 9 and 11 (consistent with theoretical *pIs* of pilosulin peptides in the range 9.9-10.5 based on sequence) and MW of approximately 5-15 kDa, and two spots with *pI* between 3 and 5 and MW of approximately 9 and 13 kDa, respectively (Figure S1, panel A).

3.3 | Analysis of JJAV allergenome

Non-reduced JJAV resolved by SDS-PAGE and immunoblotted using pooled sera from JJAV-allergic patients. Densitometry analysis revealed three diffuse IgE-binding bands <20 kDa, previously identified as the Myr p 1-3 peptides (Figure 1, lanes 5 and 6, filled

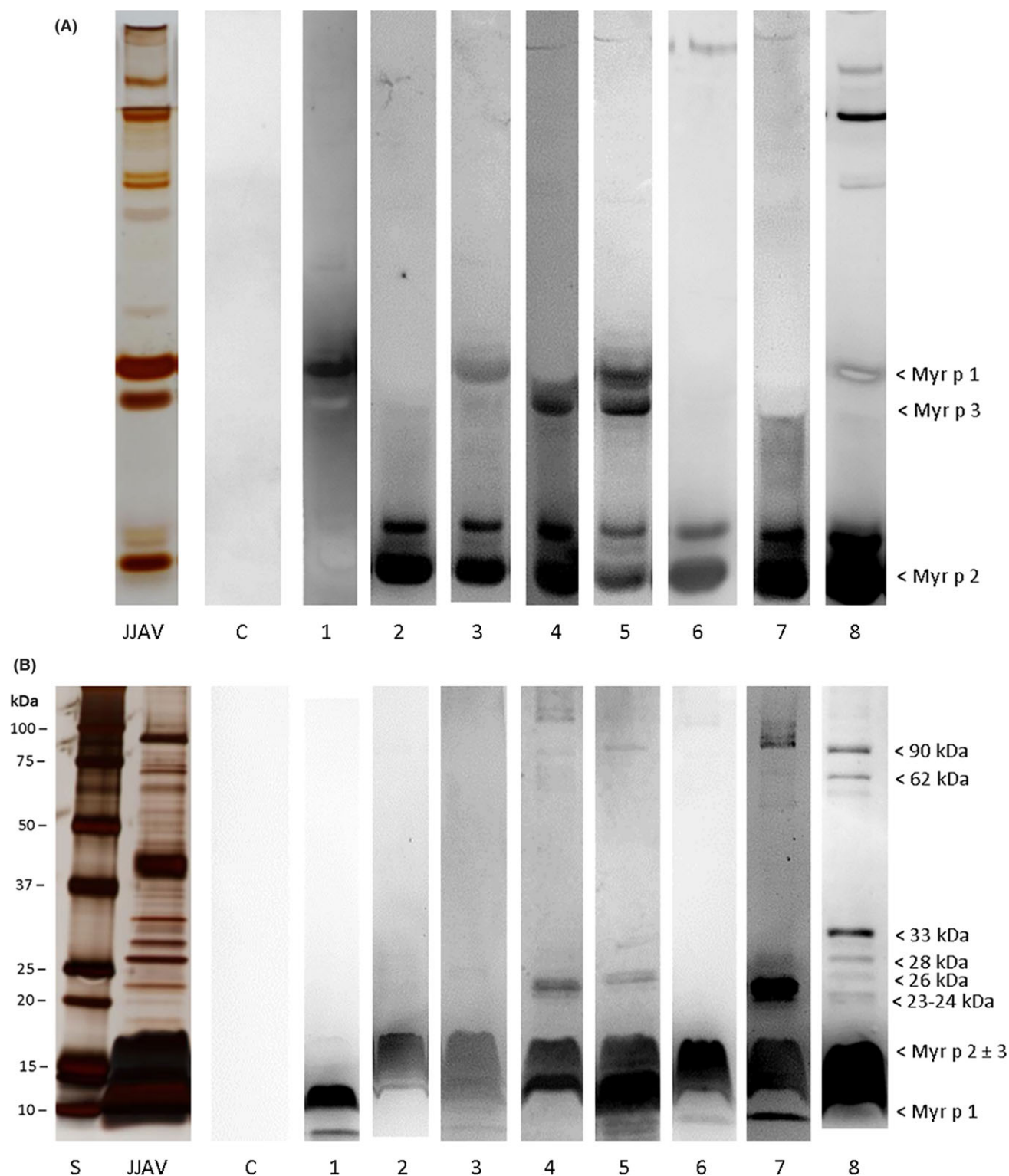


FIGURE 2 Representative results of non-reduced Jjav components resolved on AU-PAGE and stained with silver or immunoblotted using individual serum samples (A), or on 10%-20% Tris-Glycine SDS-PAGE and stained with silver or immunoblotted using the same individual serum samples (B). Lane S, Precision Plus WesternC Standards; Lane 1, exclusive recognition of Myr p 1; Lane 2, exclusive recognition of Myr p 2; Lane 3, recognition to Myr p 1 and Myr p 2; Lane 4, recognition to Myr p 2, Myr p 3 and 23 - 24 kDa band; Lane 5, recognition to Myr p 1-3 and 23 - 24 kDa band; Lane 6, recognition to Myr p 2 and 9 kDa band; Lane 7, recognition to Myr p 2, 9 kDa and 23 - 24 kDa bands; Lane 8, recognition to Myr p 2, 23 - 24 kDa, 26, 28, 33, 62 and 90 kDa bands. Lane C is control containing antibody dilution solution devoid of serum sample

arrows).¹² Additionally, there were seven high MW IgE-binding bands between 20 and 120 kDa, giving a total of ten IgE-binding bands over the MW range of 10–120 kDa (Figure 1, lanes 5 and 6, arrows). Reduction and alkylation of JJAV caused changes in the IgE-binding bands, including apparent shift in the molecular weight of some bands and weakening or disappearance of others (Figure 1, lanes 7 and 8), suggesting that some IgE-binding epitopes are dependent on the presence of intact disulfide bonds. Similarly, 2-DE immunoblots of reduced and alkylated JJAV identified a limited number of species compared to the 1D separation of non-reduced JJAV (Figure S1, panel B), suggesting that this was not a productive approach to isolate immunoreactive proteins in the native JJAV.

To analyse the proportion of patient sera that recognized each of the IgE-binding components in native JJAV, non-reduced venom was separated using SDS-PAGE and AU-PAGE, and immunoblotted using individual serum samples. All patient sera contained IgE that recognized at least one of the JJAV components between 9 and 90 kDa, but both the number of bands recognized and the pattern of immunoreactivity were highly variable (representative results are presented in Figure 2, panels A and B). The median number of IgE-binding bands recognized by individual serum was 2 (range 1–6) and proportion of patients with IgE against venom components resolved by SDS-PAGE is summarized in Figure 3. Ninety-one per cent of the patient sera recognized at least one of the low MW bands, 23% recognized the 11–14 kDa (Myr p 1; Figure 2) and 81% recognized the 14–18 kDa (Myr p 2; Figure 2) IgE-binding bands, while between 2% and 47% recognized each individual high MW band. In all, 27% of the sera exclusively recognized only low MW bands and 12% of sera only recognized high MW bands.

3.4 | Identification of JJAV components

Having established that 2-DE of reduced/alkylated JJAV yielded a limited number of immunoreactive components, we turned to SEC to

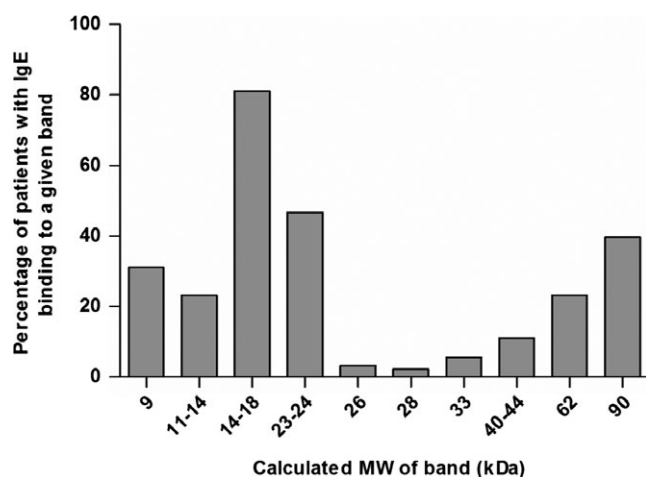


FIGURE 3 Proportion of patient sera that showed IgE-binding to each resolved non-reduced JJAV component as determined by 10%–20% Tris-Glycine SDS-PAGE followed by immunoblotting using sera from 90 JJAV allergic patients described in Table 1. Molecular weight calculation was based migration of proteins in Precision Plus Protein WesternC Standards

separate the high MW components of interest away from the more abundant and previously characterized low MW venom components. Native non-reduced venom was separated into 35 fractions (Figure S2), and based on the SDS-PAGE and immunoblotting analyses, fractions 15–24 were found to consist mostly of the high MW components and were therefore subjected to further analysis (Figure 4).

Protein bands corresponding to the low and high MW components were excised from SDS-PAGE gels and analysed by trypsin digestion and high resolution mass spectrometry, followed by database searching using PEAKS software. In addition to the previously known Myr p 1, Myr p 2, Myr p 3 and pilosulin 5 peptides, we found 17 distinct components with significant PEAKS scores that had not been previously identified in JJAV proteome (Table 2). The peptide sequences corresponding to the proteins listed in this table are presented in Table S1. Based on predicted function, these proteins were classified as possessing IgE-binding, enzymatic, structural and regulatory properties (12, 10, 4 and 2 proteins, respectively; Table 3).

3.5 | IgE-binding recognition profile and clinical correlations

Correlations (Spearman's rank) were found between IgE-binding recognition of the 14–18 kDa band (Myr p 2) with both JJAV-specific IgE ($r = 0.564$, $P < 0.0001$) and IDT threshold ($r = -0.493$, $P < 0.0001$). Correlations were found for paired IgE-binding recognition of the 26 kDa (phosphoglycerate mutase 1) and 28 kDa (venom Allergen 3-like) bands ($r = 0.802$, $P < 0.0001$), and the 40–44 kDa (arginine kinase) and 90 kDa (venom dipeptidyl peptidase IV) bands ($r = 0.448$, $P < 0.0001$). A correlation was also found for the 90 kDa band (venom dipeptidyl peptidase IV) to exist as part of multiple IgE-binding bands recognition (poly-sensitization) ($r = 0.546$; $P < 0.0001$). Weak but significant negative correlations were found for IgE-binding recognition to the 33 kDa (hyaluronidase), 40–44 kDa (arginine kinase), 62 kDa (esterase FE4-like) and 90 kDa (venom dipeptidyl peptidase IV) bands with JJAV-specific IgE ImmunoCAP ($r = -0.224$ to -0.269 ; $P < 0.05$; Table S2). No correlation was apparent between patients' previous worst reaction grade with recognition of any specific IgE-binding band.

To explore possible relationships between the risk of developing adverse reactions to JJA VIT and recognition of specific IgE-binding band(s) prior to treatment, hierarchical clustering analysis was performed (Figure S3). Recognition to the 11–14 kDa IgE-binding band (Myr p 1) and reaction score (which categorized patients' reaction profile during and after JJA VIT into 7 groups; Table 1) was found to cluster with moderate correlation ($r = 0.363$, $P = 0.0004$). No other correlation with reaction score was apparent.

4 | DISCUSSION

In the present study, we identified 21 distinct peptides and proteins in JJAV homologous to known protein sequences within the

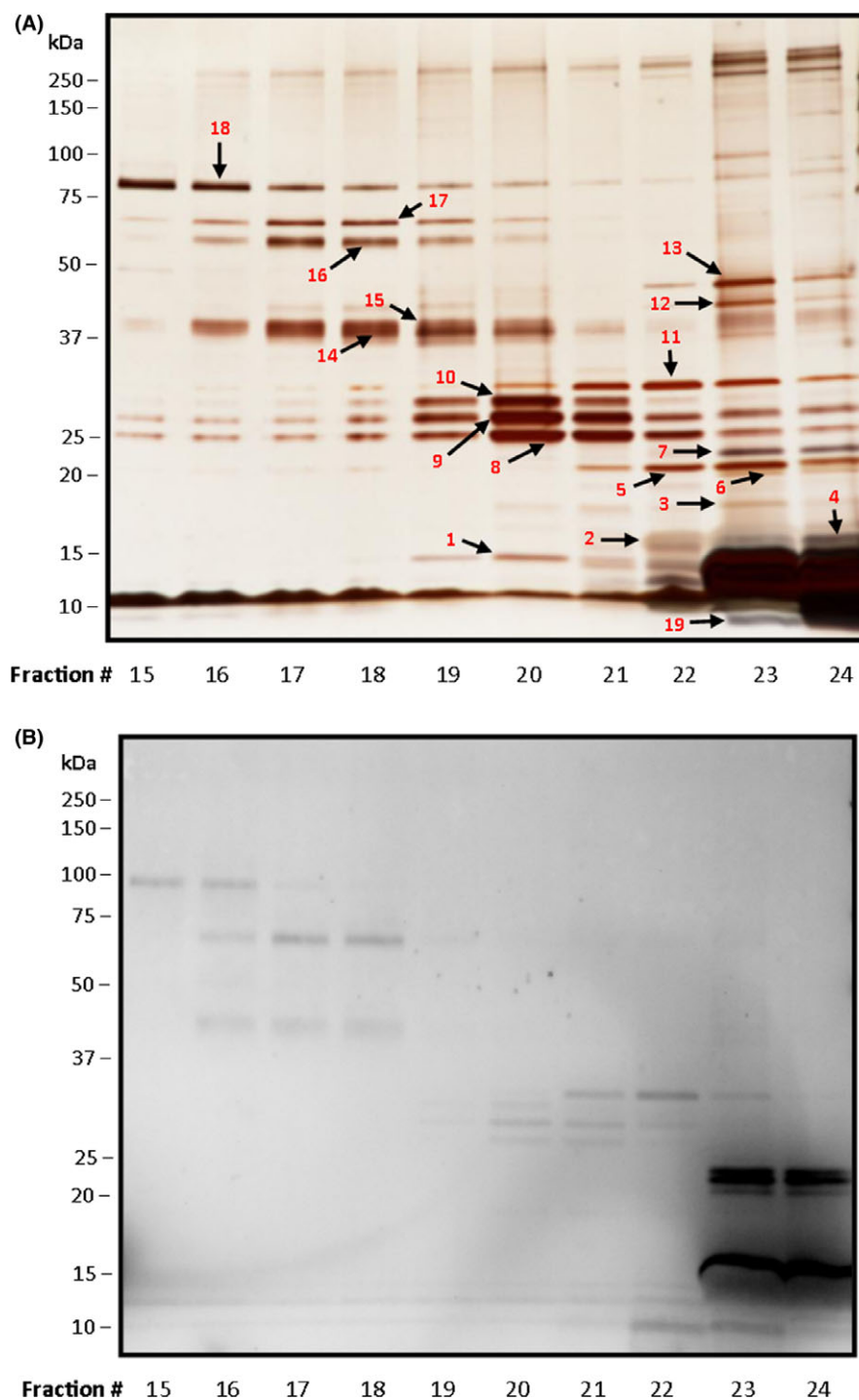


FIGURE 4 SDS-PAGE analysis of fractions from size exclusion chromatography of Jjav performed under non-reducing conditions. Selected elution fractions were separated on 10%-20% Tris-Glycine SDS-PAGE and were stained with silver (A), or immunoblotted with pooled sera from Jjav-sensitive patients (B). Molecular weight calculation was based on Precision Plus Protein WesternC Standards

Formicidae family. Seventeen of the proteins were not previously identified within Jjav, and at least 7 of these were capable of binding IgE based on their reactivity with the sera derived from Jjav-allergic patients. The four Jjav-specific peptides Myr p 1, Myr p 2 subunit pilosulin 3a, Myr p 3 and pilosulin 5 were also identified in this study. In previous work, the high relative abundance of the low MW Jjav peptides compromised detection of the low abundance venom components >20 kDa because of the tendency of the high abundance low MW venom components to streak on 1D and 2D gels (Figure S1). In this study, we used an alternative approach to

separate the low abundance venom components >20 kDa from the high-abundance low MW venom components. Separation of non-reduced Jjav by SEC and SDS-PAGE led to the successful discovery of novel IgE-binding and non-IgE-binding proteins using a combination of immunoblotting, in-gel protein digestion and mass spectrometry. Based on the SEC peak absorbance at 235 nm (Figure S2), the high MW fraction was estimated to account for 5% of the total protein components in Jjav by mass, consistent with previous estimation.¹⁷ Venom fractionation by SEC enabled the visualization of an increased number of the lower abundance high MW proteins

TABLE 2 Identification of fractionated JJAV components by tandem mass spectrometry

Band no. ^a	Protein (Allergen)	NCBI accession number	Molecular weight (kDa)		Matched peptides ^d	PEAKS score ^e
			Observed ^b	Target ^c		
1	Cu-Zn superoxide dismutase	gi 815812192 ref XP_012227043.1	15	15.49	3	137.88
2	Cofilin/actin-depolymerizing factor	gi 749756765 ref XP_011140861.1	16	16.86	6	151.79
	Phospholipid hydroperoxide glutathione peroxidase isoforms	gi 951523050 ref XP_014488366.1		19.09	5	137.54
	Pilosulin 4 (Myr p 3)	gi 51241753 dbj BAD36780.1		9.02	1	75.92
3	Muscle-specific protein 20-like	gi 752896490 ref XP_011266505.1	18	20.34	4	112.37
4	Peptidyl-prolyl cis-trans isomerase-like	gi 749749329 ref XP_011136874.1	17	22.9	9	192.41
	Pilosulin 1 (Myr p 1)	gi 730091 sp Q07932.1 MYR1_MYRPI		11.85	2	94.40
	Pilosulin 3a (Myr p 2)	gi 1911818 gb AAB50882.1		8.15	1	91.98
5	Acidic phospholipase A2, PA4 isoform X2	gi 751219056 ref XP_011162596.1	22	25.50	7	168.69
6	Acidic phospholipase A2, PA4 isoform X2	gi 751219056 ref XP_011162596.1	22	25.50	4	98.67
	Peptidyl-prolyl cis-trans isomerase B	gi 751221702 ref XP_011164043.1		21.84	3	96.70
7	Acidic phospholipase A2, PA4 isoform X2	gi 751219056 ref XP_011162596.1	23	25.50	2	105.47
8	Phosphoglycerate mutase 1	gi 826414896 ref XP_012522151.1	26	28.80	7	158.09
9	Venom allergen 3-like	gi 815804483 ref XP_012222952.1	28	26.37	2	90.63
10	Annexin B9	gi 752876495 ref XP_011255648.1	30	36.10	4	115.93
	Apolipoprotein D-like	gi 769852441 ref XP_011637689.1		30.70	3	106.83
11	Hyaluronidase-like	gi 826428058 ref XP_012527752.1	33	41.40	2	143.76
12	Elongation factor 1-alpha	gi 795085211 ref XP_011878235.1	46	50.25	3	81.87
13	Elongation factor 1-alpha isoform	gi 407021090 gb AFS65405.1	48	13.10	2	63.99
14	Arginine kinase isoform X2	gi 951526129 ref XP_014467326.1	40	39.71	5	133.36
15	Phosphoglycerate kinase	gi 769857915 ref XP_011640613.1	44	44.96	5	104.06
16	Esterase FE4-like	gi 861647540 gb KMQ95962.1	62	62.72	3	131.28
17	Transferrin	gi 815803678 ref XP_012222542.1	70	77.86	17	221.61
18	Venom dipeptidyl peptidase 4	gi 769837606 ref XP_011629993.1	90	87.45	4	125.91
19	Pilosulin 1 (Myr p 1)	gi 1911819 gb AAB50883.1	9	11.82	4	149.12
	Pilosulin 5	gi 161788856 dbj BAF95069.1		9.82	3	109.17

^aCorrespond to the serial number of SDS-PAGE protein band in Figure 4A.

^bBased on estimation of molecular weight in Figure 4A.

^cMolecular weight of matched protein based on sequence.

^dNumber of matched peptides that met PEAKS filter criteria (see Methods).

^eBased on calculated $-\log_{10} P$.

without overcrowding the SDS-PAGE lanes with the more abundant low MW venom components (Figure 4). The novel JJAV proteins were identified by searching for homologous proteins in the more distantly related members of the *Formicidae* family due to the minimal level of protein sequence information available for the *Myrmecia* genus, with the exception of the well-characterized low MW Myr p peptides.

The use of silver and SYPRO Ruby staining improved the sensitivity of protein detection compared to previous reports^{14,30} and lead to a higher number of protein able to be identified in the current study. The intensity of IgE-binding bands observed in 1D SDS-PAGE and 2-DE immunoblotting under reduced/alkylated condition was lower than expected when compared to the non-reduced sample. One possibility is that reduction and/or alkylation might have

destroyed epitopes dependent on the presence of disulfide bonds, leading to the diminished IgE detection. Similar findings have been reported by Wiese et al¹² and Street et al²⁶ when reduced/alkylated venom was resolved by tricine SDS-PAGE. The previous report that JJAV contains a glycoprotein with apparent MW of 45 kDa¹² was confirmed in the present study as part of the 40 - 44 kDa IgE-binding band (arginine kinase). Additionally, the 90 kDa IgE-binding band (venom dipeptidyl peptidase IV) was also found to be glycosylated (Figure 1, lane 9).

The proportion of patient sera that recognized individual IgE-binding bands in JJAV in this study was mostly consistent with previous report.¹² Using a larger study population, we confirmed that Myr p 2 is the major allergen in JJAV, being recognized by 81% of the population, and that the high MW IgE-binding bands 23-24 kDa

TABLE 3 Bioactivities of identified JJAV components

Band no. ^a	Protein (Allergen)	Putative function	IgE-binding capacity ^b
1	Cu-Zn superoxide dismutase	Antioxidant	
2	Cofilin/actin-depolymerizing factor	Regulator of actin dynamics	
	Phospholipid hydroperoxide glutathione peroxidase isoforms	Antioxidant	
	Pilosulin 4 (Myr p 3)	Antibiosis; histamine-releasing activity	Yes
3	Muscle-specific protein 20-like	Actin binding	
4	Peptidyl-prolyl cis-trans isomerase-like	Protein synthesis	Yes ^c
	Pilosulin 1 (Myr p 1)	Antibiosis	Yes
	Pilosulin 3a (Myr p 2)	Cytotoxic; hypotensive activity	Yes
5	Acidic phospholipase A2, PA4 isoform X2	Cytotoxic; haemolytic; anticoagulant; hypotensive activity	
6	Acidic phospholipase A2, PA4 isoform X2		Yes
	Peptidyl-prolyl cis-trans isomerase B	Protein synthesis	Yes ^c
7	Acidic phospholipase A2, PA4 isoform X2	Cytotoxic; haemolytic; anticoagulant; hypotensive activity	Yes
8	Phosphoglycerate mutase 1	Energy metabolism	Yes
9	Venom allergen 3-like	Allergen	Yes
10	Annexin B9	Actin binding	
	Apolipoprotein D-like	Transport protein	
11	Hyaluronidase-like	Facilitate venom spreading	Yes
12	Elongation factor 1-alpha	Protein synthesis	
13	Elongation factor 1-alpha isoform	Protein synthesis	
14	Arginine kinase isoform X2	Energy metabolism	Yes
15	Phosphoglycerate kinase	Energy metabolism	
16	Esterase FE4-like	Facilitate cytolysis	Yes
17	Transferrin	Transport protein; antioxidant	
18	Venom dipeptidyl peptidase 4	Activation of biomolecules	Yes
19	Pilosulin 1 (Myr p 1)	Antibiosis	Yes
	Pilosulin 5	Antibiosis; histamine-releasing	Yes ^c

^aCorrespond to the serial number of SDS-PAGE protein band in Figure 4A.

^bBased on immunoblot studies described in Figures 2 and 4B.

^cBased on indistinguishable results from SDS-PAGE immunoblot study described in Figure 4B.

(phospholipase A₂) and 90 kDa (venom dipeptidyl peptidase IV) were recognized by 47% and 40% of the population, respectively (Figure 3). The strong correlation for “paired” recognition of the 26- and 28 kDa IgE-binding bands (phosphoglycerate mutase and venom Allergen 3-like proteins, respectively) seen in this study was consistent with our previous study, which reported IgE-binding bands with apparent MWs of 30 and 32 kDa. Unlike the previous report, however, the current study found that the 40–44 kDa band (arginine kinase) is an IgE-binding band recognized by 11% of the population (Figure 3), whereas in the previous report it was recognized by 0% of the population studied.¹² Possible causes for the discrepancy might include differences in patient demography, eg only sera with RAST tracer uptake >1.0% was used in the previous study, and the different conditions used for SDS-PAGE and/or immunoblotting.

Venom preparations used in the diagnosis of JJAV allergy and in allergen immunotherapy are presently standardized only against the

well-characterized Myr p 1–3 allergenic peptides.^{7,9} However, our work suggests that current diagnostic tests are not adequate for patients who predominantly raise IgE to high MW components of the venom. Thus, patients who recognized Myr p 2 (14–18 kDa, Figure 2) were more likely to produce a high JJAV-specific IgE titre on ImmunoCAP and positive on IDT at lower test doses, whereas those who recognized IgE-binding bands of >20 kDa were more likely to produce low JJAV-specific IgE titre on ImmunoCAP. It is likely that low abundance of the non-standardized high MW components in JJAV accounts for the findings, and CRD using standardized recombinant allergens may improve detection sensitivity for these low abundance allergens.^{31,32} Likewise, the discovery that Myr p 1 (11–14 kDa, Figure 2) is correlated with an increased risk for experiencing frequent reactions during JJA VIT or sting challenge failure is potentially of clinical importance, but this must be confirmed in a larger study population. If proven, the quantification of this allergen by

CRD might help inform clinicians when assessing a patient's risk of developing frequent reactions to JJA VIT, or for treatment failure.

A prerequisite to develop the potential of CRD in JJAV is a thorough knowledge of JJAV proteome and allergenome composition.^{19,21} Besides the positive identification of pilosulins (Myr p) family of low MW peptides in the venom, this study has for the first time identified various proteins in the venom of JJA. Several of the identified proteins corresponded to enzymatic activities that had previously been identified in JJAV.^{9,17,33}

Phospholipase A₂ (PLA₂) activity in the venom of JJA has been reported,³³ and we identified putative PLA₂ enzyme(s) as components of the 22 - 24 kDa IgE-binding bands. PLAs are common in Hymenoptera venoms and are known to have IgE-binding capacity in various insects.¹⁸ They are able to disrupt the phospholipid layers of biological membranes, causing pore formation, cell lysis, inflammation and tissue damage³⁴ and are responsible for the haemolytic, cytotoxic, hypotensive and anticoagulant activities in Hymenoptera venoms.³⁵ The PLA₂ superfamily is known for its 6 conserved disulfide bonds,³⁶ and it is possible that the disappearance of the 22 - 24 kDa IgE-binding bands upon reduction/alkylation reactions results from loss of an epitope that was stabilized by these disulfide links. Previous studies have shown that the 22 - 24 kDa IgE-binding bands in JJAV are prone to degradation^{8,9} and it is possible that PLA₂ was the heat-sensitive haemolytic factor previously described by Matuszek et al.³⁷ In addition to PLA₂, the enzyme peptidyl-prolyl cis-trans isomerase (PPIase), was also detected as a component of the 22 - 24 kDa band. PPIases are ubiquitous enzymes that catalyse the cis-trans isomerization of peptidyl-prolyl bonds, an otherwise slow process that can hamper protein folding.³⁸ Together with elongation factor, which was identified as the component of the 46 and 48 kDa bands in JJAV, they play potentially important roles in peptide and protein synthesis.³⁹

Jack Jumper ant venom has previously been shown to exhibit phosphatases activities in separate studies.^{9,33} Analysis of the 26 kDa IgE-binding band showed the presence of phosphoglycerate mutase (PGM), a member of the alkaline phosphatase superfamily,^{40,41} known to catalyse the internal transfer of phosphate groups within phosphoglycerates, an essential component in energy metabolism.⁴² PGM has also been detected in honeybee venom.⁴³ The 28 kDa IgE-binding band in JJAV was found to contain venom Allergen 3-like protein, which is one of the major allergenic proteins of the fire ant (*Solenopsis invicta*) venom and is structurally related to the vespid venom Antigen 5, members of the cysteine-rich secretory proteins (CRISP) family.^{34,44,45}

Hyaluronidases are widely distributed enzymes in animal venoms, including Hymenoptera.^{33,46} Recently, we showed that the venom of JJA exhibits glycosidases activities⁹; it is likely that hyaluronidase, a glycosidase enzyme found as the component of the 33 kDa IgE-binding band was responsible for this activity. Hyaluronidases have been described as "spreading factors", facilitating the penetration of venom components through the tissues and into the blood stream by promoting the hydrolysis of glycosaminoglycans, one of the major components of the extracellular matrix of vertebrates.³⁵

Hyaluronidases are known allergenic components of honeybee and vespid venoms.¹⁸

Analysis of the 40 - 44 kDa IgE-binding glycoprotein band revealed the presence of 2 transferases, arginine kinase (AK) and phosphoglycerate kinase (PGK). AK is a 40 kDa enzyme that is involved in energy metabolism in invertebrates.⁴⁷ AK has been reported as a cross-reactive pan-allergen found in several invertebrate species, including in honeybee and wasps.^{43,47-52} Similar to the venom of the social wasp *Polybia paulista*,⁴⁸ the AK present in JJAV was also glycosylated. Like AK, PGK is an enzyme involved in energy metabolism, and it has also been detected in the venom of *Neoponera villosa* ant.⁵³

Matuszek et al.³³ reported the absence of esterase activity in JJAV. Contrary to this earlier finding, the presence of esterase FE4-like enzyme was identified in the current study as a component of the 62 kDa IgE-binding band. It has been proposed that esterases in insect venoms participate in completing the hydrolytic action of hyaluronidase and PLAs, aiding the process of cell lysis and the destruction of components of lysed cells.⁵⁴ A 70 kDa carboxylesterase allergen also exists in honeybee venom.¹⁸

The identification of dipeptidylpeptidase IV (DPP4) as the component of the 90 kDa IgE-binding glycoprotein band may explain the recent finding of protease activity in JJAV.⁹ DPP4 is a highly glycosylated serine protease that selectively removes N-terminal dipeptides with proline, alanine or hydroxyproline in the penultimate position.⁵⁵ DPP4 processes the precursors of mellitin in honeybee and mastoparan B in vespid venoms, into their mature forms^{43,55,56}; it is possible that the DPP4 in JJAV has a similar role, assisting post-translational processing of the Myr p precursor peptides. DPP4 is a known allergen present in honeybee and vespid venoms.¹⁸

Similar to other Hymenoptera venoms,^{34,43,48,57} the venom of JJA also contains proteins involved in the protection against oxidative stress (Cu-Zn superoxide dismutase, phospholipids hydroperoxide glutathione peroxidase and transferrin), and cytoskeleton-regulating proteins (cofilin/actin-depolymerizing factor, annexin and elongation factor). These proteins have not been found to exhibit any IgE-binding capacity in the current study.

5 | CONCLUSION

Using an immunoproteomics approach and sera from patients with clinically proven allergy to JJAV, this study successfully verified the frequency of patients with IgE that recognize JJAV allergen's IgE binding, confirmed the existence of the four pilosulins (Myr p) peptides, and more importantly this study has established the identity of the previously unknown high MW IgE-binding components in the venom of JJA for the first time. The clinical relevance of these IgE-binding components has also been defined in this study. The putative function and IgE-binding capacity of the characterized JJAV components are summarized in Table 3. This study has paved the way for advancing the diagnosis of Hymenoptera sting allergy and the delivery of JJA VIT towards personalized treatment.

ACKNOWLEDGEMENTS

We are thankful to Dr. Christine Chuter, Rachel Hutchinson, Rhys Gunner, Joanne Rae, Jenine Keys, Anna Stubbs, Fiona Symons, Ruth Hudson and Jane Edwards for their assistance with blood sampling; Sandra Aho-kas, Judith Hawker, Jenny Gudden, Jopy Gudden, Amanda Bannister, Shaun Bannister, Simon Stubbs, Rhys Gunner and Dr. Malcom Turner for their assistance in collecting the ants; Judith Hawker, Hayley Webb, Eleanor Chiu, Joanne McKay and Dr. Emily Mulcahy for their assistance in performing venom sac dissection; Judith Hawker, Amanda Bannister, Roseanne Ford, Janella Witmore, Joanne McKay, Elizabeth Jordan and Anne Kaye for their technical assistance in the manufacture of JJAV API grade; Dr. Cesar Tovar for his technical expertise in 2-DE; Gary Lee for technical assistance with document management and Dr. Mark Ambrose, Associate Professor Subramanyam Vemulpad, Dr. Wun Yee Lau, Dr. Emily Mulcahy and Mrs. Leonie McLean for reviewing the manuscript.

CONFLICT OF INTEREST

TW, HER, SGAB and MDW are either employee or consultants to the Tasmanian Health Service, the organization owning the intellectual property over Jack Jumper Ant Venom Immunotherapy. All other authors declare no conflict of interest.

AUTHOR CONTRIBUTION

TW conceived the study and designed the study methodologies. TW, HER, RW and DG performed the experiments. TW, RW and DG analysed the data. TW prepared the manuscript. All authors participated in its revisions and have approved the final form.

ORCID

Troy Wanandy  <http://orcid.org/0000-0003-4703-0488>

Richard Wilson  <http://orcid.org/0000-0003-0152-4394>

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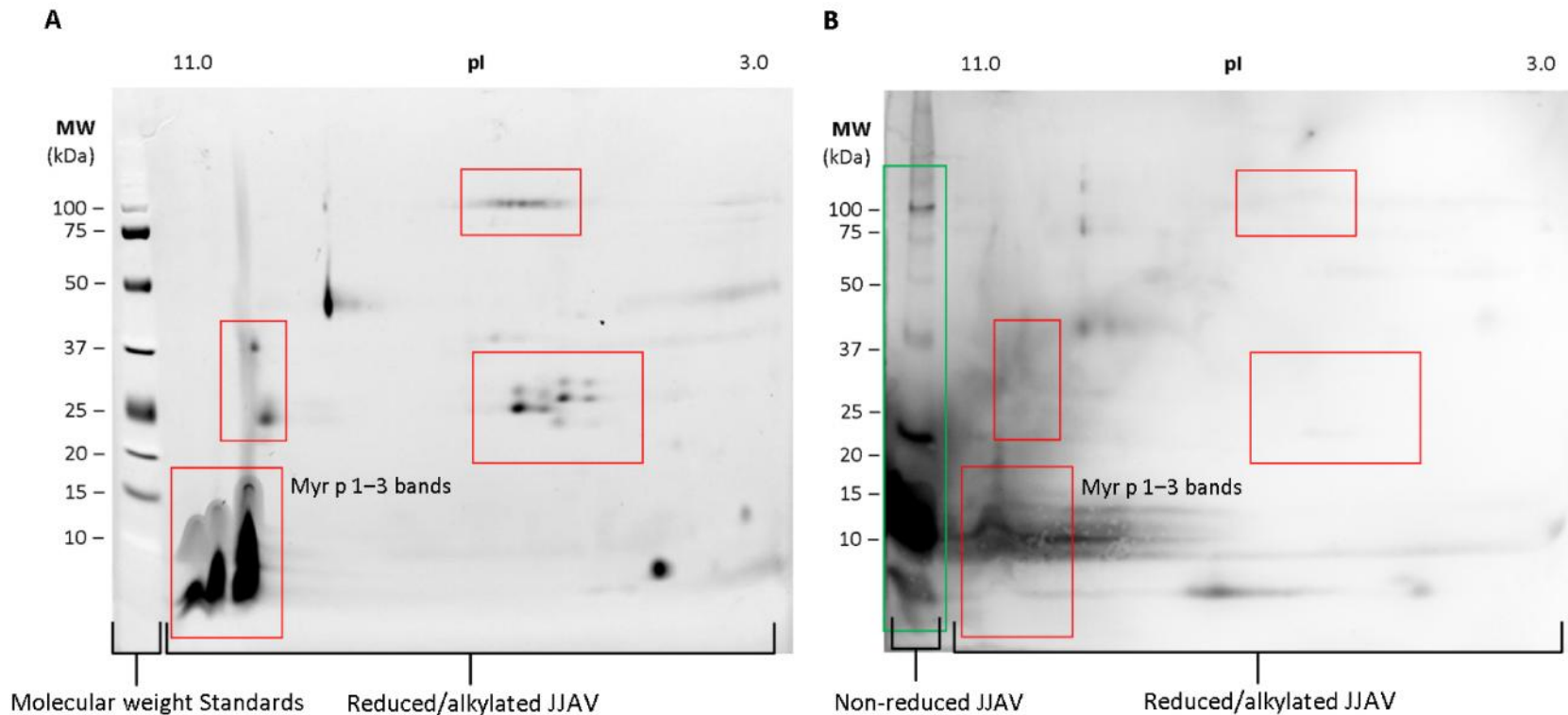
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SUPPORTING INFORMATION

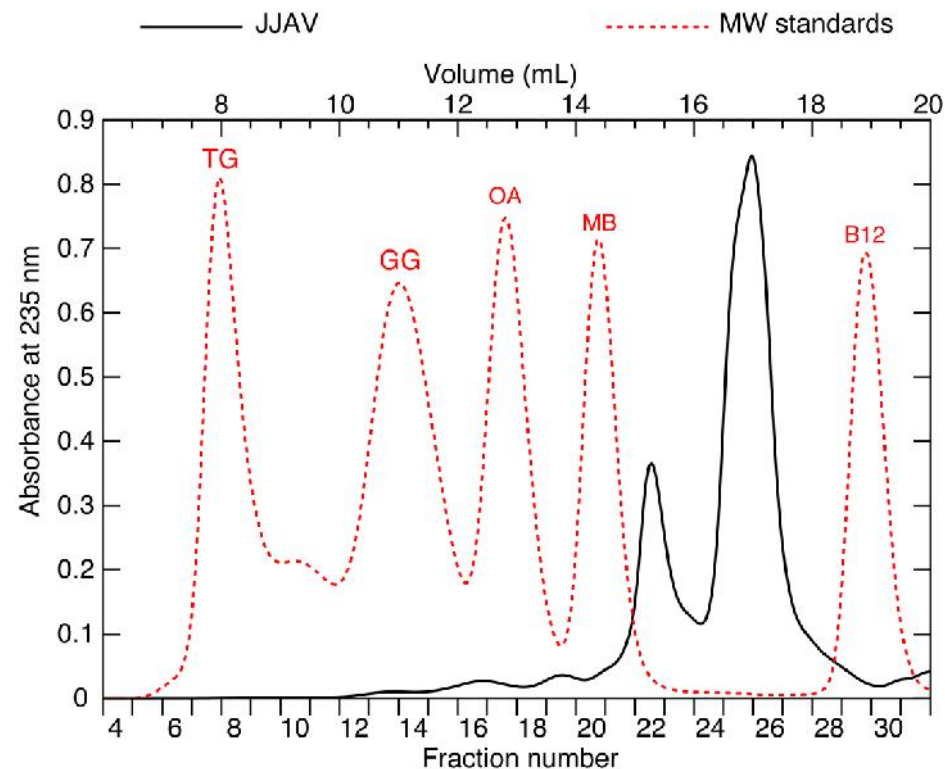
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How to cite this article: Wanandy T, Wilson R, Gell D, et al. Towards complete identification of allergens in Jack Jumper (*Myrmecia pilosula*) ant venom and their clinical relevance: An immunoproteomic approach. *Clin Exp Allergy.* 2018;48:1222–1234. <https://doi.org/10.1111/cea.13224>

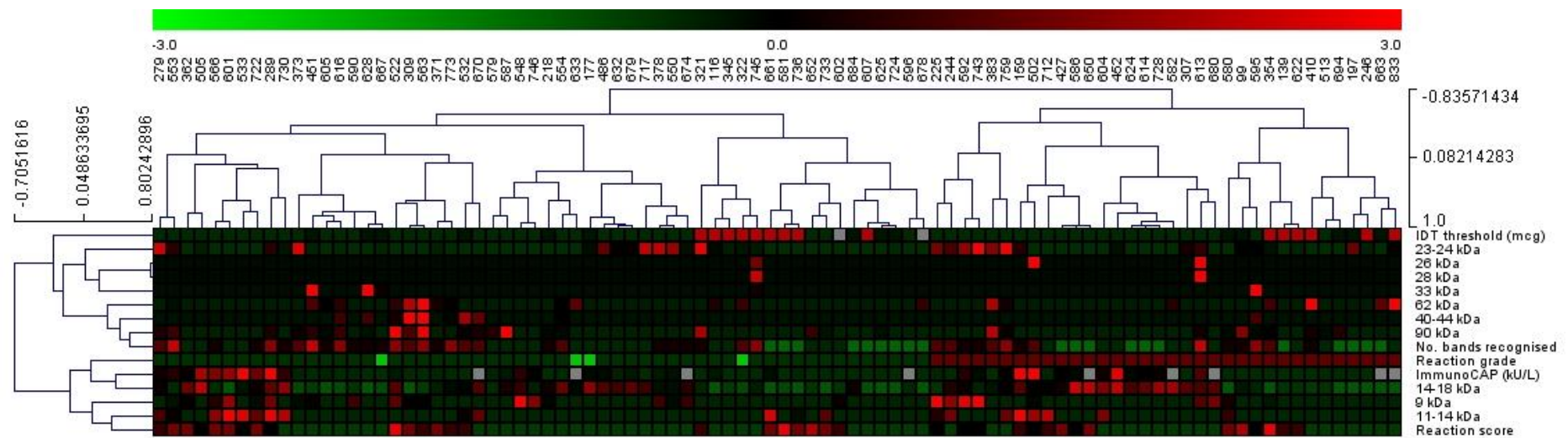
Supporting Information



Supplementary Figure 1. Representative profiles of reduced and alkylated JJAV components separated by 2-DE. The first dimension (IEF) was carried out in a non-linear pH 3–11 gradient IPG strip and the second dimension in a 4–12% Bis-Tris SDS-PAGE gel. (A) Second dimension gel was stained with SYPRO Ruby; (B) Second dimension gel was electro-transferred into a PVDF membrane and immunoblotted with a pooled sera from JJAV allergic patients. Areas marked in green and red show appearance of IgE-binding signals in non-reduced JJAV (loaded in the marker well of the second dimension gel) and disappearance of IgE-binding signals due to reduction/alkylation reactions, respectively. Molecular weight calculation was based on Precision Plus Protein WesternC Standards.



Supplementary Figure 2. Size Exclusion Chromatography profile of JJAV fractionation carried out in Superose® 12 column chromatography. Injections consisted of 0.5 mL of non-reduced JJAV at a concentration of 1 mg/mL. Elution was performed with 50 mM sodium phosphate, 150 mM sodium chloride, pH = 7. Fractions of 0.5 mL were collected at a flow rate of 0.5 mL/min and eluents were detected by absorbance at 235 nm. Molecular weight standards were thyroglobulin (TG, 670 kDa), γ -globulin (GG, 158 kDa), ovalbumin (OA, 44 kDa), myoglobin (MG, 17 kDa), and vitamin B₁₂ (B12, 1.36 kDa).



Supplementary Figure 3. Analysis of individual sera samples to determine clustering patterns in data. Data were normalised across rows and an unsupervised clustering (hierarchical clustering) was performed using a nonparametric Spearman's rank correlation distance metric and average linkage clustering method. A heat-map expression image was created to visualise results. Heat-map colour configuration: grey, black, green, and red squares represent absence of data, unchanged, low (down-regulated), and high (up-regulated) relative expression, respectively. Colour intensity of every single square in the heat-map is directly associated with the intensity of measured value, score or category. Label of dendrogram in vertical direction: 3 digits number represents patient's ID. Label of dendrogram in horizontal direction: Reaction score describes patients' reaction profile during VIT categorized numerically as described in Table 1; IDT = intradermal test; Reaction grade = severity of anaphylaxis according to the criteria of Brown (1).

Supplementary Table 2. Correlation analysis of recognition of JJAV IgE-binding bands

		Calculated molecular weight of IgE-binding band (kDa)									
		9	11–14	14–18	23–24	26	28	33	40–44	62	90
IDT threshold	r =	-0.262	-0.271	-0.493	NS	NS	NS	0.210	NS	NS	NS
	P =	0.0137	0.0107	<0.0001				0.0491			
ImmunoCAP	r =	0.270	0.486	0.564	NS	NS	NS	-0.254	-0.224	-0.269	-0.263
	P =	0.0147	<0.0001	<0.0001				0.0221	0.0445	0.0154	0.0176

IDT = intradermal test; r = Spearman's correlation coefficient; NS = not significant; Significance < 0.05.

Reference

1. Brown SG. Clinical features and severity grading of anaphylaxis. *Journal of Allergy and Clinical Immunology*. 2004;114(2):371-6.

Band # 1 Proteins

Summary

1. Notes

2. Result Statistics

Figure 1. False discovery rate (FDR) curve. X axis is the number of peptide-spectrum matches (PSM) being kept. Y axis is the corresponding FDR.

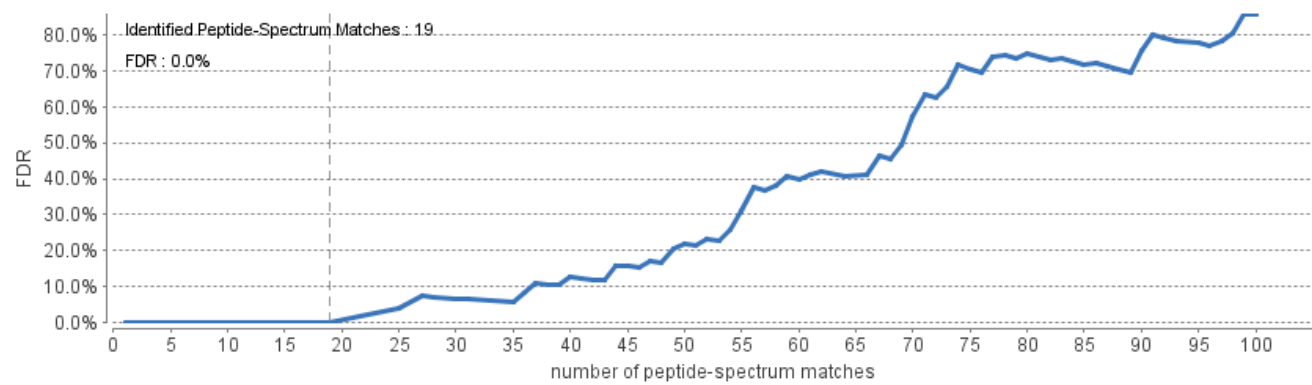


Figure 2. PSM score distribution. (a) Distribution of PEAKS peptide score; (b) Scatterplot of PEAKS peptide score versus precursor mass error.

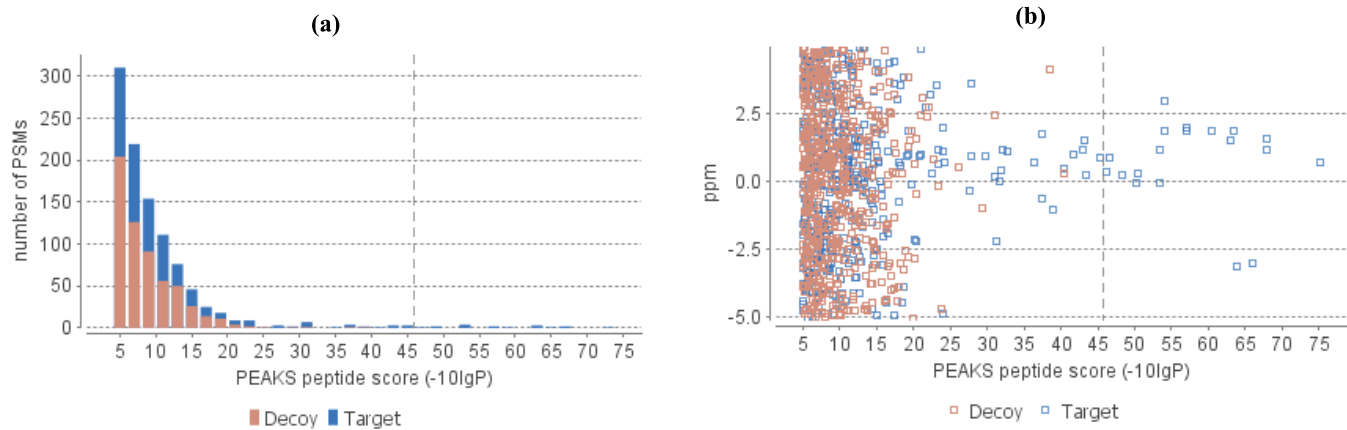


Figure 3. De novo result validation. Distribution of residue local confidence: (a) Residues in de novo sequences validated by confident database peptide assignment; (b) Residues in "de novo only" sequences.

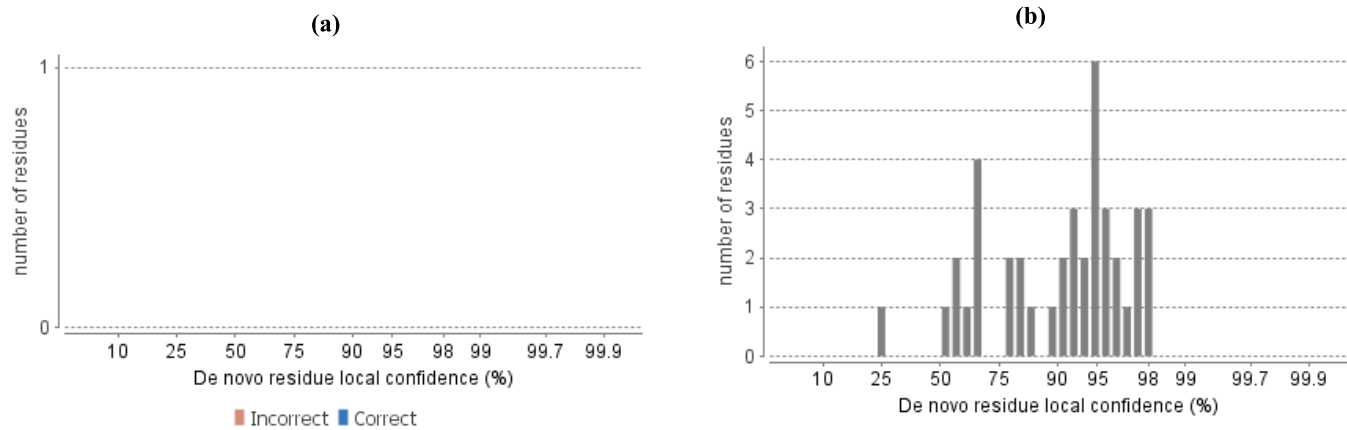


Table 1. Statistics of data.

# of MS Scans	1738
# of MS/MS Scans	2604

Table 4. PTM profile.

Name	Δ Mass	Position	#PSM	-10lgP	Area	AScore
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Table 2. Result filtration parameters.

Peptide -10lgP	≥45.8
Protein -10lgP	≥20
Proteins unique peptides	≥1
De novo ALC Score	≥80%

Table 3. Statistics of filtered result.

Peptide-Spectrum Matches	19
Peptide Sequences	15
Protein Groups	6
Proteins	64
Proteins (#Unique Peptides)	1 (>2); 28 (=2); 35 (=1);
FDR (Peptide-Spectrum Matches)	0.0%
FDR (Peptide Sequences)	0.0%
FDR (Protein)	0.0%
De Novo Only Spectra	4

3. Experiment Control

Figure 4. Precursor mass error of peptide-spectrum matches (PSM) in filtered result. **(a)** Distribution of precursor mass error in ppm; **(b)** Scatterplot of precursor m/z versus precursor mass error in ppm. 

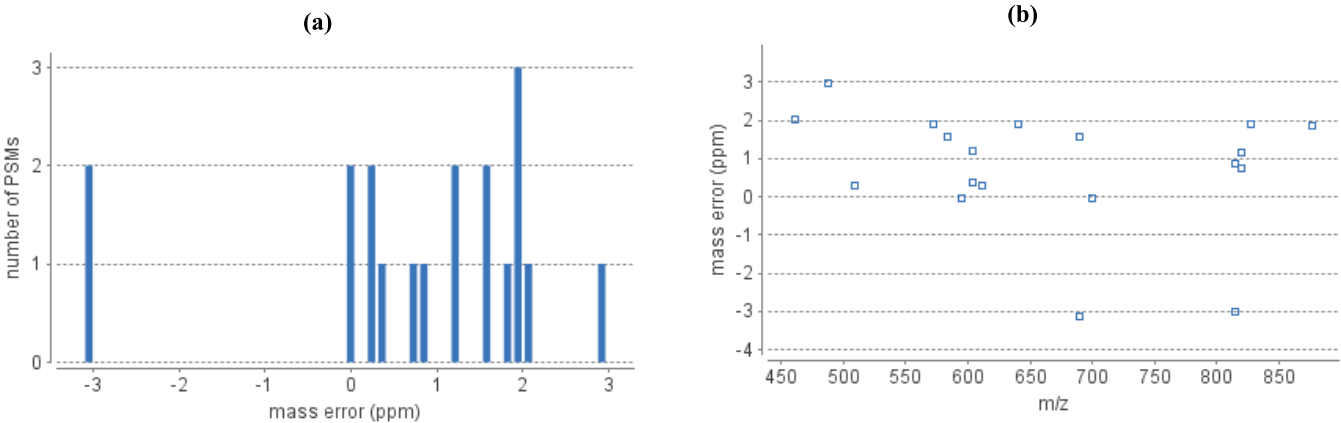


Table 5. Number of identified peptides in each sample by the number of missed cleavages

Missed Cleavages	0	1	2	3	4+
Sample 3	15	0	0	0	0

4. Other Information

Table 6. Search parameters.

Search Engine Name:	PEAKS
Parent Mass Error Tolerance:	5.0 ppm
Fragment Mass Error Tolerance:	0.5 Da
Precursor Mass Search Type:	monoisotopic
Enzyme:	Trypsin
Max Missed Cleavages:	3
Non-specific Cleavage:	one
Variable Modifications:	
Oxidation (M):	15.99
Max variable PTM per peptide:	3
Database:	Ant
Taxon:	All
Searched Entry:	473117
FDR Estimation:	Enabled
Merge Options:	no merge
Precursor Options:	corrected
Charge Options:	no correction

Table 7. Instrument parameters.

Fractions:	TW_1.raw
Ion Source:	ESI(nano-spray)
Fragmentation Mode:	CID, CAD(y and b ions)
MS Scan Mode:	FT-ICR/Orbitrap
MS/MS Scan Mode:	FT-ICR/Orbitrap

Filter Options: no filter

Process: true

Protein List

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
1	5563	gi 815812192 ref XP_012227043.1	137.88	25	3	1	N	15487	PREDICTED: LOW QUALITY PROTEIN: superoxide dismutase [Cu-Zn]-like [Linepithema humile]
2	5562	gi 951534390 ref XP_014470825.1	121.24	23	3	1	N	15998	PREDICTED: superoxide dismutase [Cu-Zn] [Dinoponera quadriceps]
3	5638	gi 751223514 ref XP_011165046.1	118.33	8	3	3	N	16026	PREDICTED: superoxide dismutase [Cu-Zn] 2 [Solenopsis invicta]
10	5608	gi 751222350 ref XP_011164407.1	90.40	19	2	2	N	18548	PREDICTED: heat shock protein Hsp-12.2-like, partial [Solenopsis invicta]
10	5609	gi 759051224 ref XP_011334715.1	90.40	17	2	2	N	20862	PREDICTED: alpha-crystallin A chain isoform X3 [Ceropachys biroï]
10	5610	gi 752872702 ref XP_011253601.1	90.40	17	2	2	N	20841	PREDICTED: alpha-crystallin A chain isoform X3 [Camponotus floridanus]
10	5611	gi 769839777 ref XP_011631058.1	90.40	17	2	2	N	20745	PREDICTED: heat shock protein beta-1 isoform X3 [Pogonomyrmex barbatus]
10	5612	gi 332024680 gb EGI64873.1	90.40	17	2	2	N	20754	Heat shock protein beta-1 [Acromyrmex echinator]
10	5613	gi 749753594 ref XP_011139193.1	90.40	17	2	2	N	20902	PREDICTED: alpha-crystallin A chain isoform X3 [Harpegnathos saltator]
10	5614	gi 759051222 ref XP_011334714.1	90.40	17	2	2	N	21562	PREDICTED: alpha-crystallin A chain isoform X2 [Ceropachys biroï]
10	5615	gi 769839775 ref XP_011631057.1	90.40	17	2	2	N	21563	PREDICTED: heat shock protein beta-1 isoform X2 [Pogonomyrmex barbatus]
10	5616	gi 780676049 ref XP_011696443.1	90.40	17	2	2	N	21604	PREDICTED: heat shock protein beta-1 isoform X2 [Wasmannia auropunctata]
10	5617	gi 746849784 ref XP_011055349.1	90.40	17	2	2	N	21590	PREDICTED: alpha-crystallin A chain isoform X2 [Acromyrmex echinator]
10	5618	gi 752872700 ref XP_011253600.1	90.40	17	2	2	N	21620	PREDICTED: alpha-crystallin A chain isoform X2 [Camponotus floridanus]
10	5619	gi 815809945 ref XP_012225858.1	90.40	17	2	2	N	21615	PREDICTED: alpha-crystallin A chain isoform X2 [Linepithema humile]
10	5620	gi 826423161 ref XP_012526611.1	90.40	17	2	2	N	21728	PREDICTED: alpha-crystallin B chain isoform X2 [Monomorium pharaonis]
10	5621	gi 951521022 ref XP_014483640.1	90.40	17	2	2	N	21678	PREDICTED: alpha-crystallin A chain isoform X1 [Dinoponera quadriceps]
10	5622	gi 749753592 ref XP_011139192.1	90.40	17	2	2	N	21678	PREDICTED: alpha-crystallin A chain isoform X2 [Harpegnathos saltator]
10	5623	gi 795042285 ref XP_011867213.1	90.40	17	2	2	N	21691	PREDICTED: heat shock protein beta-1 isoform X2 [Vollenhovia emeryi]
10	5624	gi 607362572 gb EZA56819.1	90.40	14	2	2	N	25315	Heat shock protein beta-1 [Ceropachys biroï]
10	5625	gi 759051220 ref XP_011334713.1	90.40	14	2	2	N	25920	PREDICTED: alpha-crystallin B chain isoform X1 [Ceropachys biroï]
10	5626	gi 780676045 ref XP_011696442.1	90.40	14	2	2	N	25915	PREDICTED: alpha-crystallin B chain isoform X1 [Wasmannia auropunctata]
10	5627	gi 746849782 ref XP_011055348.1	90.40	14	2	2	N	25942	PREDICTED: alpha-crystallin B chain isoform X1 [Acromyrmex echinator]
10	5628	gi 801371108 ref XP_012061833.1	90.40	14	2	2	N	25920	PREDICTED: alpha-crystallin B chain [Atta cephalotes]
10	5629	gi 815809943 ref XP_012225857.1	90.40	14	2	2	N	25931	PREDICTED: alpha-crystallin B chain isoform X1 [Linepithema humile]
10	5630	gi 769839773 ref XP_011631056.1	90.40	14	2	2	N	25921	PREDICTED: alpha-crystallin B chain isoform X1 [Pogonomyrmex barbatus]
10	5631	gi 752872698 ref XP_011253599.1	90.40	14	2	2	N	25941	PREDICTED: alpha-crystallin B chain isoform X1 [Camponotus floridanus]
10	5632	gi 749753590 ref XP_011139191.1	90.40	14	2	2	N	26032	PREDICTED: alpha-crystallin B chain isoform X1 [Harpegnathos saltator]
10	5633	gi 795042282 ref XP_011867212.1	90.40	14	2	2	N	26031	PREDICTED: alpha-crystallin B chain isoform X1 [Vollenhovia emeryi]
10	5634	gi 826423159 ref XP_012526610.1	90.40	14	2	2	N	26039	PREDICTED: alpha-crystallin B chain isoform X1 [Monomorium pharaonis]
10	5635	gi 815809947 ref XP_012225859.1	90.40	12	2	2	N	29744	PREDICTED: alpha-crystallin B chain isoform X3 [Linepithema humile]
6	77	gi 1911819 gb AAB50883.1	53.46	10	1	1	Y	11819	Myr p I=allergenic polypeptide {N-terminal} [Myrmecia pilosula=jumper ants, venom, Peptide Partial, 112 aa]
6	78	gi 312284 emb CAA49760.1	53.46	10	1	1	Y	11849	major allergen [Myrmecia pilosula]

total 64 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
6	76	gi 730091 sp Q07932.1 MYR1_MYRPI	53.46	10	1	1	Y	11849	RecName: Full=Pilosulin-1; AltName: Full=Allergen Myr p I; AltName: Full=Major allergen Myr p 1; AltName: Allergen=Myr p 1; Contains: RecName: Full=Pilosulin-1; Contains: RecName: Full=Pilosulin-1 65->112; Contains: RecNa...
30	5642	gi 751228682 ref XP_011167761.1	50.31	9	1	1	N	17087	PREDICTED: myosin light chain alkali isoform X2 [Solenopsis invicta]
30	5643	gi 815801638 ref XP_012221484.1	50.31	9	1	1	N	17041	PREDICTED: myosin light chain alkali [Linepithema humile]
30	5644	gi 769856981 ref XP_011640107.1	50.31	9	1	1	N	17133	PREDICTED: myosin light chain alkali isoform X2 [Pogonomymex barbatus]
30	128	gi 749750482 ref XP_011137501.1	50.31	9	1	1	N	17069	PREDICTED: myosin light chain alkali isoform X2 [Harpegnathos saltator]
30	5645	gi 826465315 ref XP_012535022.1	50.31	9	1	1	N	17113	PREDICTED: myosin light chain alkali isoform X2 [Monomorium pharaonis]
30	5646	gi 780687964 ref XP_011698945.1	50.31	9	1	1	N	17075	PREDICTED: myosin light chain alkali isoform X2 [Wasmannia auropunctata]
30	5647	gi 759072917 ref XP_011346087.1	50.31	9	1	1	N	17085	PREDICTED: myosin light chain alkali [Ceraaphys biroi]
30	5648	gi 951531116 ref XP_014469383.1	50.31	9	1	1	N	17026	PREDICTED: myosin light chain alkali [Dinoponera quadricaps]
30	5649	gi 759072919 ref XP_011346088.1	50.31	9	1	1	N	17085	PREDICTED: myosin light chain alkali [Ceraaphys biroi]
30	5650	gi 795063214 ref XP_011873749.1	50.31	9	1	1	N	17112	PREDICTED: myosin light chain alkali isoform X2 [Vollenhovia emeryi]
30	5651	gi 746847494 ref XP_011054119.1	50.31	9	1	1	N	17131	PREDICTED: myosin light chain alkali isoform X2 [Acromymex echinatio]
30	5652	gi 307175833 gb EFN65648.1	50.31	9	1	1	N	17026	Myosin light chain alkali [Camponotus floridanus]
30	5653	gi 752885282 ref XP_011260420.1	50.31	9	1	1	N	17026	PREDICTED: myosin light chain alkali isoform X2 [Camponotus floridanus]
30	5654	gi 307208335 gb EFN85742.1	50.31	9	1	1	N	17069	Myosin light chain alkali [Harpegnathos saltator]
30	5655	gi 1009373340 gb KYM97205.1	50.31	8	1	1	N	17233	Myosin light chain alkali [Cyphomyrmex costatus]
30	5656	gi 752885280 ref XP_011260419.1	50.31	8	1	1	N	17556	PREDICTED: myosin light chain alkali isoform X1 [Camponotus floridanus]
30	5657	gi 746847492 ref XP_011054118.1	50.31	8	1	1	N	17603	PREDICTED: myosin light chain alkali isoform X1 [Acromymex echinatio]
30	5658	gi 795063205 ref XP_011873748.1	50.31	8	1	1	N	17699	PREDICTED: myosin light chain alkali isoform X1 [Vollenhovia emeryi]
30	5659	gi 769856979 ref XP_011640106.1	50.31	8	1	1	N	17729	PREDICTED: myosin light chain alkali isoform X1 [Pogonomymex barbatus]
30	5660	gi 780687958 ref XP_011698944.1	50.31	8	1	1	N	17647	PREDICTED: myosin light chain alkali isoform X1 [Wasmannia auropunctata]
30	5661	gi 751228680 ref XP_011167760.1	50.31	8	1	1	N	17658	PREDICTED: myosin light chain alkali isoform X1 [Solenopsis invicta]
30	5662	gi 749750480 ref XP_011137500.1	50.31	8	1	1	N	17826	PREDICTED: myosin light chain alkali isoform X1 [Harpegnathos saltator]
30	5663	gi 826465309 ref XP_012535021.1	50.31	8	1	1	N	17884	PREDICTED: myosin light chain alkali isoform X1 [Monomorium pharaonis]
30	5664	gi 322786593 gb EFZ12988.1	50.31	7	1	1	N	20456	hypothetical protein SINV_04902, partial [Solenopsis invicta]
30	5665	gi 1009354327 gb KYM79681.1	50.31	7	1	1	N	20373	Myosin light chain alkali [Atta colombica]
30	5666	gi 1009388322 gb KYN10341.1	50.31	7	1	1	N	20515	Myosin light chain alkali [Trachymymex conetzi]
30	5667	gi 1009419342 gb KYN37901.1	50.31	7	1	1	N	20542	Myosin light chain alkali [Trachymymex septentrionalis]
30	5668	gi 1012980172 gb KYQ54098.1	50.31	7	1	1	N	20525	Myosin light chain alkali [Trachymymex zeteki]
30	5669	gi 801397041 ref XP_012058904.1	50.31	7	1	1	N	22153	PREDICTED: myosin light chain alkali [Atta cephalotes]
30	5670	gi 861651167 gb KMQ97620.1	50.31	3	1	1	N	56377	myosin light chain alkali-like isoform x1 protein [Lasius niger]
total 64 proteins									

Band # 2 Proteins

Summary

1. Notes

2. Result Statistics

Figure 1. False discovery rate (FDR) curve. X axis is the number of peptide-spectrum matches (PSM) being kept. Y axis is the corresponding FDR.

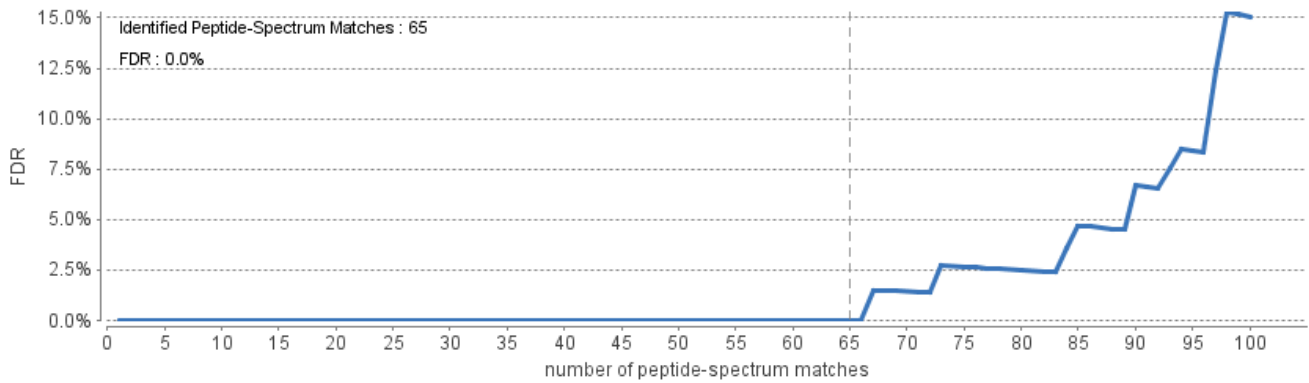


Figure 2. PSM score distribution. (a) Distribution of PEAKS peptide score; (b) Scatterplot of PEAKS peptide score versus precursor mass error.

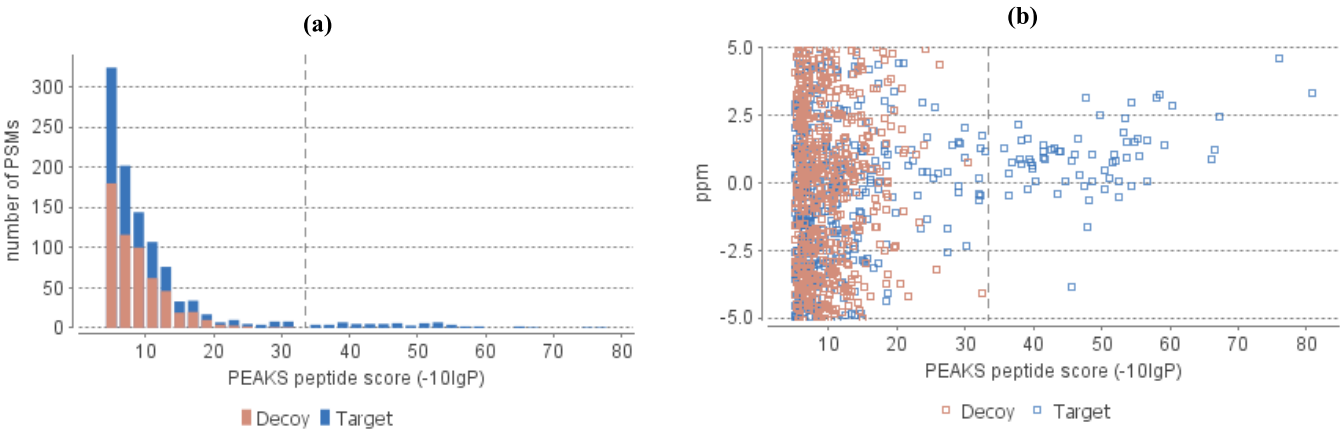


Figure 3. De novo result validation. Distribution of residue local confidence: (a) Residues in de novo sequences validated by confident database peptide assignment; (b) Residues in "de novo only" sequences.

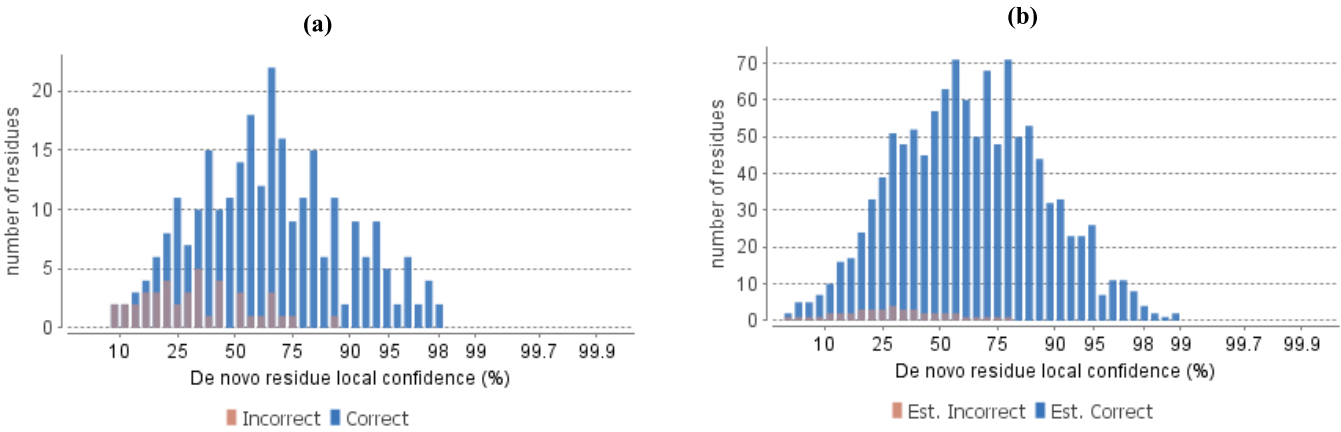


Table 1. Statistics of data.

# of MS Scans	1742
# of MS/MS Scans	2675

Table 4. PTM profile.

Name	ΔMass	Position	#PSM	-10lgP	Area	AScore
------	-------	----------	------	--------	------	--------

proteins						
Oxidation	15.99	M	7	54.26	1.44E6	69.71

Table 2. Result filtration parameters.

Peptide -10lgP	≥33.4
Protein -10lgP	≥20
Proteins unique peptides	≥1
De novo ALC Score	≥50%

Table 3. Statistics of filtered result.

Peptide-Spectrum Matches	65
Peptide Sequences	62
Protein Groups	29
Proteins	222
Proteins (#Unique Peptides)	39 (>2); 63 (=2); 120 (=1);
FDR (Peptide-Spectrum Matches)	0.0%
FDR (Peptide Sequences)	0.0%
FDR (Protein)	0.0%
De Novo Only Spectra	115

3. Experiment Control

Figure 4. Precursor mass error of peptide-spectrum matches (PSM) in filtered result. (a) Distribution of precursor mass error in ppm; (b) Scatterplot of precursor m/z versus precursor mass error in ppm.

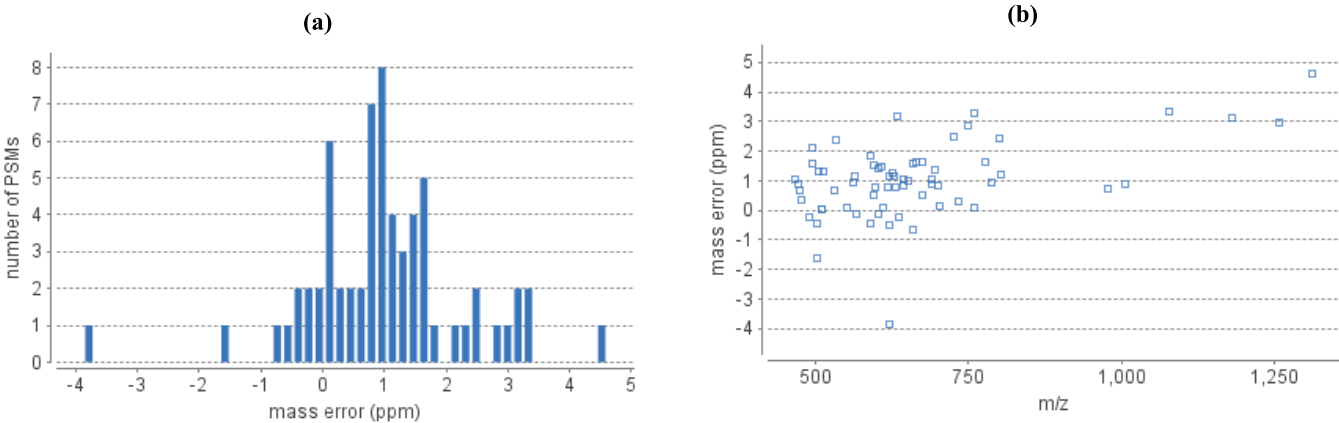


Table 5. Number of identified peptides in each sample by the number of missed cleavages

Missed Cleavages	0	1	2	3	4+
Sample 14	54	8	0	0	0

4. Other Information

Table 6. Search parameters.

Search Engine Name:	PEAKS
Parent Mass Error Tolerance:	5.0 ppm
Fragment Mass Error Tolerance:	0.5 Da
Precursor Mass Search Type:	monoisotopic
Enzyme:	Trypsin
Max Missed Cleavages:	3
Non-specific Cleavage:	one
Variable Modifications:	
Oxidation (M):	15.99
Max variable PTM per peptide:	3
Database:	Ant
Taxon:	All
Searched Entry:	473117
FDR Estimation:	Enabled
Merge Options:	no merge
Precursor Options:	corrected
Charge Options:	no correction

Table 7. Instrument parameters.

Fractions:	TW_2.raw
Ion Source:	ESI(nano-spray)
Fragmentation Mode:	CID, CAD(y and b ions)
MS Scan Mode:	FT-ICR/Orbitrap
MS/MS Scan Mode:	FT-ICR/Orbitrap

Filter Options: no filter
Process: true

Protein List

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
1	2	gi 749756765 ref XP_011140861.1	151.79	43	6	6	Y	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Harpegnathos saltator]
1	10	gi 322799134 gb EFZ20581.1	151.79	43	6	6	Y	16857	hypothetical protein SINV_11686, partial [Solenopsis invicta]
1	3	gi 795075576 ref XP_011876241.1	151.79	43	6	6	Y	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Vollenhovia emeryi]
1	4	gi 759066863 ref XP_011342896.1	151.79	43	6	6	Y	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Ceropachys biroï]
1	5	gi 751206597 ref XP_011155825.1	151.79	43	6	6	Y	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Solenopsis invicta]
1	6	gi 780650680 ref XP_011690296.1	151.79	43	6	6	Y	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Wasmannia auropunctata]
1	11	gi 607357312 gb EZA51777.1	151.79	43	6	6	Y	16860	Cofilin/actin-depolymerizing factor-like protein [Ceropachys biroï]
1	7	gi 951531070 ref XP_014469357.1	151.79	43	6	6	Y	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Dinoponera quadriceps]
1	12	gi 746872572 ref XP_011067557.1	151.79	43	6	6	Y	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Acromyrmex echinator]
1	13	gi 815823534 ref XP_012233084.1	151.79	43	6	6	Y	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Linepithema humile]
1	8	gi 826475616 ref XP_012537040.1	151.79	43	6	6	Y	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Monomorium pharaonis]
1	9	gi 752866064 ref XP_011269506.1	151.79	43	6	6	Y	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Camponotus floridanus]
1	14	gi 861649741 gb KMQ96964.1	151.79	42	6	6	Y	16974	cofilin actin-depolymerizing factor-like protein [Lasius niger]
1	15	gi 307187751 gb EFN72723.1	151.79	38	6	6	Y	19355	Cofilin/actin-depolymerizing factor-like protein [Camponotus floridanus]
1	16	gi 801383792 ref XP_012055075.1	151.79	35	6	6	Y	20394	PREDICTED: cofilin/actin-depolymerizing factor homolog [Atta cephalotes]
1	17	gi 1009357994 gb KYM83255.1	151.79	35	6	6	Y	20394	Cofilin/actin-depolymerizing factor like protein [Atta colombica]
1	18	gi 307205222 gb EFN83612.1	151.79	35	6	6	Y	20514	Cofilin/actin-depolymerizing factor-like protein [Harpegnathos saltator]
1	19	gi 1012971901 gb KYQ46466.1	151.79	34	6	6	Y	20722	Cofilin/actin-depolymerizing factor like protein [Trachymyrmex zeteki]
1	20	gi 1009394301 gb KYN15343.1	151.79	34	6	6	Y	20708	Cofilin/actin-depolymerizing factor like protein [Trachymyrmex cornetzi]
1	21	gi 332016345 gb EGI57258.1	151.79	34	6	6	Y	20654	Cofilin/actin-depolymerizing factor-like protein [Acromyrmex echinator]
1	22	gi 1009419754 gb KYN38297.1	151.79	34	6	6	Y	20608	Cofilin/actin-depolymerizing factor like protein [Trachymyrmex septentrionalis]
6	11172	gi 752896488 ref XP_011266504.1	143.62	35	4	1	Y	18907	PREDICTED: muscle-specific protein 20 [Camponotus floridanus]
2	11166	gi 951523050 ref XP_014488366.1	137.54	29	5	1	N	19085	PREDICTED: probable phospholipid hydroperoxide glutathione peroxidase isoform X3 [Dinoponera quadriceps]
2	11167	gi 749797995 ref XP_011152483.1	137.54	29	5	1	N	19094	PREDICTED: probable phospholipid hydroperoxide glutathione peroxidase isoform X2 [Harpegnathos saltator]
2	11168	gi 749797993 ref XP_011152482.1	137.54	26	5	1	N	21668	PREDICTED: probable phospholipid hydroperoxide glutathione peroxidase isoform X1 [Harpegnathos saltator]
2	11169	gi 951523048 ref XP_014488365.1	137.54	26	5	1	N	21695	PREDICTED: probable phospholipid hydroperoxide glutathione peroxidase isoform X2 [Dinoponera quadriceps]
2	11170	gi 951523046 ref XP_014488363.1	137.54	21	5	1	N	26359	PREDICTED: probable phospholipid hydroperoxide glutathione peroxidase isoform X1 [Dinoponera quadriceps]
11	11163	gi 861647111 gb KMQ95789.1	110.25	32	4	3	N	14341	muscle-specific protein 20 [Lasius niger]
11	11164	gi 815814101 ref XP_012228063.1	110.25	23	4	3	N	20180	PREDICTED: muscle-specific protein 20-like [Linepithema humile]
11	11165	gi 752896490 ref XP_011266505.1	110.25	23	4	3	N	20341	PREDICTED: muscle-specific protein 20-like [Camponotus floridanus]
11	11171	gi 307168035 gb EFN61359.1	110.25	3	4	3	N	160564	Mitogen-activated protein kinase kinase kinase 15, partial [Camponotus floridanus]
8	11250	gi 749749329 ref XP_011136874.1	100.56	11	2	2	Y	22904	PREDICTED: peptidyl-prolyl cis-trans isomerase-like [Harpegnathos saltator]
8	11251	gi 951553352 ref XP_014476232.1	100.56	11	2	2	Y	22822	PREDICTED: peptidyl-prolyl cis-trans isomerase-like [Dinoponera quadriceps]
8	11252	gi 307209006 gb EFN86206.1	100.56	11	2	2	Y	22904	Peptidyl-prolyl cis-trans isomerase [Harpegnathos saltator]

total 222 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
5	11160	gi 759032952 ref XP_011334617.1	97.35	10	3	3	N	41770	PREDICTED: actin, clone 205 [Ceropachys biroï]
5	5591	gi 751239306 ref XP_011173634.1	97.35	10	3	3	N	41783	PREDICTED: actin-5, muscle-specific [Solenopsis invicta]
5	5593	gi 752898359 ref XP_011267531.1	97.35	10	3	3	N	41783	PREDICTED: actin-5, muscle-specific [Camponotus floridanus]
5	5594	gi 752898361 ref XP_011267532.1	97.35	10	3	3	N	41783	PREDICTED: actin-5, muscle-specific [Camponotus floridanus]
5	11161	gi 752898367 ref XP_011267535.1	97.35	10	3	3	N	41756	PREDICTED: actin, muscle [Camponotus floridanus]
5	5595	gi 749790975 ref XP_011148680.1	97.35	10	3	3	N	41783	PREDICTED: actin-5, muscle-specific [Harpagophys saltator]
5	5598	gi 751239318 ref XP_011173641.1	97.35	10	3	3	N	41783	PREDICTED: actin-5, muscle-specific [Solenopsis invicta]
5	5599	gi 607368821 gb EZA62927.1	97.35	10	3	3	N	41770	Actin, clone [Ceropachys biroï]
5	5600	gi 327387361 gb AEA72282.1	97.35	10	3	3	N	41783	actin-87E isoform 1 [Solenopsis invicta]
5	11162	gi 752898365 ref XP_011267534.1	97.35	10	3	3	N	41756	PREDICTED: actin, muscle [Camponotus floridanus]
5	5603	gi 751239316 ref XP_011173639.1	97.35	10	3	3	N	41758	PREDICTED: actin, muscle [Solenopsis invicta]
5	5604	gi 746849931 ref XP_011055426.1	97.35	10	3	3	N	41684	PREDICTED: actin-5, muscle-specific [Acromyrmex echinator]
5	5605	gi 752898363 ref XP_011267533.1	97.35	10	3	3	N	41783	PREDICTED: actin-5, muscle-specific [Camponotus floridanus]
5	5606	gi 749790980 ref XP_011148681.1	97.35	10	3	3	N	41783	PREDICTED: actin-5, muscle-specific [Harpagophys saltator]
3	77	gi 1911819 gb AAB50883.1	84.36	10	2	2	Y	11819	Myr p I=allergenic polypeptide {N-termina l}; [Myrmecia pilosula=jumper ants, venom, Peptide Partial, 112 aa]
3	78	gi 312284 emb CAA49760.1	84.36	10	2	2	Y	11849	major allergen [Myrmecia pilosula]
3	76	gi 730091 sp Q07932.1 MYR1_MYRPI	84.36	10	2	2	Y	11849	RecName: Full=Pilosulin-1; AltName: Full=Allergen Myr p I; AltName: Full=Major allergen Myr p 1; AltName: Allergen=Myr p 1; Contains: RecName: Full=Pilosulin-1; Contains: RecName: Full=Pilosulin-1 65->112; Contains: RecName...
14	11227	gi 780631682 ref XP_011685618.1	80.29	15	2	2	N	15506	PREDICTED: ubiquitin-conjugating enzyme E2 variant 2 isoform X2 [Wasmannia auropunctata]
14	11228	gi 1009377667 gb KYN00943.1	80.29	15	2	2	N	15506	Ubiquitin-conjugating enzyme E2 variant 2 [Cyphomyrmex costatus]
14	11229	gi 826450604 ref XP_012532177.1	80.29	14	2	2	N	16347	PREDICTED: ubiquitin-conjugating enzyme E2 variant 2 [Monomorium pharaonis]
14	11230	gi 751200361 ref XP_011161785.1	80.29	14	2	2	N	16347	PREDICTED: ubiquitin-conjugating enzyme E2 variant 2 [Solenopsis invicta]
14	11231	gi 607364354 gb EZA58566.1	80.29	14	2	2	N	16317	Ubiquitin-conjugating enzyme E2 variant [Ceropachys biroï]
14	11232	gi 815768531 ref XP_012231623.1	80.29	14	2	2	N	16343	PREDICTED: ubiquitin-conjugating enzyme E2 variant 2 [Linepithema humile]
14	11233	gi 749734745 ref XP_011152877.1	80.29	14	2	2	N	16343	PREDICTED: ubiquitin-conjugating enzyme E2 variant 2 [Harpagophys saltator]
14	11234	gi 752880091 ref XP_011257597.1	80.29	14	2	2	N	16343	PREDICTED: ubiquitin-conjugating enzyme E2 variant 2 [Camponotus floridanus]
14	11235	gi 801368079 ref XP_012056223.1	80.29	14	2	2	N	16361	PREDICTED: ubiquitin-conjugating enzyme E2 variant 2 [Atta cephalotes]
14	11236	gi 769835200 ref XP_011647705.1	80.29	14	2	2	N	16361	PREDICTED: ubiquitin-conjugating enzyme E2 variant 2 [Pogonomyrmex barbatus]
14	11237	gi 307213098 gb EFN88620.1	80.29	14	2	2	N	16343	Ubiquitin-conjugating enzyme E2 variant 2 [Harpagophys saltator]
14	11238	gi 746830445 ref XP_011068019.1	80.29	14	2	2	N	16377	PREDICTED: ubiquitin-conjugating enzyme E2 variant 2 [Acromyrmex echinator]
14	11239	gi 780631678 ref XP_011685617.1	80.29	14	2	2	N	16361	PREDICTED: ubiquitin-conjugating enzyme E2 variant 2 isoform X1 [Wasmannia auropunctata]
14	11240	gi 759045328 ref XP_011331612.1	80.29	14	2	2	N	16317	PREDICTED: ubiquitin-conjugating enzyme E2 variant 2 [Ceropachys biroï]
14	11241	gi 307179132 gb EFN67604.1	80.29	14	2	2	N	16343	Ubiquitin-conjugating enzyme E2 variant 2 [Camponotus floridanus]
14	11242	gi 1009412549 gb KYN31474.1	80.29	14	2	2	N	16361	Ubiquitin-conjugating enzyme E2 variant 2 [Trachymyrmex septentrionalis]
14	11243	gi 332031594 gb EGI71066.1	80.29	14	2	2	N	16377	Ubiquitin-conjugating enzyme E2 variant 2 [Acromyrmex echinator]
14	11244	gi 951549119 ref XP_014474575.1	80.29	14	2	2	N	16343	PREDICTED: ubiquitin-conjugating enzyme E2 variant 2 [Dinoponera quadricapsa]
14	11245	gi 795111773 ref XP_011882525.1	80.29	14	2	2	N	16361	PREDICTED: ubiquitin-conjugating enzyme E2 variant 2 [Vollenhovia emeryi]
14	11246	gi 322802299 gb EFZ22695.1	80.29	11	2	2	N	21115	hypothetical protein SINV_09396, partial [Solenopsis invicta]
total 222 proteins									

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
14	11247	gi 1012980373 gb KYQ54296.1	80.29	10	2	2	N	21813	Ubiquitin-conjugating enzyme E2 variant 2, partial [Trachymyrmex zeteki]
14	11248	gi 1009353642 gb KYM79028.1	80.29	9	2	2	N	24457	Ubiquitin-conjugating enzyme E2 variant 2 [Atta colombica]
14	11249	gi 1009400097 gb KYN20165.1	80.29	7	2	2	N	30916	Ubiquitin-conjugating enzyme E2 variant 2, partial [Trachymyrmex cornetzi]
29	11324	gi 51241753 dbj BAD36780.1	75.92	31	1	1	N	9019	pilosulin 4 [Myrmecia banksi]
15	11272	gi 607364912 gb EZA59114.1	73.78	2	2	2	N	91494	PDZ and LIM domain protein Zasp [Cerapachys biroi]
15	11273	gi 759044497 ref XP_011331167.1	73.78	1	2	2	N	217249	PREDICTED: uncharacterized protein LOC105275764 [Cerapachys biroi]
15	11274	gi 815790568 ref XP_012215850.1	73.78	1	2	2	N	225648	PREDICTED: uncharacterized protein LOC105668197 [Linepithema humile]
16	11275	gi 951556446 ref XP_014477681.1	73.22	12	2	2	N	19927	PREDICTED: globin [Dinoponera quadricap s]
16	11276	gi 951556454 ref XP_014477684.1	73.22	12	2	2	N	19927	PREDICTED: globin [Dinoponera quadricap s]
16	11277	gi 951556451 ref XP_014477683.1	73.22	12	2	2	N	19927	PREDICTED: globin [Dinoponera quadricap s]
16	11278	gi 951556448 ref XP_014477682.1	73.22	12	2	2	N	19927	PREDICTED: globin [Dinoponera quadricap s]
17	11279	gi 780614540 ref XP_011692815.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Wasmannia auro punctata]
17	11280	gi 759055396 ref XP_011336929.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Cerapachys biroi]
17	11281	gi 752895247 ref XP_011265836.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Camponotus floridanus]
17	11282	gi 607354003 gb EZA48674.1	62.77	17	2	2	N	11381	Histone H4 [Cerapachys biroi]
17	11283	gi 307170634 gb EFN62818.1	62.77	17	2	2	N	11381	Histone H4 [Camponotus floridanus]
17	11284	gi 759039046 ref XP_011352081.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Cerapachys biroi]
17	11285	gi 769842886 ref XP_011632650.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Pogonomyrmex b arbatus]
17	11286	gi 749779952 ref XP_011144465.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Harpegnathos saltator]
17	11287	gi 1885324 emb CAA62814.1	62.77	17	2	2	N	11381	histone H4 [Myrmica ruginodis]
17	11288	gi 752892506 ref XP_011264341.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Camponotus floridanus]
17	11289	gi 752864853 ref XP_011268846.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Camponotus floridanus]
17	11290	gi 749795303 ref XP_011151030.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Harpegnathos saltator]
17	11291	gi 759076093 ref XP_011347770.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Cerapachys biroi]
17	11292	gi 751220158 ref XP_011163197.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Solenopsis invicta]
17	11293	gi 607359346 gb EZA53713.1	62.77	17	2	2	N	11381	Histone H4 [Cerapachys biroi]
17	11294	gi 607361199 gb EZA55492.1	62.77	17	2	2	N	11381	Histone H4 [Cerapachys biroi]
17	11295	gi 746853976 ref XP_011057614.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Acromyrmex echinator]
17	11296	gi 769841794 ref XP_011632090.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Pogonomyrmex b arbatus]
17	11297	gi 746834677 ref XP_011068001.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Acromyrmex echinator]
17	11298	gi 769843894 ref XP_011633178.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Pogonomyrmex b arbatus]
17	11299	gi 751207411 ref XP_011156268.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Solenopsis invicta]
17	11300	gi 780614711 ref XP_011693190.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Wasmannia auro punctata]
17	11301	gi 607366553 gb EZA60715.1	62.77	17	2	2	N	11381	Histone H4 [Cerapachys biroi]
17	11302	gi 780662547 ref XP_011693208.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Wasmannia auro punctata]
17	11303	gi 780616263 ref XP_011696983.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Wasmannia auro punctata]
17	11304	gi 759061006 ref XP_011339814.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Cerapachys biroi]
17	11305	gi 746863041 ref XP_011062464.1	62.77	17	2	2	N	11381	PREDICTED: histone H4 [Acromyrmex echinator]
18	60	gi 1009367592 gb KYM92576.1	58.01	5	1	1	Y	20432	Muscle-specific protein 20 [Atta colombica]
18	11349	gi 749734166 ref XP_011149886.1	58.01	5	1	1	Y	20504	PREDICTED: muscle-specific protein 20 [Harpegnathos saltator]
18	11350	gi 752871825 ref XP_011253128.1	58.01	5	1	1	Y	20415	PREDICTED: muscle-specific protein 20-like [Camponotus floridanus]
18	11351	gi 815806494 ref XP_012224022.1	58.01	5	1	1	Y	20479	PREDICTED: muscle-specific protein 20-like [Linepithema humile]
18	11352	gi 826416958 ref XP_012523258.1	58.01	5	1	1	Y	20537	PREDICTED: muscle-specific protein 20 [Monomorium pharaonis]

total 222 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
18	61	gi 801385197 ref XP_012055851.1	58.01	5	1	1	Y	20432	PREDICTED: muscle-specific protein 20 [At ta cephalotes]
18	62	gi 746847374 ref XP_011054061.1	58.01	5	1	1	Y	20432	PREDICTED: muscle-specific protein 20 [Acromyrmex echinator]
18	11353	gi 307183813 gb EFN70461.1	58.01	5	1	1	Y	20415	Muscle-specific protein 20 [Camponotus floridanus]
18	11354	gi 861645559 gb KMQ95150.1	58.01	4	1	1	Y	27541	muscle-specific protein 20-like protein [Lasius niger]
18	11377	gi 332025551 gb EGI65714.1	58.01	1	1	1	Y	107842	Alpha-N-acetylglactosaminidase [Acromyrmex echinator]
18	11381	gi 307213390 gb EFN88826.1	58.01	1	1	1	Y	160374	Alpha-N-acetylglactosaminidase [Harpegnathos saltator]
50	11326	gi 861657813 gb KMR03009.1	56.61	15	1	1	N	9318	small ubiquitin-related modifier 3 [Lasius niger]
50	11327	gi 1009420265 gb KYN38771.1	56.61	14	1	1	N	9814	Small ubiquitin-related modifier 3, partial [Trachymyrmex septentrionalis]
50	11328	gi 749786562 ref XP_011146906.1	56.61	13	1	1	N	10400	PREDICTED: small ubiquitin-related modifier 3 [Harpegnathos saltator]
50	11329	gi 307198848 gb EFN79624.1	56.61	13	1	1	N	10400	Small ubiquitin-related modifier 3 [Harpegnathos saltator]
50	11330	gi 1009351046 gb KYM76532.1	56.61	13	1	1	N	10405	Small ubiquitin-related modifier 3 [Atta colombica]
50	11331	gi 801388751 ref XP_012057150.1	56.61	13	1	1	N	10405	PREDICTED: small ubiquitin-related modifier 3 [Atta cephalotes]
50	11332	gi 307181428 gb EFN69023.1	56.61	13	1	1	N	10370	Small ubiquitin-related modifier 3 [Camponotus floridanus]
50	11333	gi 759040550 ref XP_011329066.1	56.61	13	1	1	N	10370	PREDICTED: small ubiquitin-related modifier 3 [Ceraopachys biro]
50	11334	gi 746853241 ref XP_011057212.1	56.61	13	1	1	N	10405	PREDICTED: small ubiquitin-related modifier 3 [Acromyrmex echinator]
50	11335	gi 752875772 ref XP_011255252.1	56.61	13	1	1	N	10370	PREDICTED: small ubiquitin-related modifier 3 [Camponotus floridanus]
50	11336	gi 607366216 gb EZA60387.1	56.61	13	1	1	N	10370	Small ubiquitin-related modifier [Ceraopachys biro]
50	11337	gi 815819782 ref XP_012231082.1	56.61	13	1	1	N	10384	PREDICTED: small ubiquitin-related modifier 3 [Linepithema humile]
50	11338	gi 826408405 ref XP_012525791.1	56.61	13	1	1	N	10517	PREDICTED: small ubiquitin-related modifier 3 [Monomorium pharaonis]
50	11339	gi 751202229 ref XP_011171067.1	56.61	13	1	1	N	10516	PREDICTED: small ubiquitin-related modifier 3-like [Solenopsis invicta]
50	11340	gi 780677887 ref XP_011696863.1	56.61	13	1	1	N	10547	PREDICTED: small ubiquitin-related modifier 3-like [Wasmannia auropunctata]
50	11341	gi 1012976187 gb KYQ50338.1	56.61	13	1	1	N	10533	Small ubiquitin-related modifier 3 [Trachymyrmex zeteki]
50	11342	gi 795022706 ref XP_011860689.1	56.61	13	1	1	N	10487	PREDICTED: small ubiquitin-related modifier 3 [Vollenhovia emeryi]
50	11343	gi 769831430 ref XP_011636433.1	56.61	13	1	1	N	10533	PREDICTED: small ubiquitin-related modifier 3-like [Pogonomyrmex barbatus]
50	11344	gi 1009378062 gb KYN01311.1	56.61	12	1	1	N	11231	Small ubiquitin-related modifier 3, partial [Cyphomyrmex costatus]
50	11345	gi 1009407782 gb KYN27195.1	56.61	12	1	1	N	11282	Small ubiquitin-related modifier 3, partial [Trachymyrmex cornetzi]
50	11346	gi 322801459 gb EFZ22120.1	56.61	12	1	1	N	11638	hypothetical protein SINV_07820, partial [Solenopsis invicta]
50	11347	gi 951570203 ref XP_014483434.1	56.61	11	1	1	N	12375	PREDICTED: small ubiquitin-related modifier 3 [Dinoponera quadricaps]
50	11348	gi 332023547 gb EGI63783.1	56.61	7	1	1	N	17717	Small ubiquitin-related modifier 3 [Acromyrmex echinator]
51	6846	gi 749750028 ref XP_011137253.1	54.24	4	1	1	N	71477	PREDICTED: heat shock 70 kDa protein cognate 4 [Harpegnathos saltator]
52	11355	gi 607367429 gb EZA61576.1	53.62	2	1	1	N	45434	Galectin-9 [Ceraopachys biro]
52	11356	gi 759037086 ref XP_011347838.1	53.62	2	1	1	N	48019	PREDICTED: collagen alpha-1(III) chain-like [Ceraopachys biro]
52	11357	gi 951562511 ref XP_014480159.1	53.62	2	1	1	N	48035	PREDICTED: uncharacterized PE-PGRS family protein PE_PGRS54-like [Dinoponera quadricaps]
52	11358	gi 815820387 ref XP_012231412.1	53.62	2	1	1	N	49082	PREDICTED: spidroin-2-like [Linepithema humile]
52	11359	gi 795059281 ref XP_011872801.1	53.62	2	1	1	N	49561	PREDICTED: basic salivary proline-rich protein 2-like [Vollenhovia emeryi]
52	11360	gi 861624938 gb KMQ88406.1	53.62	2	1	1	N	49918	hornerin-like isoform x1 protein [Lasius niger]
52	11361	gi 1009421966 gb KYN40359.1	53.62	2	1	1	N	50092	Galectin-4 [Trachymyrmex septentrionalis]
52	11362	gi 1009350716 gb KYM76208.1	53.62	2	1	1	N	50217	Galectin-4 [Atta colombica]
52	11363	gi 1012980535 gb KYQ54453.1	53.62	2	1	1	N	50254	Galectin-4 [Trachymyrmex zeteki]
52	10742	gi 1009386387 gb KYN08584.1	53.62	2	1	1	N	50390	Galectin-4 [Cyphomyrmex costatus]

total 222 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
52	11364	gi 322790899 gb EFZ15565.1	53.62	2	1	1	N	50386	hypothetical protein SINV_06789, partial [Solenopsis invicta]
52	11365	gi 780711346 ref XP_011704603.1	53.62	2	1	1	N	50248	PREDICTED: pro-resilin-like [Wasmannia a uropunctata]
52	11366	gi 752894339 ref XP_011265348.1	53.62	2	1	1	N	50039	PREDICTED: spidroin-2-like isoform X2 [Camponotus floridanus]
52	11367	gi 752894337 ref XP_011265347.1	53.62	2	1	1	N	50168	PREDICTED: pro-resilin-like isoform X1 [Camponotus floridanus]
52	11368	gi 307169505 gb EFN62153.1	53.62	2	1	1	N	50168	Galectin-4 [Camponotus floridanus]
52	11369	gi 746833194 ref XP_011062117.1	53.62	2	1	1	N	50676	PREDICTED: pro-resilin-like [Acromyrmex echinator]
52	11370	gi 332030600 gb EGI70288.1	53.62	2	1	1	N	50676	Galectin-4 [Acromyrmex echinator]
52	11371	gi 769850824 ref XP_011636833.1	53.62	2	1	1	N	50687	PREDICTED: spidroin-2-like [Pogonomyrmex barbatus]
52	11372	gi 769850822 ref XP_011636832.1	53.62	2	1	1	N	50687	PREDICTED: spidroin-2-like [Pogonomyrmex barbatus]
52	11373	gi 751221151 ref XP_011163747.1	53.62	2	1	1	N	51296	PREDICTED: spidroin-2-like [Solenopsis invicta]
52	11374	gi 307215020 gb EFN89847.1	53.62	2	1	1	N	50668	Galectin-12 [Harpegnathos saltator]
52	11375	gi 749731542 ref XP_011135485.1	53.62	2	1	1	N	50668	PREDICTED: spidroin-2-like [Harpegnathos saltator]
52	11376	gi 1009399777 gb KYN19893.1	53.62	2	1	1	N	52563	Galectin-4, partial [Trachymyrmex cornetzi]
53	11378	gi 769830873 ref XP_011633246.1	52.46	3	1	1	N	41991	PREDICTED: uncharacterized protein LOC105424622, partial [Pogonomyrmex barbatus]
19	11379	gi 322792560 gb EFZ16493.1	51.95	11	1	1	N	10553	hypothetical protein SINV_01717, partial [Solenopsis invicta]
19	11380	gi 1009376845 gb KYN00228.1	51.95	2	1	1	N	70039	hypothetical protein ALC62_09023 [Cyphomyrmex costatus]
54	5638	gi 751223514 ref XP_011165046.1	51.76	8	1	1	N	16026	PREDICTED: superoxide dismutase [Cu-Zn] 2 [Solenopsis invicta]
56	11387	gi 769839653 ref XP_011630992.1	46.16	5	1	1	N	17310	PREDICTED: protein NPC2 homolog [Pogonomyrmex barbatus]
56	11388	gi 826485498 ref XP_012538993.1	46.16	5	1	1	N	17149	PREDICTED: protein NPC2 homolog [Monomorium pharaonis]
55	11383	gi 332018975 gb EGI59514.1	45.53	7	1	1	N	16341	Peroxisome dismutase-5, mitochondrial, partial [Acromyrmex echinator]
55	11384	gi 746865869 ref XP_011063975.1	45.53	6	1	1	N	20208	PREDICTED: peroxisome dismutase-5, mitochondrial [Acromyrmex echinator]
55	11385	gi 1009422102 gb KYN40495.1	45.53	2	1	1	N	76922	Importin subunit alpha-7 [Trachymyrmex septentrionalis]
55	11386	gi 1012971870 gb KYQ46435.1	45.53	2	1	1	N	77092	Importin subunit alpha-7 [Trachymyrmex zetekii]
57	5579	gi 749772542 ref XP_011141800.1	44.60	7	1	1	N	13845	PREDICTED: superoxide dismutase [Cu-Zn], partial [Harpegnathos saltator]
57	5580	gi 307204104 gb EFN82974.1	44.60	7	1	1	N	13845	Superoxide dismutase [Cu-Zn], partial [Harpegnathos saltator]
57	5585	gi 759057450 ref XP_011337976.1	44.60	7	1	1	N	15500	PREDICTED: superoxide dismutase [Cu-Zn] [Ceratophyllus biroii]
57	5586	gi 607360315 gb EZA54646.1	44.60	7	1	1	N	15500	Superoxide dismutase [Cu-Zn] [Ceratophyllus biroii]
57	5563	gi 815812192 ref XP_012227043.1	44.60	7	1	1	N	15487	PREDICTED: LOW QUALITY PROTEIN: superoxide dismutase [Cu-Zn]-like [Linepithema humile]
57	5587	gi 752872840 ref XP_011253679.1	44.60	7	1	1	N	15495	PREDICTED: superoxide dismutase [Cu-Zn] [Camponotus floridanus]
57	5564	gi 34733404 gb AAQ81639.1	44.60	7	1	1	N	15553	Cu-Zn superoxide dismutase 1 [Lasius niger]
57	5588	gi 307183176 gb EFN70085.1	44.60	7	1	1	N	15495	Superoxide dismutase [Cu-Zn] [Camponotus floridanus]
57	5584	gi 861628645 gb KMQ89459.1	44.60	2	1	1	N	55250	superoxide dismutase, partial [Lasius niger]
58	11389	gi 815825120 ref XP_012233927.1	43.79	2	1	1	N	77023	PREDICTED: importin subunit alpha-7 isoform X2 [Linepithema humile]
30	128	gi 749750482 ref XP_011137501.1	41.70	9	1	1	N	17069	PREDICTED: myosin light chain alkali isoform X2 [Harpegnathos saltator]
59	11395	gi 861629303 gb KMQ89714.1	39.04	11	1	1	N	12334	thioredoxin 2 [Lasius niger]
61	11397	gi 751207176 ref XP_011156141.1	38.27	5	1	1	N	15163	PREDICTED: sorting nexin-12 [Solenopsis invicta]
61	11398	gi 746869742 ref XP_011066034.1	38.27	4	1	1	N	18650	PREDICTED: sorting nexin-12 isoform X2 [Acromyrmex echinator]
61	11399	gi 1009379701 gb KYN02764.1	38.27	4	1	1	N	19063	Sorting nexin-12 [Cyphomyrmex costatus]
61	11400	gi 746869740 ref XP_011066033.1	38.27	4	1	1	N	19049	PREDICTED: sorting nexin-12 isoform X1 [Acromyrmex echinator]
61	11401	gi 1012976830 gb KYQ50937.1	38.27	4	1	1	N	19049	Sorting nexin-12 [Trachymyrmex zetekii]

total 222 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
61	11402	gi 752860835 ref XP_011254124.1	38.27	4	1	1	N	19049	PREDICTED: sorting nexin-12 [Camponotus floridanus]
61	11403	gi 1009424367 gb KYN42572.1	38.27	4	1	1	N	19049	Sorting nexin-12 [Trachymyrmex septentrionalis]
61	11404	gi 780704999 ref XP_011702991.1	38.27	4	1	1	N	19049	PREDICTED: sorting nexin-12 [Wasmannia auropunctata]
61	11405	gi 759071563 ref XP_011345384.1	38.27	4	1	1	N	19093	PREDICTED: sorting nexin-12 [Cerapachys biroi]
61	11406	gi 951568075 ref XP_014482580.1	38.27	4	1	1	N	19023	PREDICTED: sorting nexin-12 isoform X2 [Dinoponera quadricaps]
61	11407	gi 769867655 ref XP_011645850.1	38.27	4	1	1	N	19049	PREDICTED: sorting nexin-12 [Pogonomyrmex barbatus]
61	11408	gi 607355702 gb EZA50262.1	38.27	4	1	1	N	19093	Sorting nexin-12 [Cerapachys biroi]
61	11409	gi 1009387209 gb KYN09346.1	38.27	4	1	1	N	19049	Sorting nexin-12 [Trachymyrmex cornetzi]
61	11410	gi 815798123 ref XP_012219729.1	38.27	4	1	1	N	19049	PREDICTED: sorting nexin-12 [Linepithema humile]
61	11411	gi 307190553 gb EFN74540.1	38.27	4	1	1	N	19049	Sorting nexin-12 [Camponotus floridanus]
61	11412	gi 1009367671 gb KYM92655.1	38.27	4	1	1	N	19049	Sorting nexin-12 [Atta colombica]
61	11413	gi 307212628 gb EFN88331.1	38.27	4	1	1	N	19023	Sorting nexin-12 [Harpegnathos saltator]
61	11414	gi 826435644 ref XP_012529251.1	38.27	4	1	1	N	19049	PREDICTED: sorting nexin-12 [Monomorium pharaonis]
61	11415	gi 801402232 ref XP_012061324.1	38.27	4	1	1	N	19049	PREDICTED: sorting nexin-12 [Atta cephalotes]
61	11416	gi 749735611 ref XP_011153980.1	38.27	4	1	1	N	19023	PREDICTED: sorting nexin-12 [Harpegnathos saltator]
61	11417	gi 795048973 ref XP_011869407.1	38.27	4	1	1	N	19049	PREDICTED: sorting nexin-12 [Vollenhovia emeryi]
61	11418	gi 951568072 ref XP_014482579.1	38.27	3	1	1	N	25465	PREDICTED: sorting nexin-3 isoform X1 [Dinoponera quadricaps]
60	11396	gi 746853980 ref XP_011057616.1	38.03	7	1	1	N	13377	PREDICTED: histone H2A-like [Acromyrmex echinator]
62	11419	gi 1009359326 gb KYM84467.1	36.74	7	1	1	N	17136	Ecdysteroid-regulated 16 kDa protein [Atta colombica]
62	11420	gi 307199781 gb EFN80227.1	36.74	7	1	1	N	17591	Epididymal secretory protein E1 [Harpegnathos saltator]
62	11421	gi 1009389483 gb KYN11307.1	36.74	7	1	1	N	17896	Ecdysteroid-regulated 16 kDa protein [Trachymyrmex cornetzi]
62	11422	gi 749783952 ref XP_011145903.1	36.74	6	1	1	N	20104	PREDICTED: MD-2-related lipid-recognition protein-like [Harpegnathos saltator]
62	11423	gi 801398443 ref XP_012059676.1	36.74	5	1	1	N	24322	PREDICTED: MD-2-related lipid-recognition protein-like [Atta cephalotes]
63	143	gi 307184709 gb EFN71038.1	36.38	4	1	1	N	22151	hypothetical protein EAG_09928 [Camponotus floridanus]
63	4127	gi 861653549 gb KMQ99191.1	36.38	1	1	1	N	108034	dynamitin-like mitochondrial protein [Lasius niger]
63	195	gi 801397101 ref XP_012058936.1	36.38	1	1	1	N	113731	PREDICTED: dynamitin-like 120 kDa protein, mitochondrial isoform X3 [Atta cephalotes]
63	4128	gi 801397099 ref XP_012058935.1	36.38	1	1	1	N	113933	PREDICTED: dynamitin-like 120 kDa protein, mitochondrial isoform X2 [Atta cephalotes]
63	4129	gi 801397097 ref XP_012058934.1	36.38	1	1	1	N	114004	PREDICTED: dynamitin-like 120 kDa protein, mitochondrial isoform X1 [Atta cephalotes]
total 222 proteins									

Band # 3 Proteins

Summary

1. Notes

2. Result Statistics

Figure 1. False discovery rate (FDR) curve. X axis is the number of peptide-spectrum matches (PSM) being kept. Y axis is the corresponding FDR.

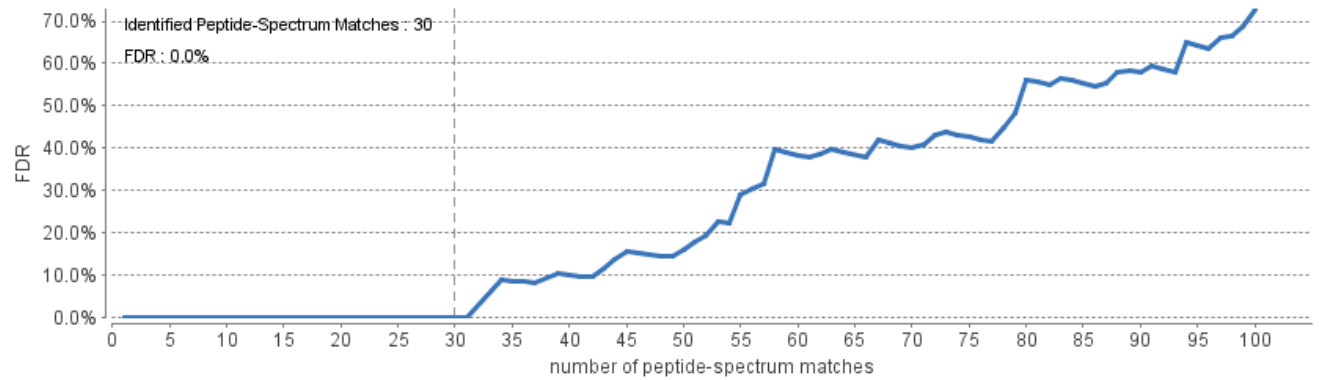


Figure 2. PSM score distribution. (a) Distribution of PEAKS peptide score; (b) Scatterplot of PEAKS peptide score versus precursor mass error.

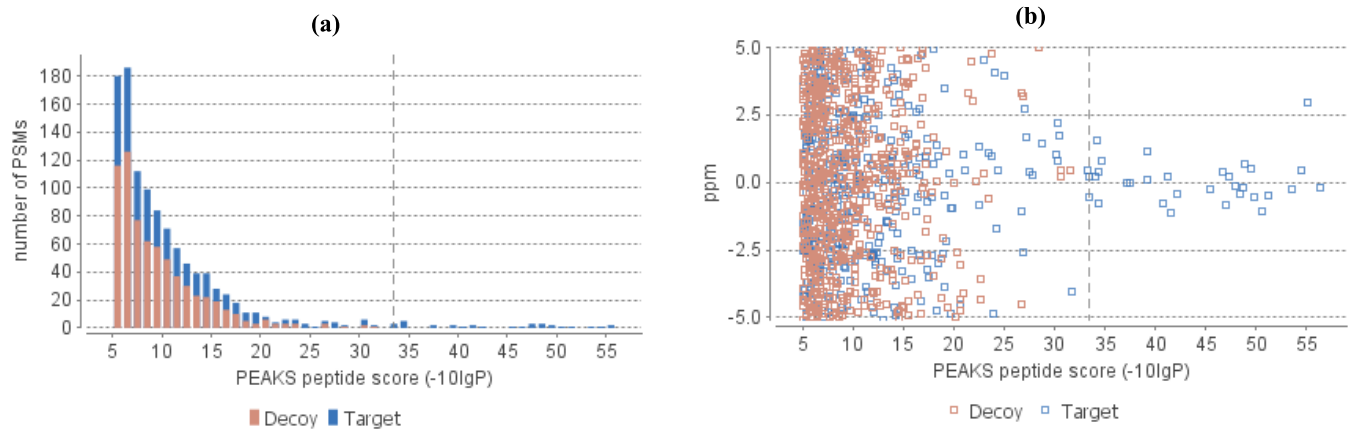


Figure 3. De novo result validation. Distribution of residue local confidence: (a) Residues in de novo sequences validated by confident database peptide assignment; (b) Residues in "de novo only" sequences.

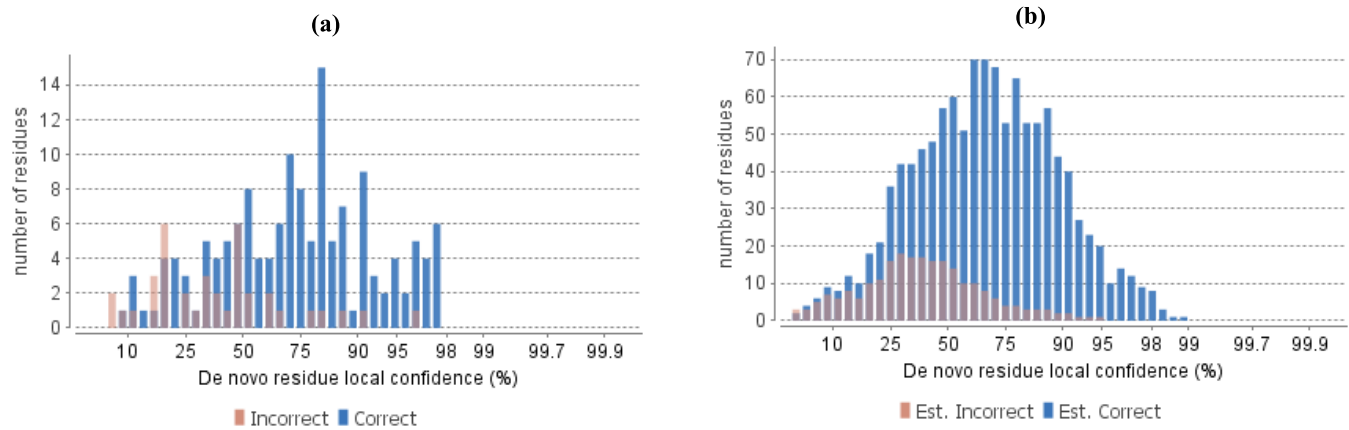


Table 1. Statistics of data.

# of MS Scans	1725
# of MS/MS Scans	2797

Table 4. PTM profile.

Name	Δ Mass	Position	#PSM	-10lgP	Area	AScore
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Table 2. Result filtration parameters.

Peptide -10lgP	≥33.4
Protein -10lgP	≥20
Proteins unique peptides	≥1
De novo ALC Score	≥50%

Table 3. Statistics of filtered result.

Peptide-Spectrum Matches	30
Peptide Sequences	24
Protein Groups	11
Proteins	103
Proteins (#Unique Peptides)	6 (>2); 20 (=2); 77 (=1);
FDR (Peptide-Spectrum Matches)	0.0%
FDR (Peptide Sequences)	0.0%
FDR (Protein)	0.0%
De Novo Only Spectra	130

3. Experiment Control

Figure 4. Precursor mass error of peptide-spectrum matches (PSM) in filtered result. **(a)** Distribution of precursor mass error in ppm; **(b)** Scatterplot of precursor m/z versus precursor mass error in ppm. ?

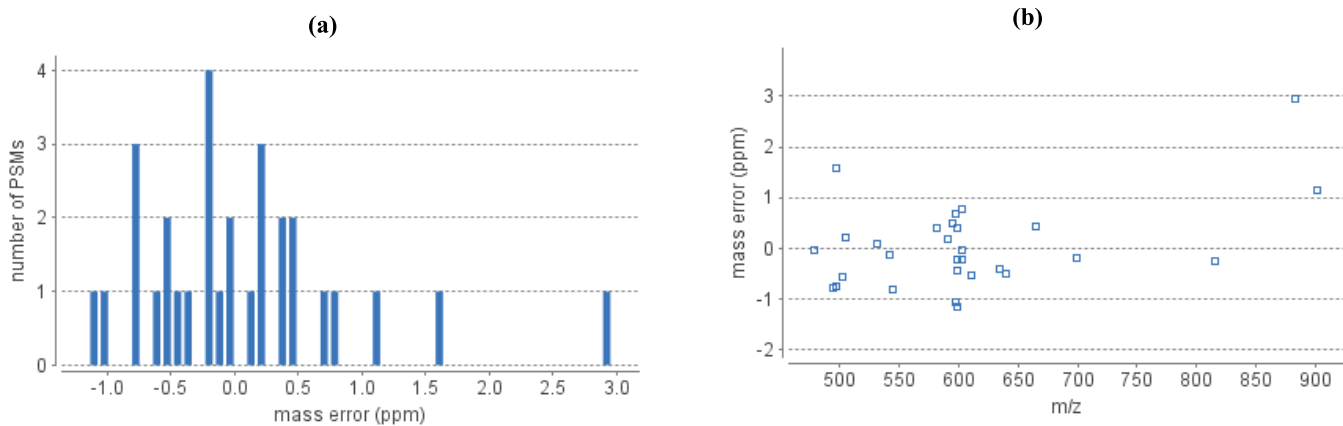


Table 5. Number of identified peptides in each sample by the number of missed cleavages

Missed Cleavages	0	1	2	3	4+
Sample 19	21	3	0	0	0

4. Other Information

Table 6. Search parameters.

Search Engine Name:	PEAKS
Parent Mass Error Tolerance:	5.0 ppm
Fragment Mass Error Tolerance:	0.5 Da
Precursor Mass Search Type:	monoisotopic
Enzyme:	Trypsin
Max Missed Cleavages:	3
Non-specific Cleavage:	one
Variable Modifications:	
Oxidation (M):	15.99
Max variable PTM per peptide:	3
Database:	Ant
Taxon:	All
Searched Entry:	473117
FDR Estimation:	Enabled
Merge Options:	no merge
Precursor Options:	corrected
Charge Options:	no correction

Table 7. Instrument parameters.

Fractions:	TW_3.raw
Ion Source:	ESI(nano-spray)
Fragmentation Mode:	CID, CAD(y and b ions)
MS Scan Mode:	FT-ICR/Orbitrap
MS/MS Scan Mode:	FT-ICR/Orbitrap

Filter Options: no filter
Process: true

Protein List

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
1	79	gi 752883275 ref XP_011259333.1	115.81	19	6	6	Y	25675	PREDICTED: acidic phospholipase A2 PA4 isoform X2 [Camponotus floridanus]
1	81	gi 752883277 ref XP_011259334.1	115.81	19	6	6	Y	25675	PREDICTED: acidic phospholipase A2 PA4 isoform X2 [Camponotus floridanus]
1	87	gi 801374599 ref XP_012063030.1	115.81	19	6	6	Y	25985	PREDICTED: acidic phospholipase A2 PA4-like [Atta cephalotes]
1	90	gi 752883273 ref XP_011259332.1	115.81	17	6	6	Y	28503	PREDICTED: acidic phospholipase A2 PA4 isoform X1 [Camponotus floridanus]
3	11165	gi 752896490 ref XP_011266505.1	112.37	25	4	4	N	20341	PREDICTED: muscle-specific protein 20-like [Camponotus floridanus]
3	11181	gi 826418146 ref XP_012523893.1	112.37	25	4	4	N	20235	PREDICTED: muscle-specific protein 20-like [Monomorium pharaonis]
4	12642	gi 752893810 ref XP_011265060.1	88.11	14	2	2	N	20707	PREDICTED: ADP-ribosylation factor 1 [Camponotus floridanus]
4	12643	gi 752893806 ref XP_011265058.1	88.11	14	2	2	N	20707	PREDICTED: ADP-ribosylation factor 1 [Camponotus floridanus]
4	12644	gi 749787291 ref XP_011147198.1	88.11	14	2	2	N	20707	PREDICTED: ADP-ribosylation factor 1 [Harpagathos saltator]
4	12645	gi 751201678 ref XP_011168539.1	88.11	14	2	2	N	20707	PREDICTED: ADP-ribosylation factor 1 [Sol enopsis invicta]
4	12646	gi 780614376 ref XP_011692370.1	88.11	14	2	2	N	20707	PREDICTED: ADP-ribosylation factor 1 [Wasmannia auropunctata]
4	12647	gi 795044039 ref XP_011867790.1	88.11	14	2	2	N	20707	PREDICTED: ADP-ribosylation factor 1 [Vollenhovia emeryi]
4	12648	gi 759034310 ref XP_011333078.1	88.11	14	2	2	N	20707	PREDICTED: ADP-ribosylation factor 1 [Cera-pachys biroi]
4	12649	gi 759034308 ref XP_011333070.1	88.11	14	2	2	N	20707	PREDICTED: ADP-ribosylation factor 1 [Cera-pachys biroi]
4	12650	gi 607368472 gb EZA62585.1	88.11	14	2	2	N	20707	ADP-ribosylation factor [Cera-pachys biroi]
4	12651	gi 749787288 ref XP_011147197.1	88.11	14	2	2	N	20707	PREDICTED: ADP-ribosylation factor 1 [Harpagathos saltator]
4	12652	gi 749787297 ref XP_011147201.1	88.11	14	2	2	N	20707	PREDICTED: ADP-ribosylation factor 1 [Harpagathos saltator]
4	12653	gi 746869013 ref XP_011065651.1	88.11	14	2	2	N	20707	PREDICTED: ADP-ribosylation factor 1 [Acromyrmex echinator]
4	12654	gi 746869015 ref XP_011065652.1	88.11	14	2	2	N	20707	PREDICTED: ADP-ribosylation factor 1 [Acromyrmex echinator]
4	12655	gi 795044042 ref XP_011867791.1	88.11	14	2	2	N	20707	PREDICTED: ADP-ribosylation factor 1 [Vollenhovia emeryi]
4	12656	gi 751201680 ref XP_011168548.1	88.11	14	2	2	N	20707	PREDICTED: ADP-ribosylation factor 1 [Sol enopsis invicta]
4	12657	gi 769844204 ref XP_011633341.1	88.11	14	2	2	N	20707	PREDICTED: ADP-ribosylation factor 1 [Pogonomymex barbatus]
4	12658	gi 749787294 ref XP_011147200.1	88.11	14	2	2	N	20707	PREDICTED: ADP-ribosylation factor 1 [Harpagathos saltator]
4	12659	gi 769844206 ref XP_011633342.1	88.11	14	2	2	N	20707	PREDICTED: ADP-ribosylation factor 1 [Pogonomymex barbatus]
4	12660	gi 780614372 ref XP_011692362.1	88.11	14	2	2	N	20707	PREDICTED: ADP-ribosylation factor 1 [Wasmannia auropunctata]
4	12661	gi 752893808 ref XP_011265059.1	88.11	14	2	2	N	20707	PREDICTED: ADP-ribosylation factor 1 [Camponotus floridanus]
5	12665	gi 815812575 ref XP_012227249.1	76.55	3	1	1	N	47076	PREDICTED: troponin I-like isoform X11 [Lin epithema humile]
5	12666	gi 815812567 ref XP_012227245.1	76.55	3	1	1	N	47874	PREDICTED: troponin I-like isoform X7 [Lin epithema humile]
5	12667	gi 815812569 ref XP_012227246.1	76.55	3	1	1	N	47720	PREDICTED: troponin I-like isoform X8 [Lin epithema humile]
5	12668	gi 815812557 ref XP_012227239.1	76.55	3	1	1	N	48518	PREDICTED: troponin I-like isoform X2 [Lin epithema humile]
2	77	gi 1911819 gb AAB50883.1	63.82	10	1	1	Y	11819	Myr p I=allergenic polypeptide {N-termina-l} [Myrmecia pilosula=jumper ants, venom, Peptide Partial, 112 aa]
2	78	gi 312284 emb CAA49760.1	63.82	10	1	1	Y	11849	major allergen [Myrmecia pilosula]
2	76	gi 730091 sp Q07932.1 MYR1_MYRPI	63.82	10	1	1	Y	11849	RecName: Full=Pilosulin-1; AltName: Full=Allergen Myr p I; AltName: Full=Major allergen Myr p 1; AltName: Allergen=Myr p 1; Contains: RecName: Full=Pilosulin-1; Contains: RecName: Full=Pilosulin-1 65->112; Contains: RecNa...
15	5666	gi 1009388322 gb KYN10341.1	56.37	7	1	1	N	20515	Myosin light chain alkali [Trachymyrmex conretzi]

total 103 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
15	5642	gi 751228682 ref XP_011167761.1	56.37	9	1	1	N	17087	PREDICTED: myosin light chain alkali isoform X2 [Solenopsis invicta]
15	5643	gi 815801638 ref XP_012221484.1	56.37	9	1	1	N	17041	PREDICTED: myosin light chain alkali [Linepithema humile]
15	5644	gi 769856981 ref XP_011640107.1	56.37	9	1	1	N	17133	PREDICTED: myosin light chain alkali isoform X2 [Pogonomyrmex barbatus]
15	128	gi 749750482 ref XP_011137501.1	56.37	9	1	1	N	17069	PREDICTED: myosin light chain alkali isoform X2 [Harpegnathos saltator]
15	5645	gi 826465315 ref XP_012535022.1	56.37	9	1	1	N	17113	PREDICTED: myosin light chain alkali isoform X2 [Monomorium pharaonis]
15	5646	gi 780687964 ref XP_011698945.1	56.37	9	1	1	N	17075	PREDICTED: myosin light chain alkali isoform X2 [Wasmannia auropunctata]
15	5647	gi 759072917 ref XP_011346087.1	56.37	9	1	1	N	17085	PREDICTED: myosin light chain alkali [Cera pachys biro]
15	5648	gi 951531116 ref XP_014469383.1	56.37	9	1	1	N	17026	PREDICTED: myosin light chain alkali [Dinoponera quadriceps]
15	5649	gi 759072919 ref XP_011346088.1	56.37	9	1	1	N	17085	PREDICTED: myosin light chain alkali [Cera pachys biro]
15	5650	gi 795063214 ref XP_011873749.1	56.37	9	1	1	N	17112	PREDICTED: myosin light chain alkali isoform X2 [Vollenhovia emeryi]
15	5651	gi 746847494 ref XP_011054119.1	56.37	9	1	1	N	17131	PREDICTED: myosin light chain alkali isoform X2 [Acromyrmex echinator]
15	5652	gi 307175833 gb EFN65648.1	56.37	9	1	1	N	17026	Myosin light chain alkali [Camponotus floridanus]
15	5653	gi 752885282 ref XP_011260420.1	56.37	9	1	1	N	17026	PREDICTED: myosin light chain alkali isoform X2 [Camponotus floridanus]
15	5654	gi 307208335 gb EFN85742.1	56.37	9	1	1	N	17069	Myosin light chain alkali [Harpegnathos saltator]
15	5655	gi 1009373340 gb KYM97205.1	56.37	8	1	1	N	17233	Myosin light chain alkali [Cyphomyrmex costatus]
15	5656	gi 752885280 ref XP_011260419.1	56.37	8	1	1	N	17556	PREDICTED: myosin light chain alkali isoform X1 [Camponotus floridanus]
15	5657	gi 746847492 ref XP_011054118.1	56.37	8	1	1	N	17603	PREDICTED: myosin light chain alkali isoform X1 [Acromyrmex echinator]
15	5658	gi 795063205 ref XP_011873748.1	56.37	8	1	1	N	17699	PREDICTED: myosin light chain alkali isoform X1 [Vollenhovia emeryi]
15	5659	gi 769856979 ref XP_011640106.1	56.37	8	1	1	N	17729	PREDICTED: myosin light chain alkali isoform X1 [Pogonomyrmex barbatus]
15	5660	gi 780687958 ref XP_011698944.1	56.37	8	1	1	N	17647	PREDICTED: myosin light chain alkali isoform X1 [Wasmannia auropunctata]
15	5661	gi 751228680 ref XP_011167760.1	56.37	8	1	1	N	17658	PREDICTED: myosin light chain alkali isoform X1 [Solenopsis invicta]
15	5662	gi 749750480 ref XP_011137500.1	56.37	8	1	1	N	17826	PREDICTED: myosin light chain alkali isoform X1 [Harpegnathos saltator]
15	5663	gi 826465309 ref XP_012535021.1	56.37	8	1	1	N	17884	PREDICTED: myosin light chain alkali isoform X1 [Monomorium pharaonis]
15	5664	gi 322786593 gb EFZ12988.1	56.37	7	1	1	N	20456	hypothetical protein SINV_04902, partial [Solenopsis invicta]
15	5665	gi 1009354327 gb KYM79681.1	56.37	7	1	1	N	20373	Myosin light chain alkali [Atta colombica]
15	5667	gi 1009419342 gb KYN37901.1	56.37	7	1	1	N	20542	Myosin light chain alkali [Trachymyrmex septentrionalis]
15	5668	gi 1012980172 gb KYQ54098.1	56.37	7	1	1	N	20525	Myosin light chain alkali [Trachymyrmex zeki]
15	5669	gi 801397041 ref XP_012058904.1	56.37	7	1	1	N	22153	PREDICTED: myosin light chain alkali [Atta cephalotes]
15	5670	gi 861651167 gb KMQ97620.1	56.37	3	1	1	N	56377	myosin light chain alkali-like isoform x1 protein [Lasius niger]
31	11379	gi 322792560 gb EFZ16493.1	50.57	11	1	1	N	10553	hypothetical protein SINV_01717, partial [Solenopsis invicta]
31	11380	gi 1009376845 gb KYN00228.1	50.57	2	1	1	N	70039	hypothetical protein ALC62_09023 [Cyphomyrmex costatus]
32	12670	gi 801398031 ref XP_012059450.1	48.89	5	1	1	N	22550	PREDICTED: THO complex subunit 4-like [Atta cephalotes]
32	12671	gi 307180346 gb EFN68372.1	48.89	4	1	1	N	26614	THO complex subunit 4 [Camponotus floridanus]
32	12672	gi 307200277 gb EFN80545.1	48.89	4	1	1	N	26647	THO complex subunit 4 [Harpegnathos saltator]
32	12673	gi 759054119 ref XP_011336252.1	48.89	4	1	1	N	26932	PREDICTED: THO complex subunit 4 [Cera pachys biro]
32	12674	gi 752877294 ref XP_011256074.1	48.89	4	1	1	N	26873	PREDICTED: THO complex subunit 4 [Camponotus floridanus]
32	12675	gi 607361714 gb EZA55989.1	48.89	4	1	1	N	26932	RNA and export factor-binding protein [Cera pachys biro]
32	12676	gi 749782740 ref XP_011145476.1	48.89	4	1	1	N	26906	PREDICTED: THO complex subunit 4 [Harpegnathos saltator]
32	12677	gi 332016673 gb EGI57527.1	48.89	4	1	1	N	26763	RNA and export factor-binding protein 2 [Acromyrmex echinator]
total 103 proteins									

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
32	12678	gi 1009383875 gb KYN06420.1	48.89	4	1	1	N	26880	RNA and export factor-binding protein 2 [C yphomyrmex costatus]
32	12679	gi 951569456 ref XP_014483137.1	48.89	4	1	1	N	26864	PREDICTED: THO complex subunit 4 [Dino ponera quadriceps]
32	12680	gi 1009400220 gb KYN20287.1	48.89	4	1	1	N	27055	RNA and export factor-binding protein 2 [T rachymyrmex cornetzi]
32	12681	gi 746871666 ref XP_011067067.1	48.89	4	1	1	N	27022	PREDICTED: THO complex subunit 4 [Acro myrmex echinator]
32	12682	gi 1009355829 gb KYM81132.1	48.89	4	1	1	N	27109	RNA and export factor-binding protein 2 [A tta colombica]
32	12683	gi 1009412751 gb KYN31662.1	48.89	4	1	1	N	27022	RNA and export factor-binding protein 2 [T rachymyrmex septentrionalis]
32	12684	gi 1012982018 gb KYQ55838.1	48.89	4	1	1	N	27140	RNA and export factor-binding protein 2 [T rachymyrmex zeteki]
32	12685	gi 751217225 ref XP_011161593.1	48.89	4	1	1	N	27134	PREDICTED: THO complex subunit 4 [Sole nopsis invicta]
32	12686	gi 826455402 ref XP_012533099.1	48.89	4	1	1	N	27194	PREDICTED: THO complex subunit 4 [Mono morium pharaonis]
32	12687	gi 780718794 ref XP_011706383.1	48.89	4	1	1	N	27192	PREDICTED: THO complex subunit 4 [Was mannia auropunctata]
32	12688	gi 769855670 ref XP_011639405.1	48.89	4	1	1	N	27212	PREDICTED: THO complex subunit 4 [Pogo nomyrmex barbatus]
32	12689	gi 322793642 gb EFZ17092.1	48.89	4	1	1	N	27434	hypothetical protein SINV_14629, partial [Solenopsis invicta]
32	12690	gi 795052497 ref XP_011870534.1	48.89	4	1	1	N	27424	PREDICTED: THO complex subunit 4 [Volle nhovia emeryi]
32	12691	gi 815821906 ref XP_012232208.1	48.89	4	1	1	N	27628	PREDICTED: THO complex subunit 4 [Linep ithema humile]
32	12692	gi 861607823 gb KMQ84724.1	48.89	4	1	1	N	29079	tho complex subunit 4-like protein, partial [Lasius niger]
6	12703	gi 815816306 ref XP_012229239.1	46.65	6	1	1	N	22465	PREDICTED: histone H1B-like [Linepithema humile]
6	12704	gi 751207409 ref XP_011156267.1	46.65	5	1	1	N	23837	PREDICTED: late histone H1-like [Solenops is invicta]
6	12705	gi 322798610 gb EFZ20214.1	46.65	5	1	1	N	23837	hypothetical protein SINV_05737, partial [Solenopsis invicta]
33	12706	gi 746841606 ref XP_011050991.1	37.25	5	1	1	N	22099	PREDICTED: muscle LIM protein Mlp84B-lik e isoform X3 [Acromyrmex echinator]
33	12707	gi 749757112 ref XP_011140957.1	37.25	2	1	1	N	53514	PREDICTED: LOW QUALITY PROTEIN: mus cle LIM protein Mlp84B [Harpegnathos salt ator]
33	12708	gi 746841604 ref XP_011050990.1	37.25	2	1	1	N	53653	PREDICTED: muscle LIM protein Mlp84B-lik e isoform X2 [Acromyrmex echinator]
33	12709	gi 751209662 ref XP_011157487.1	37.25	2	1	1	N	53526	PREDICTED: muscle LIM protein Mlp84B-lik e isoform X2 [Solenopsis invicta]
33	12710	gi 795045767 ref XP_011868348.1	37.25	2	1	1	N	53756	PREDICTED: muscle LIM protein Mlp84B-lik e isoform X1 [Vollenhovia emeryi]
33	12711	gi 746841601 ref XP_011050989.1	37.25	2	1	1	N	53997	PREDICTED: muscle LIM protein Mlp84B-lik e isoform X1 [Acromyrmex echinator]
33	12712	gi 751209660 ref XP_011157486.1	37.25	2	1	1	N	53884	PREDICTED: muscle LIM protein Mlp84B-lik e isoform X1 [Solenopsis invicta]
35	143	gi 307184709 gb EFN71038.1	33.46	4	1	1	N	22151	hypothetical protein EAG_09928 [Campono tus floridanus]
35	4127	gi 861653549 gb KMQ99191.1	33.46	1	1	1	N	108034	dynammin-like mitochondrial protein [Lasius niger]
35	195	gi 801397101 ref XP_012058936.1	33.46	1	1	1	N	113731	PREDICTED: dynammin-like 120 kDa protei n, mitochondrial isoform X3 [Atta cephalot es]
35	4128	gi 801397099 ref XP_012058935.1	33.46	1	1	1	N	113933	PREDICTED: dynammin-like 120 kDa protei n, mitochondrial isoform X2 [Atta cephalot es]
35	4129	gi 801397097 ref XP_012058934.1	33.46	1	1	1	N	114004	PREDICTED: dynammin-like 120 kDa protei n, mitochondrial isoform X1 [Atta cephalot es]
total 103 proteins									

Band # 4 Proteins

Summary

1. Notes

2. Result Statistics

Figure 1. False discovery rate (FDR) curve. X axis is the number of peptide-spectrum matches (PSM) being kept. Y axis is the corresponding FDR.

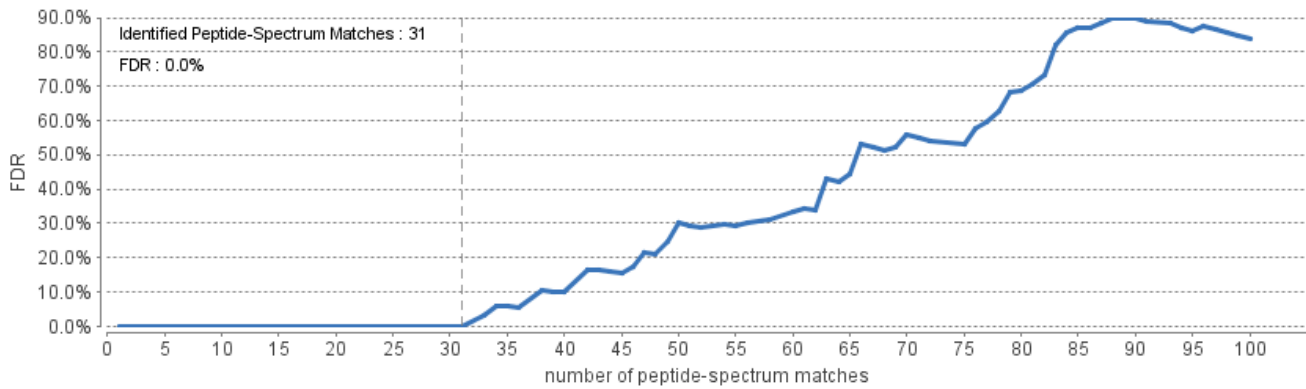


Figure 2. PSM score distribution. (a) Distribution of PEAKS peptide score; (b) Scatterplot of PEAKS peptide score versus precursor mass error.

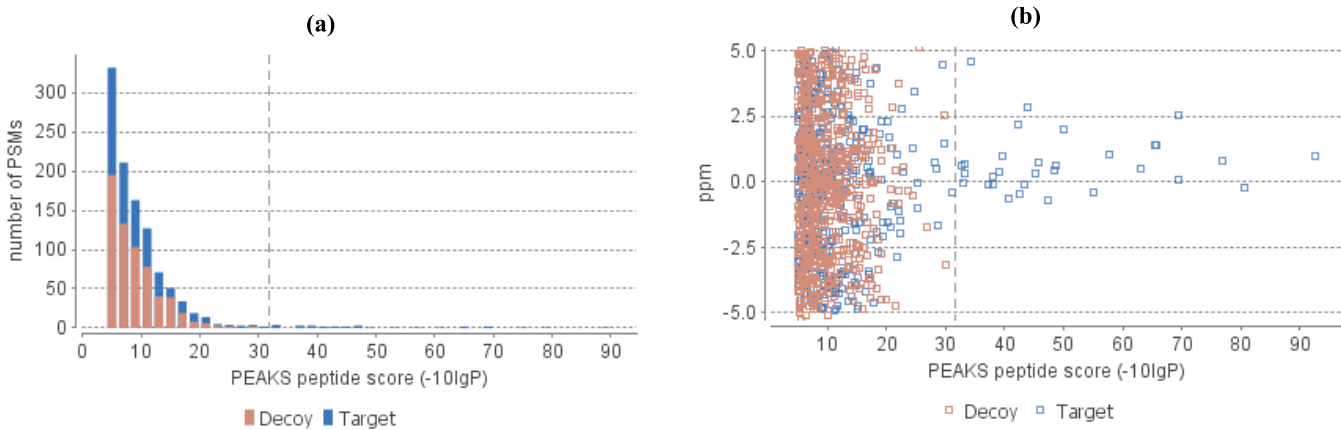


Figure 3. De novo result validation. Distribution of residue local confidence: (a) Residues in de novo sequences validated by confident database peptide assignment; (b) Residues in "de novo only" sequences.

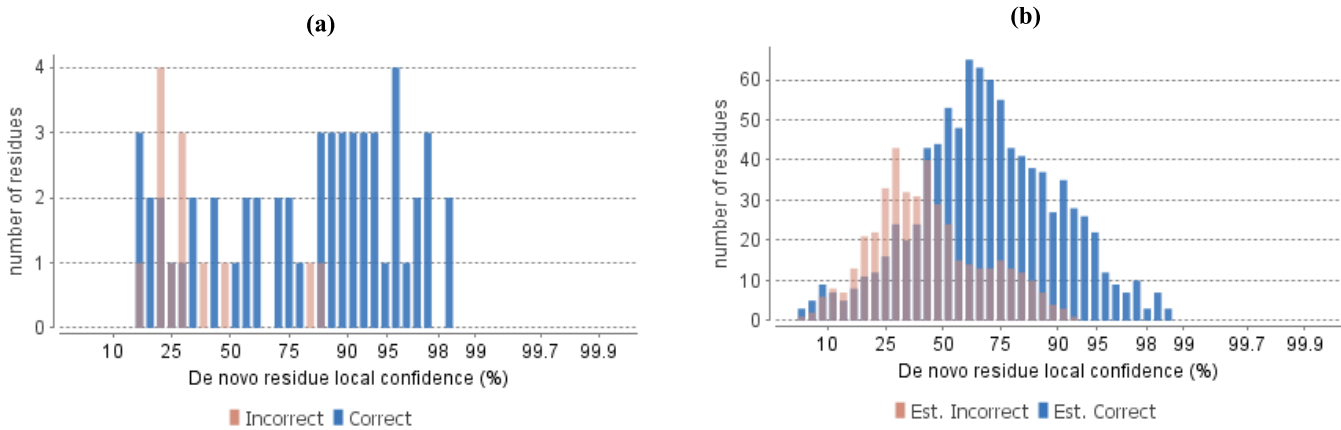


Table 1. Statistics of data.

# of MS Scans	1737
# of MS/MS Scans	2885

Table 4. PTM profile.

Name	Δ Mass	Position	#PSM	-10lgP	Area	AScore
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Table 2. Result filtration parameters.

Peptide -10lgP	≥31.7
Protein -10lgP	≥20
Proteins unique peptides	≥1
De novo ALC Score	≥50%

Table 3. Statistics of filtered result.

Peptide-Spectrum Matches	31
Peptide Sequences	24
Protein Groups	8
Proteins	60
Proteins (#Unique Peptides)	3 (>2); 5 (=2); 52 (=1);
FDR (Peptide-Spectrum Matches)	0.0%
FDR (Peptide Sequences)	0.0%
FDR (Protein)	0.0%
De Novo Only Spectra	128

3. Experiment Control

Figure 4. Precursor mass error of peptide-spectrum matches (PSM) in filtered result. (a) Distribution of precursor mass error in ppm; (b) Scatterplot of precursor m/z versus precursor mass error in ppm.

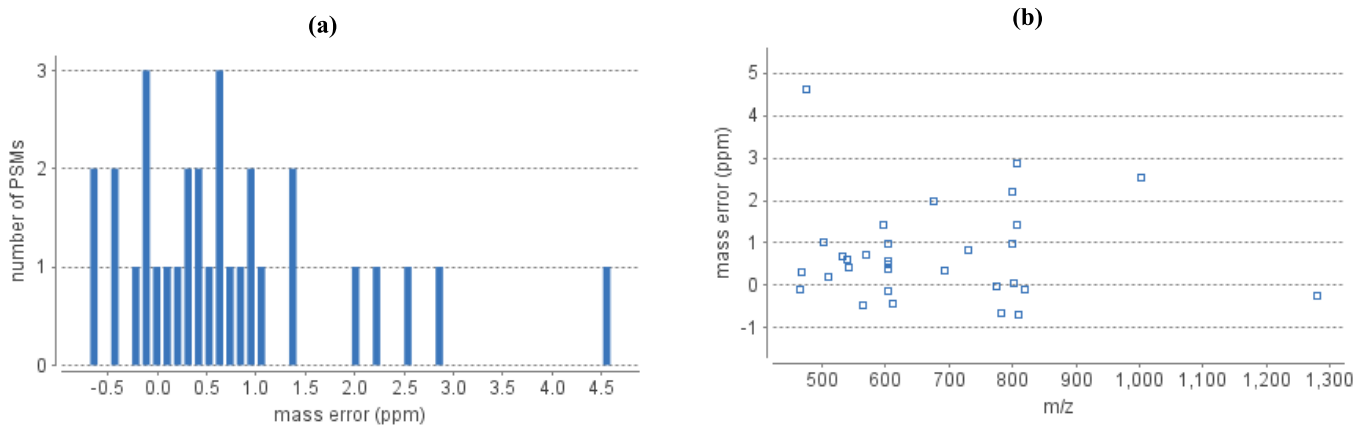


Table 5. Number of identified peptides in each sample by the number of missed cleavages

Missed Cleavages	0	1	2	3	4+
Sample 20	20	4	0	0	0

4. Other Information

Table 6. Search parameters.

Search Engine Name:	PEAKS
Parent Mass Error Tolerance:	5.0 ppm
Fragment Mass Error Tolerance:	0.5 Da
Precursor Mass Search Type:	monoisotopic
Enzyme:	Trypsin
Max Missed Cleavages:	3
Non-specific Cleavage:	one
Variable Modifications:	
Oxidation (M):	15.99
Max variable PTM per peptide:	3
Database:	Ant
Taxon:	All
Searched Entry:	473117
FDR Estimation:	Enabled
Merge Options:	no merge
Precursor Options:	corrected
Charge Options:	no correction

Table 7. Instrument parameters.

Fractions:	TW_4.raw
Ion Source:	ESI(nano-spray)
Fragmentation Mode:	CID, CAD(y and b ions)
MS Scan Mode:	FT-ICR/Orbitrap
MS/MS Scan Mode:	FT-ICR/Orbitrap

Filter Options: no filter
Process: true

Protein List

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
1	11250	gi 749749329 ref XP_011136874.1	192.41	33	9	9	Y	22904	PREDICTED: peptidyl-prolyl cis-trans isomerase-like [Harpegnathos saltator]
1	11251	gi 951553352 ref XP_014476232.1	192.41	33	9	9	Y	22822	PREDICTED: peptidyl-prolyl cis-trans isomerase-like [Dinoponera quadriceps]
1	11252	gi 307209006 gb EFN86206.1	192.41	33	9	9	Y	22904	Peptidyl-prolyl cis-trans isomerase [Harpegnathos saltator]
7	14086	gi 1009374605 gb KYM98331.1	100.49	2	2	2	N	75845	Transferrin [Cyphomyrmex costatus]
7	14087	gi 1012977385 gb KYQ51459.1	100.49	2	2	2	N	78006	Transferrin [Trachymyrmex zeteki]
2	77	gi 1911819 gb AAB50883.1	94.40	12	2	2	Y	11819	Myr p I=allergenic polypeptide {N-terminal} [Myrmecia pilosula=jumper ants, venom, Peptide Partial, 112 aa]
2	78	gi 312284 emb CAA49760.1	94.40	12	2	2	Y	11849	major allergen [Myrmecia pilosula]
2	76	gi 730091 sp Q07932.1 MYR1_MYRPI	94.40	12	2	2	Y	11849	RecName: Full=Pilosulin-1; AltName: Full=Allergen Myr p I; AltName: Full=Major allergen Myr p 1; AltName: Allergen=Myr p 1; Contains: RecName: Full=Pilosulin-1; Contains: RecName: Full=Pilosulin-1 65->112; Contains: RecName...
6	14082	gi 1911818 gb AAB50882.1	91.98	33	1	1	N	8145	Myr p II=allergenic polypeptide {N-terminal} [Myrmecia pilosula=jumper ants, venom, Peptide Partial, 75 aa]
6	14083	gi 2498604 sp Q26464.1 MYR3A_MYRPI	91.98	33	1	1	N	8145	RecName: Full=Pilosulin-3a; AltName: Full=Allergen Myr p II; AltName: Full=Pilosulin-2; AltName: Allergen=Myr p 2; Flags: Precursor
6	14084	gi 1438761 gb AAB36316.1	91.98	33	1	1	N	8145	Myr p II [Myrmecia pilosula]
6	14085	gi 1839305 gb AAB47023.1	91.98	33	1	1	N	8145	Myr p II=allergen [Myrmecia pilosula=Australian jumper ants, venom, Peptide, 75 aa]
5	11202	gi 746853393 ref XP_011057295.1	79.14	8	1	1	N	19210	PREDICTED: probable phospholipid hydroperoxide glutathione peroxidase isoform X2 [Acromyrmex echinator]
5	11210	gi 746853391 ref XP_011057294.1	79.14	7	1	1	N	21881	PREDICTED: probable phospholipid hydroperoxide glutathione peroxidase isoform X1 [Acromyrmex echinator]
5	11200	gi 861635716 gb KMQ91644.1	79.14	8	1	1	N	17626	putative phospholipid hydroperoxide glutathione peroxidase isoform x1 [Lasius niger]
5	11257	gi 795090249 ref XP_011879301.1	79.14	8	1	1	N	19100	PREDICTED: probable phospholipid hydroperoxide glutathione peroxidase isoform X2 [Vollenhovia emeryi]
5	11204	gi 769858058 ref XP_011640688.1	79.14	8	1	1	N	19024	PREDICTED: probable phospholipid hydroperoxide glutathione peroxidase isoform X2 [Pogonomyrmex barbatus]
5	11205	gi 769858060 ref XP_011640689.1	79.14	8	1	1	N	19024	PREDICTED: probable phospholipid hydroperoxide glutathione peroxidase isoform X2 [Pogonomyrmex barbatus]
5	11219	gi 751198850 ref XP_011168979.1	79.14	8	1	1	N	19135	PREDICTED: probable phospholipid hydroperoxide glutathione peroxidase isoform X2 [Solenopsis invicta]
5	11167	gi 749797995 ref XP_011152483.1	79.14	8	1	1	N	19094	PREDICTED: probable phospholipid hydroperoxide glutathione peroxidase isoform X2 [Harpegnathos saltator]
5	11206	gi 815808366 ref XP_012225017.1	79.14	8	1	1	N	19223	PREDICTED: probable phospholipid hydroperoxide glutathione peroxidase isoform X2 [Linepithema humile]
5	11220	gi 826422357 ref XP_012526177.1	79.14	8	1	1	N	18906	PREDICTED: probable phospholipid hydroperoxide glutathione peroxidase isoform X2 [Monomorium pharaonis]
5	11221	gi 826422355 ref XP_012526176.1	79.14	8	1	1	N	18906	PREDICTED: probable phospholipid hydroperoxide glutathione peroxidase isoform X2 [Monomorium pharaonis]
5	11222	gi 826422351 ref XP_012526174.1	79.14	7	1	1	N	21650	PREDICTED: probable phospholipid hydroperoxide glutathione peroxidase isoform X1 [Monomorium pharaonis]
5	11223	gi 826422349 ref XP_012526173.1	79.14	7	1	1	N	21650	PREDICTED: probable phospholipid hydroperoxide glutathione peroxidase isoform X1 [Monomorium pharaonis]
5	11208	gi 815808362 ref XP_012225015.1	79.14	7	1	1	N	21837	PREDICTED: probable phospholipid hydroperoxide glutathione peroxidase isoform X1 [Linepithema humile]
5	11258	gi 795090239 ref XP_011879298.1	79.14	7	1	1	N	21763	PREDICTED: probable phospholipid hydroperoxide glutathione peroxidase isoform X1 [Vollenhovia emeryi]

total 60 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
5	11209	gi 769858056 ref XP_011640687.1	79.14	7	1	1	N	21766	PREDICTED: probable phospholipid hyd roperoxide glutathione peroxidase isofo rm X1 [Pogonomyrmex barbatus]
5	11224	gi 751198848 ref XP_011168899.1	79.14	7	1	1	N	21846	PREDICTED: probable phospholipid hyd roperoxide glutathione peroxidase isofo rm X1 [Solenopsis invicta]
5	11225	gi 826422353 ref XP_012526175.1	79.14	7	1	1	N	21650	PREDICTED: probable phospholipid hyd roperoxide glutathione peroxidase isofo rm X1 [Monomorium pharaonis]
5	11168	gi 749797993 ref XP_011152482.1	79.14	7	1	1	N	21668	PREDICTED: probable phospholipid hyd roperoxide glutathione peroxidase isofo rm X1 [Harpegnathos saltator]
5	11169	gi 951523048 ref XP_014488365.1	79.14	7	1	1	N	21695	PREDICTED: probable phospholipid hyd roperoxide glutathione peroxidase isofo rm X2 [Dinoponera quadriceps]
5	11211	gi 815808364 ref XP_012225016.1	79.14	7	1	1	N	21837	PREDICTED: probable phospholipid hyd roperoxide glutathione peroxidase isofo rm X1 [Linepithema humile]
5	11212	gi 769858054 ref XP_011640686.1	79.14	7	1	1	N	21766	PREDICTED: probable phospholipid hyd roperoxide glutathione peroxidase isofo rm X1 [Pogonomyrmex barbatus]
5	11259	gi 795090244 ref XP_011879300.1	79.14	7	1	1	N	21763	PREDICTED: probable phospholipid hyd roperoxide glutathione peroxidase isofo rm X1 [Vollenhovia emeryi]
5	11170	gi 951523046 ref XP_014488363.1	79.14	6	1	1	N	26359	PREDICTED: probable phospholipid hyd roperoxide glutathione peroxidase isofo rm X1 [Dinoponera quadriceps]
8	5688	gi 801403344 ref XP_012061624.1	45.57	0	1	1	N	1817097	PREDICTED: LOW QUALITY PROTEIN: t itin-like [Atta cephalotes]
35	132	gi 1009372276 gb KYM96404.1	42.54	7	1	1	N	16728	Cofilin/actin-depolymerizing factor like protein, partial [Cyphomyrmex costatu s]
35	2	gi 749756765 ref XP_011140861.1	42.54	7	1	1	N	16860	PREDICTED: cofilin/actin-depolymerizi ng factor homolog [Harpegnathos salta tor]
35	10	gi 322799134 gb EFZ20581.1	42.54	7	1	1	N	16857	hypothetical protein SINV_11686, parti al [Solenopsis invicta]
35	3	gi 795075576 ref XP_011876241.1	42.54	7	1	1	N	16860	PREDICTED: cofilin/actin-depolymerizi ng factor homolog [Vollenhovia emery i]
35	4	gi 759066863 ref XP_011342896.1	42.54	7	1	1	N	16860	PREDICTED: cofilin/actin-depolymerizi ng factor homolog [Ceropachys biroi]
35	5	gi 751206597 ref XP_011155825.1	42.54	7	1	1	N	16860	PREDICTED: cofilin/actin-depolymerizi ng factor homolog [Solenopsis invicta]
35	6	gi 780650680 ref XP_011690296.1	42.54	7	1	1	N	16860	PREDICTED: cofilin/actin-depolymerizi ng factor homolog [Wasmannia auropu nctata]
35	11	gi 607357312 gb EZA51777.1	42.54	7	1	1	N	16860	Cofilin/actin-depolymerizing factor-like protein [Ceropachys biroi]
35	7	gi 951531070 ref XP_014469357.1	42.54	7	1	1	N	16860	PREDICTED: cofilin/actin-depolymerizi ng factor homolog [Dinoponera quadric eps]
35	12	gi 746872572 ref XP_011067557.1	42.54	7	1	1	N	16860	PREDICTED: cofilin/actin-depolymerizi ng factor homolog [Acromyrmex echin atior]
35	13	gi 815823534 ref XP_012233084.1	42.54	7	1	1	N	16860	PREDICTED: cofilin/actin-depolymerizi ng factor homolog [Linepithema humil e]
35	8	gi 826475616 ref XP_012537040.1	42.54	7	1	1	N	16860	PREDICTED: cofilin/actin-depolymerizi ng factor homolog [Monomorium phara onis]
35	9	gi 752866064 ref XP_011269506.1	42.54	7	1	1	N	16860	PREDICTED: cofilin/actin-depolymerizi ng factor homolog [Camponotus florida nus]
35	14	gi 861649741 gb KMQ96964.1	42.54	7	1	1	N	16974	cofilin actin-depolymerizing factor-like protein [Lasius niger]
35	15	gi 307187751 gb EFN72723.1	42.54	6	1	1	N	19355	Cofilin/actin-depolymerizing factor-like protein [Camponotus floridanus]
35	16	gi 801383792 ref XP_012055075.1	42.54	5	1	1	N	20394	PREDICTED: cofilin/actin-depolymerizi ng factor homolog [Atta cephalotes]
35	17	gi 1009357994 gb KYM83255.1	42.54	5	1	1	N	20394	Cofilin/actin-depolymerizing factor like protein [Atta colombica]
35	18	gi 307205222 gb EFN83612.1	42.54	5	1	1	N	20514	Cofilin/actin-depolymerizing factor-like protein [Harpegnathos saltator]
35	19	gi 1012971901 gb KYQ46466.1	42.54	5	1	1	N	20722	Cofilin/actin-depolymerizing factor like protein [Trachymyrmex zeteki]
35	20	gi 1009394301 gb KYN15343.1	42.54	5	1	1	N	20708	Cofilin/actin-depolymerizing factor like protein [Trachymyrmex cornetzi]
35	21	gi 332016345 gb EGI57258.1	42.54	5	1	1	N	20654	Cofilin/actin-depolymerizing factor-like protein [Acromyrmex echinator]

total 60 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
35	22	gi 1009419754 gb KYN38297.1	42.54	5	1	1	N	20608	Cofilin/actin-depolymerizing factor like protein [Trachymyrmex septentrionalis]
36	179	gi 751202763 ref XP_011173546.1	33.36	1	1	1	N	93364	PREDICTED: histone deacetylase 4-like [Solenopsis invicta]
total 60 proteins									

Prepared with PEAKS™ (bioinform.com)

Band # 5 Proteins

Summary

1. Notes

2. Result Statistics

Figure 1. False discovery rate (FDR) curve. X axis is the number of peptide-spectrum matches (PSM) being kept. Y axis is the corresponding FDR.

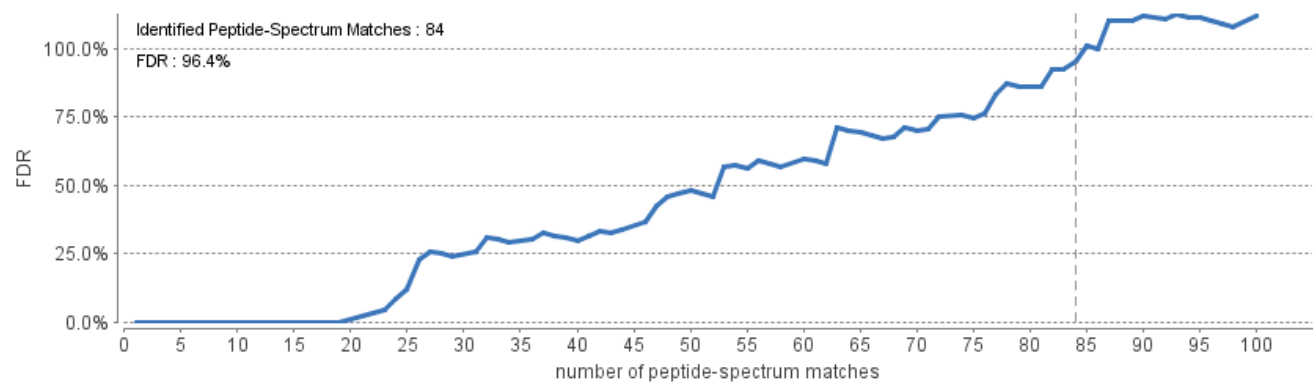


Figure 2. PSM score distribution. (a) Distribution of PEAKS peptide score; (b) Scatterplot of PEAKS peptide score versus precursor mass error.

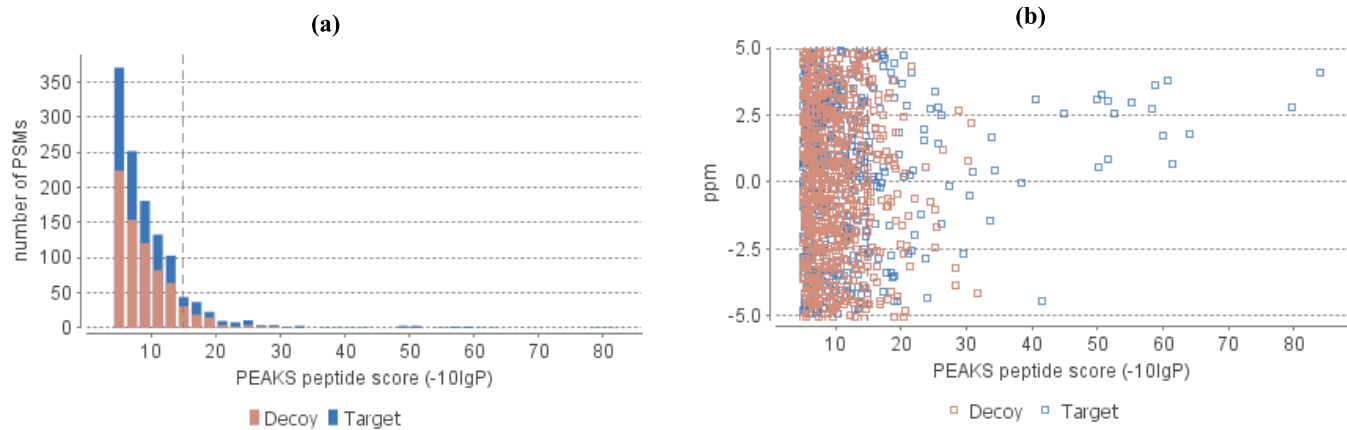


Figure 3. De novo result validation. Distribution of residue local confidence: (a) Residues in de novo sequences validated by confident database peptide assignment; (b) Residues in "de novo only" sequences.

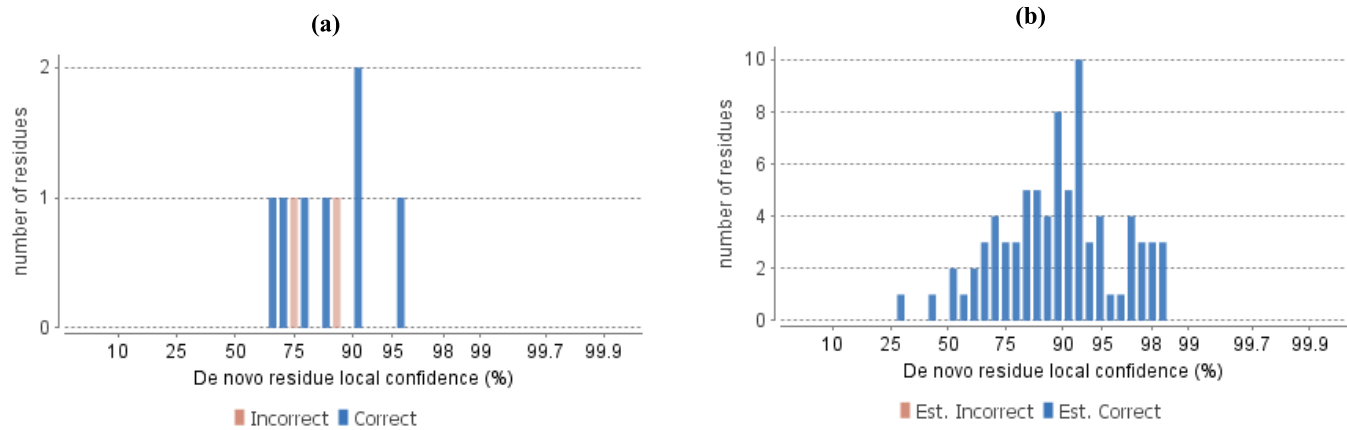


Table 1. Statistics of data.

# of MS Scans	1613
# of MS/MS Scans	3336

Table 4. PTM profile.

Name	Δ Mass	Position	#PSM	-10lgP	Area	AScore
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Table 2. Result filtration parameters.

Peptide -10lgP	≥15
Protein -10lgP	≥20
Proteins unique peptides	≥1
De novo ALC Score	≥80%

Table 3. Statistics of filtered result.

Peptide-Spectrum Matches	84
Peptide Sequences	78
Protein Groups	29
Proteins	118
Proteins (#Unique Peptides)	32 (>2); 1 (=2); 85 (=1);
FDR (Peptide-Spectrum Matches)	96.4%
FDR (Peptide Sequences)	101.3%
FDR (Protein)	0.0%
De Novo Only Spectra	8

3. Experiment Control

Figure 4. Precursor mass error of peptide-spectrum matches (PSM) in filtered result. **(a)** Distribution of precursor mass error in ppm; **(b)** Scatterplot of precursor m/z versus precursor mass error in ppm. 

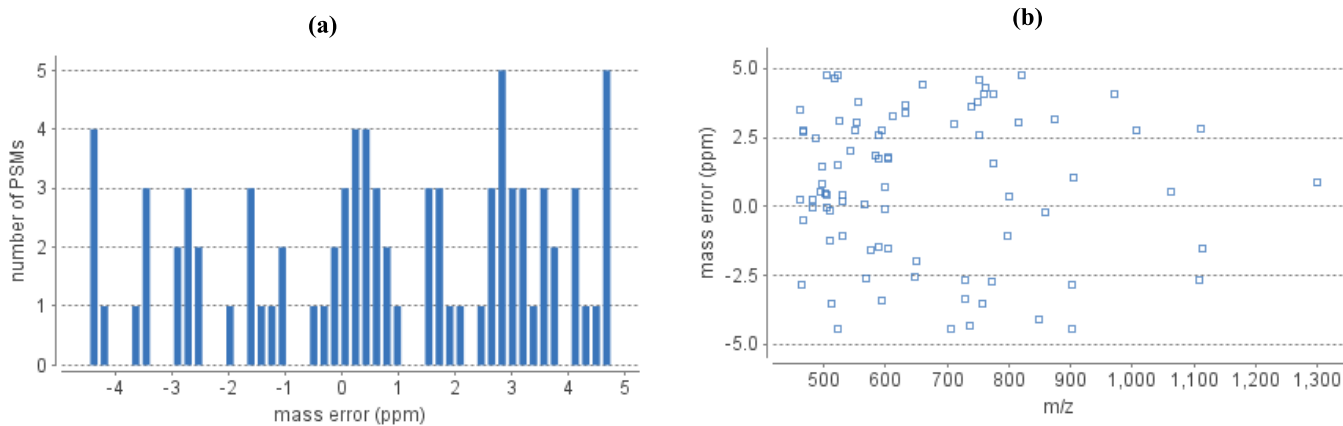


Table 5. Number of identified peptides in each sample by the number of missed cleavages

Missed Cleavages	0	1	2	3	4+
Sample 21	40	24	8	6	0

4. Other Information

Table 6. Search parameters.

Search Engine Name:	PEAKS
Parent Mass Error Tolerance:	5.0 ppm
Fragment Mass Error Tolerance:	0.5 Da
Precursor Mass Search Type:	monoisotopic
Enzyme:	Trypsin
Max Missed Cleavages:	3
Non-specific Cleavage:	one
Variable Modifications:	
Oxidation (M):	15.99
Max variable PTM per peptide:	3
Database:	Ant
Taxon:	All
Searched Entry:	473117
FDR Estimation:	Enabled
Merge Options:	no merge
Precursor Options:	corrected
Charge Options:	no correction

Oxidation	15.99	M	17	64.01	4.37E5	64.94
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Table 7. Instrument parameters.

Fractions:	TW_5.raw
Ion Source:	ESI(nano-spray)
Fragmentation Mode:	CID, CAD(y and b ions)
MS Scan Mode:	FT-ICR/Orbitrap
MS/MS Scan Mode:	FT-ICR/Orbitrap

Filter Options: no filter
Process: true

Protein List

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
1	63	gi 322792410 gb EFZ16394.1	168.69	20	7	7	Y	25370	hypothetical protein SINV_12161, partial [Solenopsis invicta]
1	64	gi 751219056 ref XP_011162596.1	168.69	20	7	7	Y	25498	PREDICTED: acidic phospholipase A2 PA4 isoform X2 [Solenopsis invicta]
1	66	gi 607361739 gb EZA56014.1	168.69	19	7	7	Y	25661	Group 3 secretory phospholipase A2 [Cera-pachys biroi]
1	67	gi 780637978 ref XP_011687259.1	168.69	19	7	7	Y	26007	PREDICTED: phospholipase A2 isozymes P A3A/PA3B/PA5 isoform X2 [Wasmannia auropunctata]
1	69	gi 751219054 ref XP_011162595.1	168.69	18	7	7	Y	28045	PREDICTED: uncharacterized protein LOC1 05197765 isoform X1 [Solenopsis invicta]
1	70	gi 759054210 ref XP_011336300.1	168.69	18	7	7	Y	28030	PREDICTED: uncharacterized protein LOC1 05278712 isoform X3 [Cera-pachys biroi]
1	71	gi 759054208 ref XP_011336299.1	168.69	18	7	7	Y	28800	PREDICTED: uncharacterized protein LOC1 05278712 isoform X2 [Cera-pachys biroi]
1	73	gi 780637966 ref XP_011687254.1	168.69	18	7	7	Y	28793	PREDICTED: uncharacterized protein LOC1 05449644 isoform X1 [Wasmannia auropunctata]
1	72	gi 780637974 ref XP_011687258.1	168.69	18	7	7	Y	28793	PREDICTED: uncharacterized protein LOC1 05449644 isoform X1 [Wasmannia auropunctata]
1	74	gi 780637970 ref XP_011687255.1	168.69	18	7	7	Y	28793	PREDICTED: uncharacterized protein LOC1 05449644 isoform X1 [Wasmannia auropunctata]
1	75	gi 759054206 ref XP_011336298.1	168.69	16	7	7	Y	31169	PREDICTED: uncharacterized protein LOC1 05278712 isoform X1 [Cera-pachys biroi]
3	2	gi 749756765 ref XP_011140861.1	120.24	26	3	3	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Harpegnathos saltator]
3	10	gi 322799134 gb EFZ20581.1	120.24	26	3	3	N	16857	hypothetical protein SINV_11686, partial [Solenopsis invicta]
3	3	gi 795075576 ref XP_011876241.1	120.24	26	3	3	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Vollenhovia emeryi]
3	4	gi 759066863 ref XP_011342896.1	120.24	26	3	3	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Cera-pachys biroi]
3	5	gi 751206597 ref XP_011155825.1	120.24	26	3	3	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Solenopsis invicta]
3	6	gi 780650680 ref XP_011690296.1	120.24	26	3	3	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Wasmannia auropunctata]
3	11	gi 607357312 gb EZA51777.1	120.24	26	3	3	N	16860	Cofilin/actin-depolymerizing factor-like protein [Cera-pachys biroi]
3	7	gi 951531070 ref XP_014469357.1	120.24	26	3	3	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Dinoponera quadriceps]
3	12	gi 746872572 ref XP_011067557.1	120.24	26	3	3	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Acromyrmex echinatio]
3	13	gi 815823534 ref XP_012233084.1	120.24	26	3	3	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Linepithema humile]
3	8	gi 826475616 ref XP_012537040.1	120.24	26	3	3	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Monomorium pharaonis]
3	9	gi 752866064 ref XP_011269506.1	120.24	26	3	3	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Camponotus floridanus]
3	14	gi 861649741 gb KMQ96964.1	120.24	26	3	3	N	16974	cofilin actin-depolymerizing factor-like protein [Lasius niger]
3	15	gi 307187751 gb EFN72723.1	120.24	23	3	3	N	19355	Cofilin/actin-depolymerizing factor-like protein [Camponotus floridanus]
3	16	gi 801383792 ref XP_012055075.1	120.24	21	3	3	N	20394	PREDICTED: cofilin/actin-depolymerizing factor homolog [Atta cephalotes]
3	17	gi 1009357994 gb KYM83255.1	120.24	21	3	3	N	20394	Cofilin/actin-depolymerizing factor like protein [Atta colombica]
3	18	gi 307205222 gb EFN83612.1	120.24	21	3	3	N	20514	Cofilin/actin-depolymerizing factor-like protein [Harpegnathos saltator]
3	19	gi 1012971901 gb KYQ46466.1	120.24	21	3	3	N	20722	Cofilin/actin-depolymerizing factor like protein [Trachymyrmex zeteki]
3	20	gi 1009394301 gb KYN15343.1	120.24	21	3	3	N	20708	Cofilin/actin-depolymerizing factor like protein [Trachymyrmex cornetzi]
3	21	gi 332016345 gb EGI57258.1	120.24	21	3	3	N	20654	Cofilin/actin-depolymerizing factor-like protein [Acromyrmex echinatio]
3	22	gi 1009419754 gb KYN38297.1	120.24	21	3	3	N	20608	Cofilin/actin-depolymerizing factor like protein [Trachymyrmex septentrionalis]
7	10073	gi 826461821 ref XP_012534360.1	78.44	5	2	2	N	26025	PREDICTED: venom allergen 3-like [Monomorium pharaonis]

total 118 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
2	77	gi 1911819 gb AAB50883.1	64.01	10	1	1	Y	11819	Myr p I=allergenic polypeptide {N-termina l} [Myrmecia pilosula=jumper ants, veno m, Peptide Partial, 112 aa]
2	78	gi 312284 emb CAA49760.1	64.01	10	1	1	Y	11849	major allergen [Myrmecia pilosula]
2	76	gi 730091 sp Q07932.1 MYR1_MYRPI	64.01	10	1	1	Y	11849	RecName: Full=Pilosulin-1; AltName: Full= Allergen Myr p I; AltName: Full=Major aller gen Myr p 1; AltName: Allergen=Myr p 1; Contains: RecName: Full=Pilosulin-1; Cont ains: RecName: Full=Pilosulin-1 65->112; Contains: RecNa...
20	15314	gi 607348360 gb EZA46495.1	58.72	14	1	1	N	11732	Ras-related protein Rab-2A, partial [Cera pachys biro]
20	15315	gi 759082668 ref XP_011351220.1	58.72	11	1	1	N	14410	PREDICTED: ras-related protein Rab-2-lik e, partial [Cera pachys biro]
20	15316	gi 307176411 gb EFN65985.1	58.72	8	1	1	N	18440	Ras-related protein Rab-2A [Camponotus fl oridanus]
20	15317	gi 607368749 gb EZA62857.1	58.72	8	1	1	N	18440	Ras-related protein Rab-2 [Cera pachys bir oi]
20	15318	gi 1009377620 gb KYN00896.1	58.72	8	1	1	N	18440	Ras-related protein Rab-2 [Cyphomyrmex costatus]
20	15319	gi 752884345 ref XP_011259910.1	58.72	8	1	1	N	18440	PREDICTED: ras-related protein Rab-2 [Ca mponotus floridanus]
20	15320	gi 1009396666 gb KYN17315.1	58.72	8	1	1	N	18470	Ras-related protein Rab-2 [Trachymyrmex cornetzi]
20	15321	gi 751204485 ref XP_011175797.1	58.72	7	1	1	N	21797	PREDICTED: ras-related protein Rab-2, par tial [Solenopsis invicta]
20	15322	gi 1009417864 gb KYN36543.1	58.72	7	1	1	N	21882	Ras-related protein Rab-2, partial [Trachy myrmex septentrionalis]
20	15323	gi 795090310 ref XP_011879314.1	58.72	7	1	1	N	23635	PREDICTED: ras-related protein Rab-2 [Vol lenhovia emeryi]
20	15324	gi 951564182 ref XP_014481041.1	58.72	7	1	1	N	23688	PREDICTED: ras-related protein Rab-2 [Din oponera quadriceps]
20	15325	gi 815767114 ref XP_012224045.1	58.72	7	1	1	N	23666	PREDICTED: LOW QUALITY PROTEIN: ras-r elated protein Rab-2 [Linepithema humile]
20	15326	gi 801389723 ref XP_012057360.1	58.72	7	1	1	N	23662	PREDICTED: ras-related protein Rab-2 [Att a cephalotes]
20	15327	gi 1012985758 gb KYQ59275.1	58.72	7	1	1	N	23635	Ras-related protein Rab-2 [Trachymyrmex zeteki]
20	15328	gi 759032982 ref XP_011336753.1	58.72	7	1	1	N	23635	PREDICTED: ras-related protein Rab-2 [Ce rapachys biro]
20	15329	gi 769858048 ref XP_011640682.1	58.72	7	1	1	N	23647	PREDICTED: ras-related protein Rab-2 [Po gonomyrmex barbatus]
20	15330	gi 780630380 ref XP_011685325.1	58.72	7	1	1	N	23635	PREDICTED: ras-related protein Rab-2 [Wa smannia auropunctata]
20	15331	gi 826492406 ref XP_012540361.1	58.72	7	1	1	N	23635	PREDICTED: ras-related protein Rab-2 [Mo nomorium pharaonis]
20	15332	gi 861660462 gb KMR05082.1	58.72	7	1	1	N	23635	ras-related protein rab-2 [Lasius niger]
20	15333	gi 1009357119 gb KYM82393.1	58.72	2	1	1	N	64175	Ras-related protein Rab-2 [Atta colombica]
20	15334	gi 332024209 gb EGI64416.1	58.72	7	1	1	N	21360	Ras-related protein Rab-2 [Acromyrmex ec hinator]
20	15335	gi 749752872 ref XP_011138801.1	58.72	7	1	1	N	23675	PREDICTED: ras-related protein Rab-2 [Ha rpegnathos saltator]
20	15336	gi 307207076 gb EFN84885.1	58.72	7	1	1	N	23675	Ras-related protein Rab-2A [Harpegnathos saltator]
20	15337	gi 746851366 ref XP_011056205.1	58.72	7	1	1	N	23934	PREDICTED: LOW QUALITY PROTEIN: ras-r elated protein Rab-2 [Acromyrmex echinati or]
19	15295	gi 307199886 gb EFN80283.1	49.81	4	1	1	N	21946	Acyl-protein thioesterase 1, partial [Harpe gnathos saltator]
19	15296	gi 861658817 gb KMR03924.1	49.81	4	1	1	N	22387	acyl-protein thioesterase 1-like protein [La sius niger]
19	15297	gi 815815129 ref XP_012228610.1	49.81	4	1	1	N	23715	PREDICTED: acyl-protein thioesterase 2 [Li nepithema humile]
19	15298	gi 769866680 ref XP_011645328.1	49.81	4	1	1	N	23614	PREDICTED: acyl-protein thioesterase 2 [P ogonomyrmex barbatus]
19	15299	gi 801387181 ref XP_012056747.1	49.81	4	1	1	N	23575	PREDICTED: acyl-protein thioesterase 2 [A tta cephalotes]
19	15300	gi 826410384 ref XP_012538793.1	49.81	4	1	1	N	23564	PREDICTED: acyl-protein thioesterase 2 [M onomorium pharaonis]
19	15301	gi 307177259 gb EFN66437.1	49.81	4	1	1	N	23612	Acyl-protein thioesterase 2 [Camponotus fl oridanus]
19	15302	gi 749783883 ref XP_011145876.1	49.81	4	1	1	N	23557	PREDICTED: acyl-protein thioesterase 1 [H arpegnathos saltator]
19	15303	gi 751220778 ref XP_011163537.1	49.81	4	1	1	N	23598	PREDICTED: acyl-protein thioesterase 1 [S olenopsis invicta]
19	15304	gi 752882877 ref XP_011259114.1	49.81	4	1	1	N	23612	PREDICTED: acyl-protein thioesterase 2 [C amponotus floridanus]

total 118 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
19	15305	gi 332019861 gb EGI60322.1	49.81	4	1	1	N	23575	Acyl-protein thioesterase 1 [Acromyrmex echinator]
19	15306	gi 815815131 ref XP_012228611.1	49.81	4	1	1	N	23715	PREDICTED: acyl-protein thioesterase 2 [Lepithema humile]
19	15307	gi 1012984581 gb KYQ58213.1	49.81	4	1	1	N	23605	Acyl-protein thioesterase 2 [Trachymyrmex zeteki]
19	15308	gi 746863870 ref XP_011062908.1	49.81	4	1	1	N	23575	PREDICTED: acyl-protein thioesterase 2 [Acromyrmex echinator]
19	15309	gi 1009354900 gb KYM80235.1	49.81	4	1	1	N	23851	Acyl-protein thioesterase 1 [Atta colombica]
19	15310	gi 795072718 ref XP_011875663.1	49.81	3	1	1	N	25483	PREDICTED: acyl-protein thioesterase 1 [Vollenhovia emeryi]
19	15311	gi 322791151 gb EFZ15713.1	49.81	3	1	1	N	33892	hypothetical protein SINV_15507, partial [Solenopsis invicta]
19	15312	gi 1009420631 gb KYN39126.1	49.81	2	1	1	N	38698	Acyl-protein thioesterase 1 [Trachymyrmex septentrionalis]
19	15313	gi 1009397129 gb KYN17697.1	49.81	2	1	1	N	38529	Acyl-protein thioesterase 2 [Trachymyrmex cornetzi]
19	15340	gi 780606413 ref XP_011687237.1	49.81	4	1	1	N	22469	PREDICTED: acyl-protein thioesterase 2 isoform X2 [Wasmannia auropunctata]
19	15341	gi 951551611 ref XP_014475535.1	49.81	4	1	1	N	23584	PREDICTED: acyl-protein thioesterase 1 [Dinoponera quadriceps]
19	15342	gi 780606409 ref XP_011687227.1	49.81	3	1	1	N	25364	PREDICTED: acyl-protein thioesterase 1 isoform X1 [Wasmannia auropunctata]
39	143	gi 307184709 gb EFN71038.1	34.24	4	1	1	N	22151	hypothetical protein EAG_09928 [Camponotus floridanus]
39	4127	gi 861653549 gb KMQ99191.1	34.24	1	1	1	N	108034	dynammin-like mitochondrial protein [Lasius niger]
39	195	gi 801397101 ref XP_012058936.1	34.24	1	1	1	N	113731	PREDICTED: dynammin-like 120 kDa protein, mitochondrial isoform X3 [Atta cephalotes]
39	4128	gi 801397099 ref XP_012058935.1	34.24	1	1	1	N	113933	PREDICTED: dynammin-like 120 kDa protein, mitochondrial isoform X2 [Atta cephalotes]
39	4129	gi 801397097 ref XP_012058934.1	34.24	1	1	1	N	114004	PREDICTED: dynammin-like 120 kDa protein, mitochondrial isoform X1 [Atta cephalotes]
40	15346	gi 795030040 ref XP_011863145.1	33.68	1	1	1	N	166587	PREDICTED: GTPase-activating protein and VPS9 domain-containing protein 1 isoform X3 [Vollenhovia emeryi]
9	179	gi 751202763 ref XP_011173546.1	30.48	1	1	1	N	93364	PREDICTED: histone deacetylase 4-like [Solenopsis invicta]
4	15351	gi 607364075 gb EZA58296.1	29.62	1	1	1	Y	101425	Transforming acidic coiled-coil-containing protein, partial [Cerapachys biroi]
4	15352	gi 759046656 ref XP_011332322.1	29.62	1	1	1	Y	101554	PREDICTED: uncharacterized protein LOC105276428 isoform X1 [Cerapachys biroi]
4	15353	gi 759046658 ref XP_011332323.1	29.62	1	1	1	Y	101554	PREDICTED: uncharacterized protein LOC105276428 isoform X2 [Cerapachys biroi]
45	15356	gi 746857887 ref XP_011059694.1	27.43	0	1	1	N	361294	PREDICTED: protein furry isoform X1 [Acromyrmex echinator]
45	15357	gi 746857885 ref XP_011059693.1	27.43	0	1	1	N	361294	PREDICTED: protein furry isoform X1 [Acromyrmex echinator]
47	15359	gi 746839325 ref XP_011050086.1	26.25	9	1	1	Y	63850	PREDICTED: heparan-alpha-glucosaminide N-acetyltransferase-like isoform X2 [Acromyrmex echinator]
47	15360	gi 746839323 ref XP_011050085.1	26.25	9	1	1	Y	64421	PREDICTED: heparan-alpha-glucosaminide N-acetyltransferase-like isoform X1 [Acromyrmex echinator]
49	2693	gi 801403936 ref XP_012061765.1	26.07	4	1	1	N	22557	PREDICTED: protein Tube [Atta cephalotes]
49	2694	gi 1009355112 gb KYM80438.1	26.07	4	1	1	N	22505	Protein Tube [Atta colombica]
49	2695	gi 746851807 ref XP_011056440.1	26.07	4	1	1	N	22669	PREDICTED: protein Tube [Acromyrmex echinator]
49	2696	gi 1009383369 gb KYN05973.1	26.07	4	1	1	N	22811	Protein Tube [Cyphomyrmex costatus]
49	2697	gi 861631825 gb KMQ90464.1	26.07	3	1	1	N	28203	protein tube [Lasius niger]
51	15363	gi 826418588 ref XP_012524138.1	25.63	3	1	1	N	26315	PREDICTED: venom allergen 3-like [Monomorium pharaonis]
50	15362	gi 1009386137 gb KYN08390.1	25.29	1	1	1	N	441973	Heparanase [Cyphomyrmex costatus]
11	15367	gi 1009394709 gb KYN15692.1	25.09	1	1	1	N	195567	Leukocyte elastase inhibitor [Trachymyrmex cornetzi]
10	12717	gi 749732468 ref XP_011140395.1	25.09	4	1	1	N	33173	PREDICTED: uncharacterized protein LOC105183755 [Harpegnathos saltator]
55	6569	gi 1009377814 gb KYN01090.1	23.73	1	1	1	N	530292	Dynein beta chain, ciliary [Cyphomyrmex costatus]
57	15399	gi 951534108 ref XP_014470714.1	23.64	3	1	1	N	114337	PREDICTED: polycomb group protein Psc-like isoform X1 [Dinoponera quadriceps]

total 118 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
31	4148	gi 752895858 ref XP_011266169.1	23.59	3	1	1	N	36893	PREDICTED: uncharacterized protein LOC105257314 [Camponotus floridanus]
58	15403	gi 826452331 ref XP_012532497.1	23.06	4	1	1	Y	21957	PREDICTED: uncharacterized protein LOC105834506 isoform X2 [Monomorium pharaonis]
32	15407	gi 751213951 ref XP_011159805.1	22.14	1	1	1	N	103462	PREDICTED: zinc finger protein 493-like [Solenopsis invicta]
21	15369	gi 780614447 ref XP_011692571.1	21.93	0	1	1	N	253508	PREDICTED: uncharacterized protein LOC105452816 [Wasmannia auropunctata]
33	15411	gi 759043595 ref XP_011330691.1	21.64	1	1	1	N	243916	PREDICTED: phosphatidylinositol 4-kinase alpha isoform X2 [Cerapachys biroi]
61	15412	gi 307211557 gb EFN87635.1	21.52	2	1	1	Y	246178	Rotatin [Harpegnathos saltator]
71	15425	gi 769861541 ref XP_011642546.1	21.25	1	1	1	N	54176	PREDICTED: KAT8 regulatory NSL complex subunit 2 [Pogonomyrmex barbatus]
26	15384	gi 1009398702 gb KYN18977.1	21.02	3	1	1	Y	172036	Putative odorant receptor 67c [Trachymyrmex cornetzi]
64	12910	gi 749735202 ref XP_011153757.1	20.83	3	1	1	Y	176215	PREDICTED: zinc finger protein 423-like isoform X2 [Harpegnathos saltator]
69	805	gi 746868767 ref XP_011065518.1	20.45	1	1	1	N	200243	PREDICTED: protein abnormal spindle [Acromyrmex echinator]
69	15422	gi 746868771 ref XP_011065520.1	20.45	1	1	1	N	200243	PREDICTED: protein abnormal spindle [Acromyrmex echinator]
total 118 proteins									

Prepared with PEAKS™ (bioinform.com)

Band # 6 Proteins

Summary

1. Notes

2. Result Statistics

Figure 1. False discovery rate (FDR) curve. X axis is the number of peptide-spectrum matches (PSM) being kept. Y axis is the corresponding FDR.

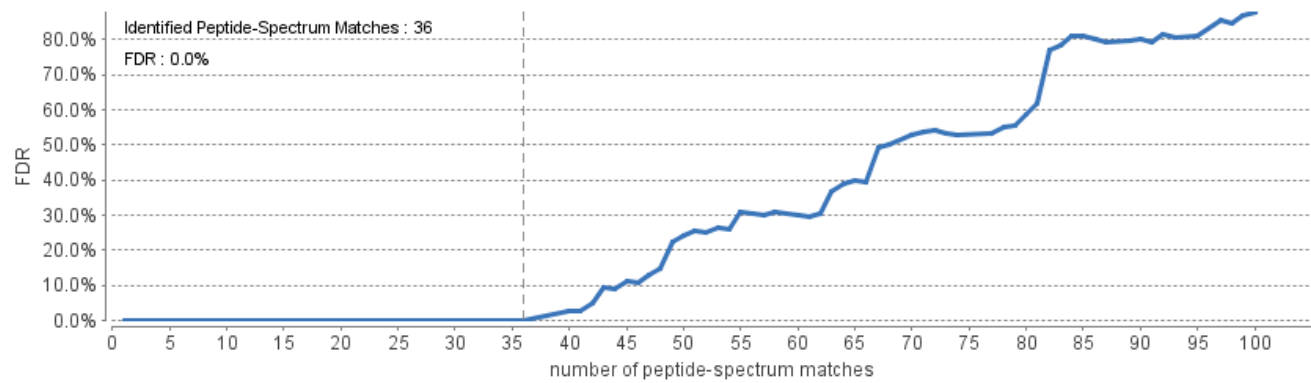


Figure 2. PSM score distribution. (a) Distribution of PEAKS peptide score; (b) Scatterplot of PEAKS peptide score versus precursor mass error.

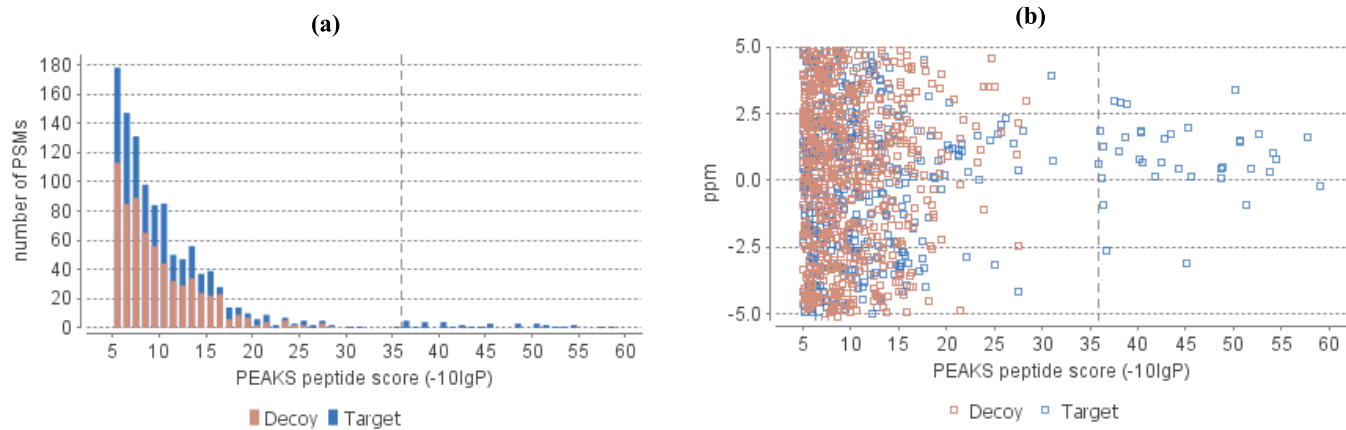


Figure 3. De novo result validation. Distribution of residue local confidence: (a) Residues in de novo sequences validated by confident database peptide assignment; (b) Residues in "de novo only" sequences.

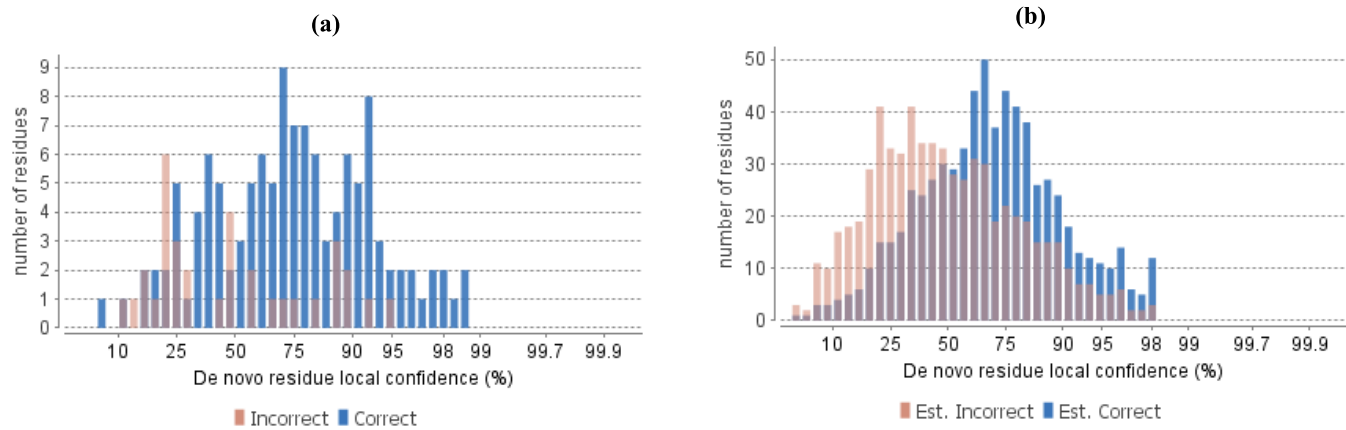


Table 1. Statistics of data.

# of MS Scans	1667
# of MS/MS Scans	3039

Table 4. PTM profile.

Name	Δ Mass	Position	#PSM	-10lgP	Area	AScore
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Table 2. Result filtration parameters.

Peptide -10lgP	≥35.9
Protein -10lgP	≥20
Proteins unique peptides	≥1
De novo ALC Score	≥50%

Table 3. Statistics of filtered result.

Peptide-Spectrum Matches	36
Peptide Sequences	34
Protein Groups	15
Proteins	175
Proteins (#Unique Peptides)	64 (>2); 63 (=2); 48 (=1);
FDR (Peptide-Spectrum Matches)	0.0%
FDR (Peptide Sequences)	0.0%
FDR (Protein)	0.0%
De Novo Only Spectra	124

3. Experiment Control

Figure 4. Precursor mass error of peptide-spectrum matches (PSM) in filtered result. (a) Distribution of precursor mass error in ppm; (b) Scatterplot of precursor m/z versus precursor mass error in ppm.

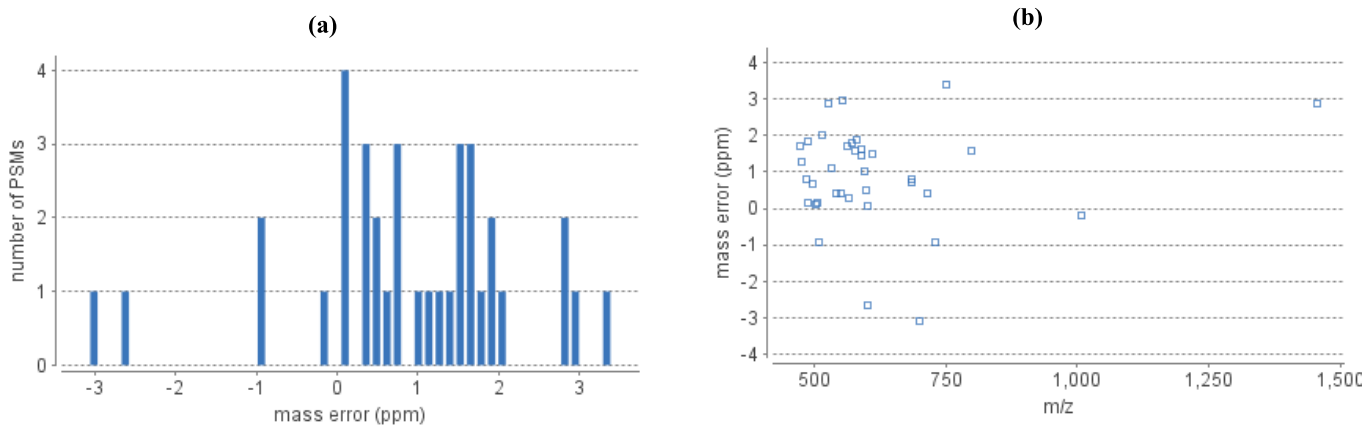


Table 5. Number of identified peptides in each sample by the number of missed cleavages

Missed Cleavages	0	1	2	3	4+
Sample 22	30	4	0	0	0

4. Other Information

Table 6. Search parameters.

Search Engine Name:	PEAKS
Parent Mass Error Tolerance:	5.0 ppm
Fragment Mass Error Tolerance:	0.5 Da
Precursor Mass Search Type:	monoisotopic
Enzyme:	Trypsin
Max Missed Cleavages:	3
Non-specific Cleavage:	one
Variable Modifications:	
Oxidation (M):	15.99
Max variable PTM per peptide:	3
Database:	Ant
Taxon:	All
Searched Entry:	473117
FDR Estimation:	Enabled
Merge Options:	no merge
Precursor Options:	corrected
Charge Options:	no correction

Table 7. Instrument parameters.

Fractions:	TW_6.raw
Ion Source:	ESI(nano-spray)
Fragmentation Mode:	CID, CAD(y and b ions)
MS Scan Mode:	FT-ICR/Orbitrap
MS/MS Scan Mode:	FT-ICR/Orbitrap

Filter Options: no filter

Process: true

Protein List

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
4	2	gi 749756765 ref XP_011140861.1	109.13	33	4	4	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Harpegnathos saltator]
4	10	gi 322799134 gb EFZ20581.1	109.13	33	4	4	N	16857	hypothetical protein SINV_11686, partial [Solenopsis invicta]
4	3	gi 795075576 ref XP_011876241.1	109.13	33	4	4	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Vollenhovia emeryi]
4	4	gi 759066863 ref XP_011342896.1	109.13	33	4	4	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Cera-pachys biroi]
4	5	gi 751206597 ref XP_011155825.1	109.13	33	4	4	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Solenopsis invicta]
4	6	gi 780650680 ref XP_011690296.1	109.13	33	4	4	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Wasmannia auropunctata]
4	11	gi 607357312 gb EZA51777.1	109.13	33	4	4	N	16860	Cofilin/actin-depolymerizing factor-like protein [Cera-pachys biroi]
4	7	gi 951531070 ref XP_014469357.1	109.13	33	4	4	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Dinoponera quadriceps]
4	12	gi 746872572 ref XP_011067557.1	109.13	33	4	4	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Acromyrmex echinator]
4	13	gi 815823534 ref XP_012233084.1	109.13	33	4	4	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Linepithema humile]
4	8	gi 826475616 ref XP_012537040.1	109.13	33	4	4	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Monomorium pharaonis]
4	9	gi 752866064 ref XP_011269506.1	109.13	33	4	4	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Camponotus floridanus]
4	14	gi 861649741 gb KMQ96964.1	109.13	33	4	4	N	16974	cofilin actin-depolymerizing factor-like protein [Lasius niger]
4	15	gi 307187751 gb EFN72723.1	109.13	29	4	4	N	19355	Cofilin/actin-depolymerizing factor-like protein [Camponotus floridanus]
4	16	gi 801383792 ref XP_012055075.1	109.13	27	4	4	N	20394	PREDICTED: cofilin/actin-depolymerizing factor homolog [Atta cephalotes]
4	17	gi 1009357994 gb KYM83255.1	109.13	27	4	4	N	20394	Cofilin/actin-depolymerizing factor like protein [Atta colombica]
4	18	gi 307205222 gb EFN83612.1	109.13	27	4	4	N	20514	Cofilin/actin-depolymerizing factor-like protein [Harpegnathos saltator]
4	19	gi 1012971901 gb KYQ46466.1	109.13	26	4	4	N	20722	Cofilin/actin-depolymerizing factor like protein [Trachymyrmex zeteki]
4	20	gi 1009394301 gb KYN15343.1	109.13	26	4	4	N	20708	Cofilin/actin-depolymerizing factor like protein [Trachymyrmex cornetzi]
4	21	gi 332016345 gb EGI57258.1	109.13	26	4	4	N	20654	Cofilin/actin-depolymerizing factor-like protein [Acromyrmex echinator]
4	22	gi 1009419754 gb KYN38297.1	109.13	26	4	4	N	20608	Cofilin/actin-depolymerizing factor like protein [Trachymyrmex septentrionalis]
1	63	gi 322792410 gb EFZ16394.1	98.67	14	4	4	Y	25370	hypothetical protein SINV_12161, partial [Solenopsis invicta]
1	64	gi 751219056 ref XP_011162596.1	98.67	14	4	4	Y	25498	PREDICTED: acidic phospholipase A2 PA4 isoform X2 [Solenopsis invicta]
1	79	gi 752883275 ref XP_011259333.1	98.67	13	4	4	Y	25675	PREDICTED: acidic phospholipase A2 PA4 isoform X2 [Camponotus floridanus]
1	12640	gi 307202432 gb EFN81852.1	98.67	13	4	4	Y	25812	Phospholipase A2 isozyme PA4 [Harpegnathos saltator]
1	81	gi 752883277 ref XP_011259334.1	98.67	13	4	4	Y	25675	PREDICTED: acidic phospholipase A2 PA4 isoform X2 [Camponotus floridanus]
1	82	gi 795027450 ref XP_011862285.1	98.67	13	4	4	Y	25771	PREDICTED: acidic phospholipase A2 PA4 [Vollenhovia emeryi]
1	83	gi 795027459 ref XP_011862288.1	98.67	13	4	4	Y	25771	PREDICTED: acidic phospholipase A2 PA4 [Vollenhovia emeryi]
1	65	gi 769852445 ref XP_011637691.1	98.67	13	4	4	Y	25718	PREDICTED: acidic phospholipase A2 PA4 isoform X2 [Pogonomyrmex barbatus]
1	84	gi 795027456 ref XP_011862287.1	98.67	13	4	4	Y	25771	PREDICTED: acidic phospholipase A2 PA4 [Vollenhovia emeryi]
1	85	gi 795027453 ref XP_011862286.1	98.67	13	4	4	Y	25771	PREDICTED: acidic phospholipase A2 PA4 [Vollenhovia emeryi]
1	66	gi 607361739 gb EZA56014.1	98.67	13	4	4	Y	25661	Group 3 secretory phospholipase A2 [Cera-pachys biroi]
1	86	gi 746846018 ref XP_011053315.1	98.67	13	4	4	Y	25913	PREDICTED: acidic phospholipase A2 PA4-like isoform X1 [Acromyrmex echinator]
1	87	gi 801374599 ref XP_012063030.1	98.67	13	4	4	Y	25985	PREDICTED: acidic phospholipase A2 PA4-like [Atta cephalotes]
1	12638	gi 332025853 gb EGI66009.1	98.67	13	4	4	Y	25913	Phospholipase A2 isozyme PA4 [Acromyrmex echinator]

total 175 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
1	12639	gi 1009378592 gb KYN01798.1	98.67	13	4	4	Y	25958	Phospholipase A2 isozyme PA4 [Cyphomyr mex costatus]
1	68	gi 769852443 ref XP_011637690.1	98.67	13	4	4	Y	27251	PREDICTED: acidic phospholipase A2 PA4 i soform X1 [Pogonomyrmex barbatus]
1	88	gi 749777653 ref XP_011143637.1	98.67	13	4	4	Y	27531	PREDICTED: acidic phospholipase A2 PA4 i soform X6 [Harpegnathos saltator]
1	70	gi 759054210 ref XP_011336300.1	98.67	12	4	4	Y	28030	PREDICTED: uncharacterized protein LOC1 05278712 isoform X3 [Cerapachys biroi]
1	90	gi 752883273 ref XP_011259332.1	98.67	12	4	4	Y	28503	PREDICTED: acidic phospholipase A2 PA4 i soform X1 [Camponotus floridanus]
1	91	gi 749777649 ref XP_011143635.1	98.67	12	4	4	Y	28548	PREDICTED: acidic phospholipase A2 PA4 i soform X4 [Harpegnathos saltator]
3	16696	gi 751221702 ref XP_011164043.1	96.70	18	3	3	N	21841	PREDICTED: peptidyl-prolyl cis-trans isom erase B [Solenopsis invicta]
3	16697	gi 795061048 ref XP_011873371.1	96.70	18	3	3	N	21909	PREDICTED: peptidyl-prolyl cis-trans isom erase B [Vollenhovia emeryi]
3	16698	gi 746846708 ref XP_011053699.1	96.70	18	3	3	N	21925	PREDICTED: peptidyl-prolyl cis-trans isom erase B [Acromyrmex echinator]
3	16699	gi 1009391715 gb KYN13004.1	96.70	18	3	3	N	21921	Peptidyl-prolyl cis-trans isomerase 5 [Trac hymyrmex cornetzi]
3	16700	gi 801377887 ref XP_012064602.1	96.70	18	3	3	N	21891	PREDICTED: peptidyl-prolyl cis-trans isom erase B [Atta cephalotes]
3	16701	gi 780687601 ref XP_011698873.1	96.70	18	3	3	N	21948	PREDICTED: peptidyl-prolyl cis-trans isom erase 5 [Wasmania auropunctata]
3	16702	gi 332025731 gb EGI65889.1	96.70	18	3	3	N	21925	Peptidyl-prolyl cis-trans isomerase 5 [Acro myrmex echinator]
3	16703	gi 861634825 gb KMQ91382.1	96.70	18	3	3	N	22006	peptidyl-prolyl cis-trans isomerase 5 [Lasius niger]
3	16704	gi 815766609 ref XP_012221080.1	96.70	18	3	3	N	22111	PREDICTED: peptidyl-prolyl cis-trans isom erase 5 [Linepithema humile]
3	16705	gi 769850192 ref XP_011636506.1	96.70	18	3	3	N	22190	PREDICTED: peptidyl-prolyl cis-trans isom erase 5 [Pogonomyrmex barbatus]
3	16706	gi 759080743 ref XP_011350217.1	96.70	18	3	3	N	22128	PREDICTED: peptidyl-prolyl cis-trans isom erase 5 [Cerapachys biroi]
3	16707	gi 951532288 ref XP_014470014.1	96.70	18	3	3	N	22095	PREDICTED: peptidyl-prolyl cis-trans isom erase 5 [Dinoponera quadricaps]
3	16708	gi 307211461 gb EFN87567.1	96.70	18	3	3	N	22267	Peptidyl-prolyl cis-trans isomerase 5 [Harp egnathos saltator]
3	16709	gi 607352114 gb EZA47135.1	96.70	18	3	3	N	22128	Peptidyl-prolyl cis-trans isomerase [Cera pa chys biroi]
3	16710	gi 1009353784 gb KYM79163.1	96.70	17	3	3	N	22966	Peptidyl-prolyl cis-trans isomerase B, parti al [Atta colombica]
3	16711	gi 1009381270 gb KYN04146.1	96.70	16	3	3	N	23932	Peptidyl-prolyl cis-trans isomerase B, parti al [Cyphomyrmex costatus]
3	16712	gi 749745312 ref XP_011155192.1	96.70	16	3	3	N	24725	PREDICTED: peptidyl-prolyl cis-trans isom erase 5 [Harpegnathos saltator]
3	16713	gi 322790590 gb EFZ15398.1	96.70	16	3	3	N	24569	hypothetical protein SINV_01262, partial [Solenopsis invicta]
3	16714	gi 1012974398 gb KYQ48695.1	96.70	6	3	3	N	67695	putative glutamyl-tRNA(Gln) amidotransfer ase subunit B, mitochondrial [Trachymyrm ex zeteki]
3	16715	gi 1009423997 gb KYN42249.1	96.70	6	3	3	N	67598	putative glutamyl-tRNA(Gln) amidotransfer ase subunit B, mitochondrial [Trachymyrm ex septentrionalis]
8	16716	gi 815766597 ref XP_012220907.1	89.40	14	3	3	N	22336	PREDICTED: ATP synthase subunit O, mito chondrial [Linepithema humile]
8	16717	gi 749753623 ref XP_011139209.1	89.40	14	3	3	N	22609	PREDICTED: ATP synthase subunit O, mito chondrial isoform X2 [Harpegnathos saltat or]
8	16718	gi 749753621 ref XP_011139208.1	89.40	14	3	3	N	23084	PREDICTED: ATP synthase subunit O, mito chondrial isoform X1 [Harpegnathos saltat or]
11	16725	gi 751215430 ref XP_011160621.1	71.68	18	2	2	N	20331	PREDICTED: protein D2-like isoform X3 [S olenopsis invicta]
11	16726	gi 769856580 ref XP_011639894.1	71.68	18	2	2	N	20453	PREDICTED: protein D2-like isoform X3 [P ogonomyrmex barbatus]
11	16740	gi 751215428 ref XP_011160620.1	71.68	16	2	2	N	22792	PREDICTED: protein D2-like isoform X2 [S olenopsis invicta]
11	16747	gi 751215426 ref XP_011160619.1	71.68	15	2	2	N	23405	PREDICTED: protein D2-like isoform X1 [S olenopsis invicta]
11	16748	gi 769856578 ref XP_011639893.1	71.68	15	2	2	N	23664	PREDICTED: protein D2-like isoform X2 [P ogonomyrmex barbatus]
11	16749	gi 769856576 ref XP_011639892.1	71.68	15	2	2	N	23699	PREDICTED: protein D2-like isoform X1 [P ogonomyrmex barbatus]
12	16727	gi 307213993 gb EFN89200.1	68.21	9	2	2	N	22328	40S ribosomal protein S7 [Harpegnathos s altator]
12	16728	gi 752878390 ref XP_011256677.1	68.21	9	2	2	N	22293	PREDICTED: 40S ribosomal protein S7-like [Camponotus floridanus]
total 175 proteins									

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
12	16729	gi 285027707 gb ADC34227.1	68.21	9	2	2	N	22237	ribosomal protein S7 [Solenopsis invicta]
12	16730	gi 951525111 ref XP_014489339.1	68.21	9	2	2	N	22430	PREDICTED: 40S ribosomal protein S7 [Dinoponera quadricaps]
12	16731	gi 769862079 ref XP_011642834.1	68.21	9	2	2	N	22277	PREDICTED: 40S ribosomal protein S7-like [Pogonomyrmex barbatus]
12	16732	gi 769862077 ref XP_011642832.1	68.21	9	2	2	N	22277	PREDICTED: 40S ribosomal protein S7-like [Pogonomyrmex barbatus]
12	16733	gi 307180129 gb EFN68173.1	68.21	9	2	2	N	22293	40S ribosomal protein S7 [Camponotus floridanus]
12	16734	gi 826470579 ref XP_012536038.1	68.21	9	2	2	N	22337	PREDICTED: 40S ribosomal protein S7-like [Monomorium pharaonis]
12	16735	gi 749733149 ref XP_011144334.1	68.21	9	2	2	N	22328	PREDICTED: 40S ribosomal protein S7 [Harpegnathos saltator]
12	16736	gi 780632800 ref XP_011685888.1	68.21	9	2	2	N	22216	PREDICTED: 40S ribosomal protein S7-like [Wasmannia auropunctata]
12	16737	gi 752507686 ref NP_001291532.1	68.21	9	2	2	N	22237	40S ribosomal protein S7-like [Solenopsis invicta]
12	16738	gi 795050241 ref XP_011869810.1	68.21	9	2	2	N	22460	PREDICTED: 40S ribosomal protein S7-like [Vollenhovia emeryi]
12	16739	gi 795050238 ref XP_011869809.1	68.21	9	2	2	N	22460	PREDICTED: 40S ribosomal protein S7-like [Vollenhovia emeryi]
12	16741	gi 322801251 gb EFZ21938.1	68.21	8	2	2	N	25842	hypothetical protein SINV_03506, partial [Solenopsis invicta]
12	16742	gi 801392872 ref XP_012057980.1	68.21	7	2	2	N	26184	PREDICTED: 40S ribosomal protein S7-like [Atta cephalotes]
12	16743	gi 746835438 ref XP_011068410.1	68.21	7	2	2	N	26104	PREDICTED: 40S ribosomal protein S7-like [Acromyrmex echinator]
12	16744	gi 1012976919 gb KYQ51019.1	68.21	7	2	2	N	28127	40S ribosomal protein S7 [Trachymyrmex zeteki]
12	16745	gi 1009354346 gb KYM79695.1	68.21	7	2	2	N	29332	40S ribosomal protein S7 [Atta colombica]
12	16746	gi 1009419062 gb KYN37701.1	68.21	7	2	2	N	29794	40S ribosomal protein S7 [Trachymyrmex septentrionalis]
12	16750	gi 1009408410 gb KYN27747.1	68.21	6	2	2	N	30400	40S ribosomal protein S7 [Trachymyrmex cornetzi]
12	16751	gi 332029624 gb EGI69513.1	68.21	6	2	2	N	33379	40S ribosomal protein S7 [Acromyrmex echinator]
12	16752	gi 1009370719 gb KYM95125.1	68.21	6	2	2	N	34257	40S ribosomal protein S7 [Cyphomyrmex costatus]
12	16753	gi 861633416 gb KMQ90951.1	68.21	2	2	2	N	79826	dnaj-like subfamily c member 11-like protein [Lasius niger]
2	77	gi 1911819 gb AAB50883.1	64.22	10	1	1	Y	11819	Myr p I=allergenic polypeptide {N-termina l} [Myrmecia pilosula=jumper ants, venom, Peptide Partial, 112 aa]
2	78	gi 312284 emb CAA49760.1	64.22	10	1	1	Y	11849	major allergen [Myrmecia pilosula]
2	76	gi 730091 sp Q07932.1 MYR1_MYRPI	64.22	10	1	1	Y	11849	RecName: Full=Pilosulin-1; AltName: Full=Allergen Myr p I; AltName: Full=Major allergen Myr p I; AltName: Allergen=Myr p I; Contains: RecName: Full=Pilosulin-1; Contains: RecName: Full=Pilosulin-1 65->112; Contains: RecName...
7	15297	gi 815815129 ref XP_012228610.1	63.94	8	2	2	N	23715	PREDICTED: acyl-protein thioesterase 2 [Lepidoptera humile]
7	15306	gi 815815131 ref XP_012228611.1	63.94	8	2	2	N	23715	PREDICTED: acyl-protein thioesterase 2 [Lepidoptera humile]
7	15295	gi 307199886 gb EFN80283.1	63.94	8	2	2	N	21946	Acyl-protein thioesterase 1, partial [Harpegnathos saltator]
7	15296	gi 861658817 gb KMR03924.1	63.94	8	2	2	N	22387	acyl-protein thioesterase 1-like protein [Lasius niger]
7	15298	gi 769866680 ref XP_011645328.1	63.94	8	2	2	N	23614	PREDICTED: acyl-protein thioesterase 2 [Pogonomyrmex barbatus]
7	15299	gi 801387181 ref XP_012056747.1	63.94	8	2	2	N	23575	PREDICTED: acyl-protein thioesterase 2 [Atta cephalotes]
7	15300	gi 826410384 ref XP_012538793.1	63.94	8	2	2	N	23564	PREDICTED: acyl-protein thioesterase 2 [Monomorium pharaonis]
7	15301	gi 307177259 gb EFN66437.1	63.94	8	2	2	N	23612	Acyl-protein thioesterase 2 [Camponotus floridanus]
7	15302	gi 749783883 ref XP_011145876.1	63.94	8	2	2	N	23557	PREDICTED: acyl-protein thioesterase 1 [Harpegnathos saltator]
7	15303	gi 751220778 ref XP_011163537.1	63.94	8	2	2	N	23598	PREDICTED: acyl-protein thioesterase 1 [Solenopsis invicta]
7	15304	gi 752882877 ref XP_011259114.1	63.94	8	2	2	N	23612	PREDICTED: acyl-protein thioesterase 2 [Camponotus floridanus]
7	15305	gi 332019861 gb EGI60322.1	63.94	8	2	2	N	23575	Acyl-protein thioesterase 1 [Acromyrmex echinator]
7	15307	gi 1012984581 gb KYQ58213.1	63.94	8	2	2	N	23605	Acyl-protein thioesterase 2 [Trachymyrmex zeteki]

total 175 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
7	15308	gi 746863870 ref XP_011062908.1	63.94	8	2	2	N	23575	PREDICTED: acyl-protein thioesterase 2 [Acromyrmex echinator]
7	15309	gi 1009354900 gb KYM80235.1	63.94	8	2	2	N	23851	Acyl-protein thioesterase 1 [Atta colombica]
7	15310	gi 795072718 ref XP_011875663.1	63.94	7	2	2	N	25483	PREDICTED: acyl-protein thioesterase 1 [Vollenhovia emeryi]
7	15311	gi 322791151 gb EFZ15713.1	63.94	6	2	2	N	33892	hypothetical protein SINV_15507, partial [Solenopsis invicta]
7	15312	gi 1009420631 gb KYN39126.1	63.94	5	2	2	N	38698	Acyl-protein thioesterase 1 [Trachymyrmex septentrionalis]
7	15313	gi 1009397129 gb KYN17697.1	63.94	5	2	2	N	38529	Acyl-protein thioesterase 2 [Trachymyrmex cornetzi]
13	16755	gi 759070439 ref XP_011344792.1	61.00	9	2	2	N	23683	PREDICTED: troponin I isoform X17 [Cerapachys biroi]
13	16756	gi 751217509 ref XP_011161751.1	61.00	9	2	2	N	23712	PREDICTED: troponin I isoform X6 [Solenopsis invicta]
13	16757	gi 751217507 ref XP_011161750.1	61.00	8	2	2	N	24510	PREDICTED: troponin I isoform X5 [Solenopsis invicta]
13	16758	gi 759070435 ref XP_011344790.1	61.00	8	2	2	N	24481	PREDICTED: troponin I isoform X15 [Cerapachys biroi]
13	16759	gi 759070427 ref XP_011344786.1	61.00	8	2	2	N	24680	PREDICTED: troponin I isoform X11 [Cerapachys biroi]
13	16760	gi 751217505 ref XP_011161749.1	61.00	8	2	2	N	25076	PREDICTED: troponin I isoform X4 [Solenopsis invicta]
13	16761	gi 759070415 ref XP_011344779.1	61.00	8	2	2	N	25478	PREDICTED: troponin I isoform X5 [Cerapachys biroi]
13	16762	gi 759070419 ref XP_011344781.1	61.00	8	2	2	N	25324	PREDICTED: troponin I isoform X7 [Cerapachys biroi]
13	16763	gi 751217499 ref XP_011161746.1	61.00	8	2	2	N	25874	PREDICTED: troponin I isoform X2 [Solenopsis invicta]
13	16764	gi 751217503 ref XP_011161748.1	61.00	8	2	2	N	25720	PREDICTED: troponin I isoform X3 [Solenopsis invicta]
13	16765	gi 751217501 ref XP_011161747.1	61.00	8	2	2	N	25720	PREDICTED: troponin I isoform X3 [Solenopsis invicta]
13	16766	gi 759070407 ref XP_011344775.1	61.00	8	2	2	N	26122	PREDICTED: troponin I isoform X1 [Cerapachys biroi]
13	16767	gi 751217497 ref XP_011161745.1	61.00	8	2	2	N	26518	PREDICTED: troponin I isoform X1 [Solenopsis invicta]
13	16768	gi 751217495 ref XP_011161744.1	61.00	8	2	2	N	26518	PREDICTED: troponin I isoform X1 [Solenopsis invicta]
13	16769	gi 322793267 gb EFZ16924.1	61.00	7	2	2	N	31208	hypothetical protein SINV_80140, partial [Solenopsis invicta]
45	31	gi 801404535 ref XP_012061889.1	54.50	10	1	1	N	13516	PREDICTED: LOW QUALITY PROTEIN: glutathione S-transferase 1-1-like [Atta cephalotes]
45	29	gi 1009415415 gb KYN34225.1	54.50	6	1	1	N	24624	Glutathione S-transferase 1-1 [Trachymyrmex septentrionalis]
45	32	gi 1009400887 gb KYN20914.1	54.50	6	1	1	N	24782	Glutathione S-transferase 1-1 [Trachymyrmex cornetzi]
45	33	gi 1009386107 gb KYN08360.1	54.50	5	1	1	N	25055	Glutathione S-transferase 1-1 [Cyphomyrmex costatus]
45	34	gi 1009353160 gb KYM78583.1	54.50	3	1	1	N	47998	Glutathione S-transferase 1-1 [Atta colombica]
6	16719	gi 751225557 ref XP_011166167.1	51.80	5	1	1	N	30547	PREDICTED: GTP-binding protein SAR1b isoform X1 [Solenopsis invicta]
14	16770	gi 951555859 ref XP_014477451.1	49.63	2	1	1	N	69268	PREDICTED: PDZ and LIM domain protein Zasp isoform X3 [Dinoponera quadriceps]
14	16771	gi 951555857 ref XP_014477449.1	49.63	2	1	1	N	70394	PREDICTED: PDZ and LIM domain protein Zasp isoform X2 [Dinoponera quadriceps]
14	16772	gi 951555854 ref XP_014477448.1	49.63	2	1	1	N	72097	PREDICTED: PDZ and LIM domain protein Zasp isoform X1 [Dinoponera quadriceps]
14	16773	gi 332017150 gb EGI57949.1	49.63	1	1	1	N	88870	LIM domain-binding protein 3 [Acromyrmex echinator]
14	11272	gi 607364912 gb EZA59114.1	49.63	1	1	1	N	91494	PDZ and LIM domain protein Zasp [Cerapachys biroi]
14	16774	gi 1009354544 gb KYM79885.1	49.63	1	1	1	N	167505	PDZ and LIM domain protein Zasp, partial [Atta colombica]
14	16775	gi 307178151 gb EFN66959.1	49.63	1	1	1	N	187042	LIM domain-binding protein 3 [Camponotus floridanus]
14	16776	gi 951555862 ref XP_014477452.1	49.63	1	1	1	N	186042	PREDICTED: uncharacterized protein LOC106745932 isoform X4 [Dinoponera quadriceps]
14	16777	gi 322784934 gb EFZ11705.1	49.63	1	1	1	N	201397	hypothetical protein SINV_04419, partial [Solenopsis invicta]
14	16778	gi 1009400915 gb KYN20942.1	49.63	1	1	1	N	211738	PDZ and LIM domain protein Zasp [Trachymyrmex cornetzi]

total 175 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
14	16779	gi 1009415395 gb KYN34205.1	49.63	1	1	1	N	212134	PDZ and LIM domain protein Zasp [Trachymyrmex septentrionalis]
14	16780	gi 1012983919 gb KYQ57592.1	49.63	1	1	1	N	212670	PDZ and LIM domain protein Zasp [Trachymyrmex zeteki]
14	16781	gi 752881463 ref XP_011258339.1	49.63	1	1	1	N	212815	PREDICTED: PDZ and LIM domain protein Zasp-like [Camponotus floridanus]
14	16782	gi 801386315 ref XP_012056469.1	49.63	1	1	1	N	213131	PREDICTED: uncharacterized protein LOC105619562 [Atta cephalotes]
14	16783	gi 769845784 ref XP_011634167.1	49.63	1	1	1	N	213071	PREDICTED: uncharacterized protein LOC105425203 [Pogonomyrmex barbatus]
14	16784	gi 795059904 ref XP_011872999.1	49.63	1	1	1	N	213285	PREDICTED: uncharacterized protein LOC105564872 [Vollenhovia emeryi]
14	16785	gi 780649542 ref XP_011690040.1	49.63	1	1	1	N	213934	PREDICTED: uncharacterized protein LOC105451361 [Wasmannia auropunctata]
14	16786	gi 1009383137 gb KYN05782.1	49.63	1	1	1	N	215202	PDZ and LIM domain protein Zasp [Cyphomyrmex costatus]
14	16787	gi 751232187 ref XP_011169696.1	49.63	1	1	1	N	217652	PREDICTED: uncharacterized protein LOC105202731 [Solenopsis invicta]
14	11273	gi 759044497 ref XP_011331167.1	49.63	1	1	1	N	217249	PREDICTED: uncharacterized protein LOC105275764 [Ceraopachys biroii]
14	16788	gi 826446045 ref XP_012531295.1	49.63	1	1	1	N	219494	PREDICTED: uncharacterized protein LOC105833822 [Monomorium pharaonis]
14	16789	gi 746870999 ref XP_011066707.1	49.63	1	1	1	N	227184	PREDICTED: uncharacterized protein LOC105153507 [Acromyrmex echinator]
14	11274	gi 815790568 ref XP_012215850.1	49.63	1	1	1	N	225648	PREDICTED: uncharacterized protein LOC105668197 [Linepithema humile]
46	128	gi 749750482 ref XP_011137501.1	45.10	9	1	1	N	17069	PREDICTED: myosin light chain alkali isoform X2 [Harpegnathos saltator]
47	16837	gi 801384826 ref XP_012055647.1	40.54	5	1	1	N	28599	PREDICTED: 15-hydroxyprostaglandin dehydrogenase [NAD(+)]-like [Atta cephalotes]
47	16838	gi 746863107 ref XP_011062501.1	40.54	5	1	1	N	28376	PREDICTED: 15-hydroxyprostaglandin dehydrogenase [NAD(+)]-like [Acromyrmex echinator]
47	16839	gi 826434745 ref XP_012529071.1	40.54	5	1	1	N	28678	PREDICTED: 15-hydroxyprostaglandin dehydrogenase [NAD(+)]-like isoform X3 [Monomorium pharaonis]
47	16840	gi 826434740 ref XP_012529070.1	40.54	5	1	1	N	32652	PREDICTED: 15-hydroxyprostaglandin dehydrogenase [NAD(+)]-like isoform X2 [Monomorium pharaonis]
47	16841	gi 826434735 ref XP_012529069.1	40.54	5	1	1	N	33227	PREDICTED: 15-hydroxyprostaglandin dehydrogenase [NAD(+)]-like isoform X1 [Monomorium pharaonis]
47	16842	gi 1009363272 gb KYM88327.1	40.54	3	1	1	N	56559	15-hydroxyprostaglandin dehydrogenase [NAD+] [Atta colombica]
48	5579	gi 749772542 ref XP_011141800.1	36.43	7	1	1	N	13845	PREDICTED: superoxide dismutase [Cu-Zn], partial [Harpegnathos saltator]
48	5580	gi 307204104 gb EFN82974.1	36.43	7	1	1	N	13845	Superoxide dismutase [Cu-Zn], partial [Harpegnathos saltator]
48	5585	gi 759057450 ref XP_011337976.1	36.43	7	1	1	N	15500	PREDICTED: superoxide dismutase [Cu-Zn] [Ceraopachys biroii]
48	5586	gi 607360315 gb EZA54646.1	36.43	7	1	1	N	15500	Superoxide dismutase [Cu-Zn] [Ceraopachys biroii]
48	5563	gi 815812192 ref XP_012227043.1	36.43	7	1	1	N	15487	PREDICTED: LOW QUALITY PROTEIN: superoxide dismutase [Cu-Zn]-like [Linepithema humile]
48	5587	gi 752872840 ref XP_011253679.1	36.43	7	1	1	N	15495	PREDICTED: superoxide dismutase [Cu-Zn] [Camponotus floridanus]
48	5564	gi 34733404 gb AAQ81639.1	36.43	7	1	1	N	15553	Cu-Zn superoxide dismutase 1 [Lasius niger]
48	5588	gi 307183176 gb EFN70085.1	36.43	7	1	1	N	15495	Superoxide dismutase [Cu-Zn] [Camponotus floridanus]
48	5584	gi 861628645 gb KMQ89459.1	36.43	2	1	1	N	55250	superoxide dismutase, partial [Lasius niger]
total 175 proteins									

Band # 7 Proteins

Summary

1. Notes

2. Result Statistics

Figure 1. False discovery rate (FDR) curve. X axis is the number of peptide-spectrum matches (PSM) being kept. Y axis is the corresponding FDR.

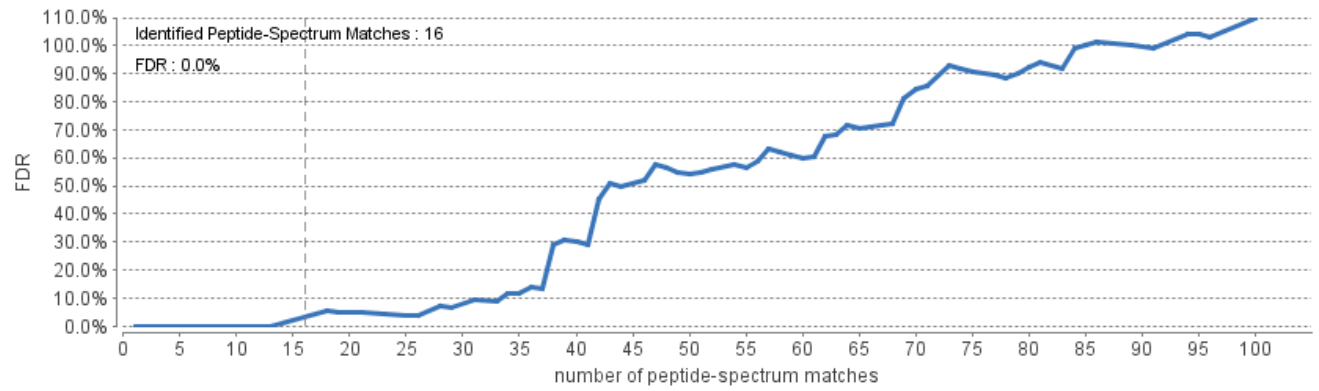


Figure 2. PSM score distribution. (a) Distribution of PEAKS peptide score; (b) Scatterplot of PEAKS peptide score versus precursor mass error.

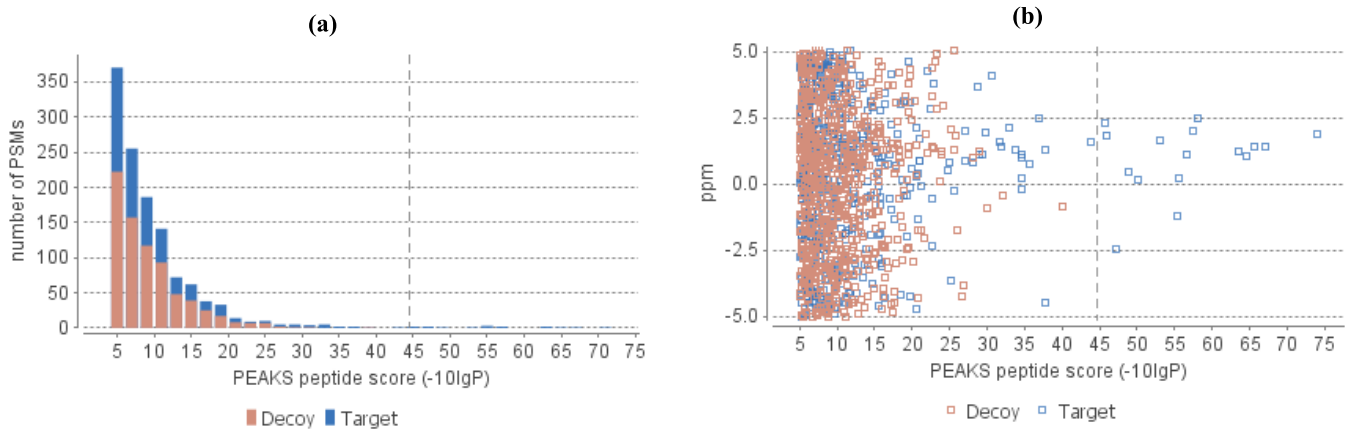


Figure 3. De novo result validation. Distribution of residue local confidence: (a) Residues in de novo sequences validated by confident database peptide assignment; (b) Residues in "de novo only" sequences.

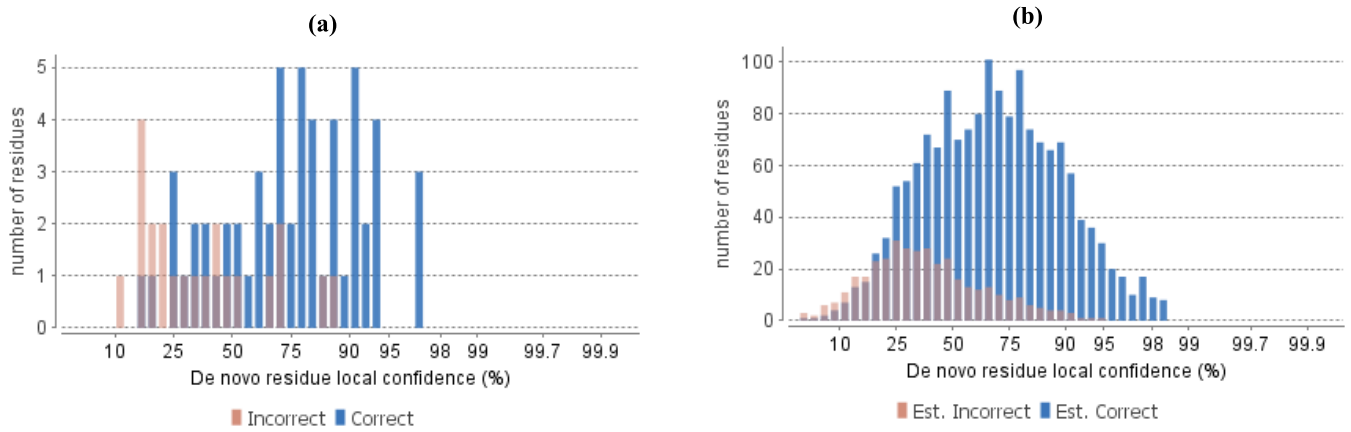


Table 1. Statistics of data.

# of MS Scans	1604
# of MS/MS Scans	3289

Table 4. PTM profile.

Name	Δ Mass	Position	#PSM	-10lgP	Area	AScore
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Table 2. Result filtration parameters.

Peptide -10lgP	≥44.6
Protein -10lgP	≥20
Proteins unique peptides	≥1
De novo ALC Score	≥50%

Table 3. Statistics of filtered result.

Peptide-Spectrum Matches	16
Peptide Sequences	16
Protein Groups	9
Proteins	88
Proteins (#Unique Peptides)	0 (>2); 34 (=2); 54 (=1);
FDR (Peptide-Spectrum Matches)	0.0%
FDR (Peptide Sequences)	0.0%
FDR (Protein)	0.0%
De Novo Only Spectra	189

3. Experiment Control

Figure 4. Precursor mass error of peptide-spectrum matches (PSM) in filtered result. **(a)** Distribution of precursor mass error in ppm; **(b)** Scatterplot of precursor m/z versus precursor mass error in ppm.

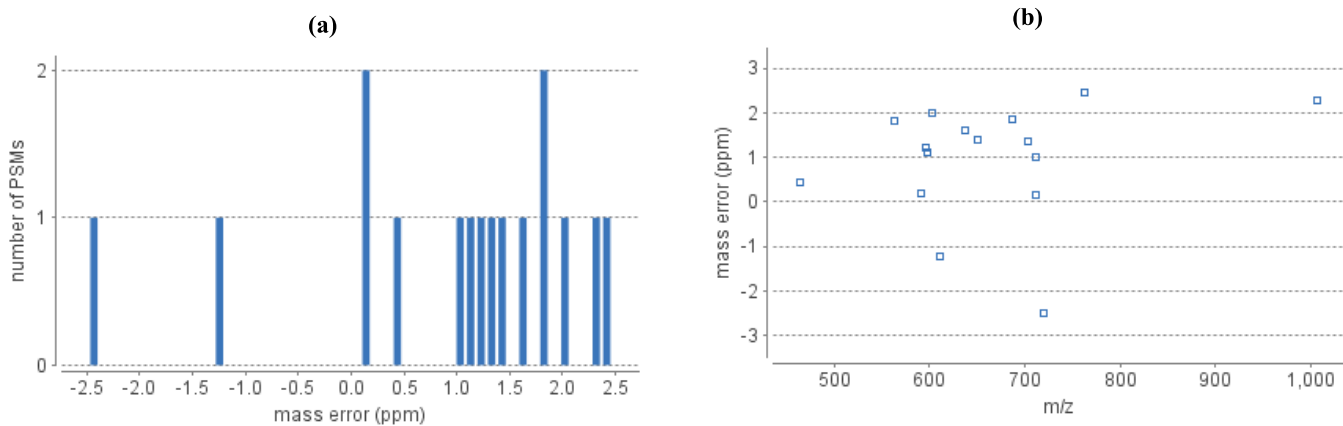


Table 5. Number of identified peptides in each sample by the number of missed cleavages

Missed Cleavages	0	1	2	3	4+
Sample 23	16	0	0	0	0

4. Other Information

Table 6. Search parameters.

Search Engine Name:	PEAKS
Parent Mass Error Tolerance:	5.0 ppm
Fragment Mass Error Tolerance:	0.5 Da
Precursor Mass Search Type:	monoisotopic
Enzyme:	Trypsin
Max Missed Cleavages:	3
Non-specific Cleavage:	one
Variable Modifications:	
Oxidation (M):	15.99
Max variable PTM per peptide:	3
Database:	Ant
Taxon:	All
Searched Entry:	473117
FDR Estimation:	Enabled
Merge Options:	no merge
Precursor Options:	corrected
Charge Options:	no correction

Filter Options: no filter

Process: true

Protein List

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
2	63	gi 322792410 gb EFZ16394.1	105.47	6	2	2	Y	25370	hypothetical protein SINV_12161, partial [Solenopsis invicta]
2	64	gi 751219056 ref XP_011162596.1	105.47	6	2	2	Y	25498	PREDICTED: acidic phospholipase A2 PA4 isoform X2 [Solenopsis invicta]
2	65	gi 769852445 ref XP_011637691.1	105.47	6	2	2	Y	25718	PREDICTED: acidic phospholipase A2 PA4 isoform X2 [Pogonomyrmex barbatus]
2	66	gi 607361739 gb EZA56014.1	105.47	6	2	2	Y	25661	Group 3 secretory phospholipase A2 [Cera-pachys biroi]
2	67	gi 780637978 ref XP_011687259.1	105.47	6	2	2	Y	26007	PREDICTED: phospholipase A2 isozymes P A3A/PA3B/PA5 isoform X2 [Wasmannia auropunctata]
2	68	gi 769852443 ref XP_011637690.1	105.47	6	2	2	Y	27251	PREDICTED: acidic phospholipase A2 PA4 isoform X1 [Pogonomyrmex barbatus]
2	69	gi 751219054 ref XP_011162595.1	105.47	6	2	2	Y	28045	PREDICTED: uncharacterized protein LOC105197765 isoform X1 [Solenopsis invicta]
2	70	gi 759054210 ref XP_011336300.1	105.47	6	2	2	Y	28030	PREDICTED: uncharacterized protein LOC105278712 isoform X3 [Cera-pachys biroi]
2	71	gi 759054208 ref XP_011336299.1	105.47	5	2	2	Y	28800	PREDICTED: uncharacterized protein LOC105278712 isoform X2 [Cera-pachys biroi]
2	73	gi 780637966 ref XP_011687254.1	105.47	5	2	2	Y	28793	PREDICTED: uncharacterized protein LOC105449644 isoform X1 [Wasmannia auropunctata]
2	72	gi 780637974 ref XP_011687258.1	105.47	5	2	2	Y	28793	PREDICTED: uncharacterized protein LOC105449644 isoform X1 [Wasmannia auropunctata]
2	74	gi 780637970 ref XP_011687255.1	105.47	5	2	2	Y	28793	PREDICTED: uncharacterized protein LOC105449644 isoform X1 [Wasmannia auropunctata]
2	75	gi 759054206 ref XP_011336298.1	105.47	5	2	2	Y	31169	PREDICTED: uncharacterized protein LOC105278712 isoform X1 [Cera-pachys biroi]
4	2639	gi 746872269 ref XP_011067393.1	86.40	1	1	1	N	102824	PREDICTED: AP-1 complex subunit beta-1 isoform X2 [Acromyrmex echinator]
4	2640	gi 746872265 ref XP_011067390.1	86.40	1	1	1	N	102824	PREDICTED: AP-1 complex subunit beta-1 isoform X2 [Acromyrmex echinator]
4	2641	gi 751234032 ref XP_011170727.1	86.40	1	1	1	N	102967	PREDICTED: AP-1 complex subunit beta-1 isoform X3 [Solenopsis invicta]
4	2642	gi 751234030 ref XP_011170725.1	86.40	1	1	1	N	103133	PREDICTED: AP-1 complex subunit beta-1 isoform X2 [Solenopsis invicta]
4	2643	gi 751234038 ref XP_011170730.1	86.40	1	1	1	N	102967	PREDICTED: AP-1 complex subunit beta-1 isoform X3 [Solenopsis invicta]
4	2644	gi 752876178 ref XP_011255475.1	86.40	1	1	1	N	103519	PREDICTED: AP-1 complex subunit beta-1 isoform X2 [Camponotus floridanus]
4	2645	gi 746872263 ref XP_011067389.1	86.40	1	1	1	N	103949	PREDICTED: AP-1 complex subunit beta-1 isoform X1 [Acromyrmex echinator]
4	1	gi 780664802 ref XP_011693761.1	86.40	1	1	1	N	104252	PREDICTED: AP-1 complex subunit beta-1 isoform X4 [Wasmannia auropunctata]
6	29	gi 1009415415 gb KYN34225.1	74.00	6	1	1	N	24624	Glutathione S-transferase 1-1 [Trachymyrmex septentrionalis]
6	31	gi 801404535 ref XP_012061889.1	74.00	10	1	1	N	13516	PREDICTED: LOW QUALITY PROTEIN: glutathione S-transferase 1-1-like [Atta cephalotes]
6	32	gi 1009400887 gb KYN20914.1	74.00	6	1	1	N	24782	Glutathione S-transferase 1-1 [Trachymyrmex cornetzi]
6	33	gi 1009386107 gb KYN08360.1	74.00	5	1	1	N	25055	Glutathione S-transferase 1-1 [Cyphomyrmex costatus]
6	34	gi 1009353160 gb KYM78583.1	74.00	3	1	1	N	47998	Glutathione S-transferase 1-1 [Atta colombica]
7	2	gi 749756765 ref XP_011140861.1	68.81	19	2	2	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Harpegnathos saltator]
7	10	gi 322799134 gb EFZ20581.1	68.81	19	2	2	N	16857	hypothetical protein SINV_11686, partial [Solenopsis invicta]
7	3	gi 795075576 ref XP_011876241.1	68.81	19	2	2	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Vollenhovia emeryi]
7	4	gi 759066863 ref XP_011342896.1	68.81	19	2	2	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Cera-pachys biroi]
7	5	gi 751206597 ref XP_011155825.1	68.81	19	2	2	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Solenopsis invicta]
7	6	gi 780650680 ref XP_011690296.1	68.81	19	2	2	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Wasmannia auropunctata]
7	11	gi 607357312 gb EZA51777.1	68.81	19	2	2	N	16860	Cofilin/actin-depolymerizing factor-like protein [Cera-pachys biroi]

total 88 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
7	7	gi 951531070 ref XP_014469357.1	68.81	19	2	2	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Dinoponera quadriceps]
7	12	gi 746872572 ref XP_011067557.1	68.81	19	2	2	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Acromyrmex echinator]
7	13	gi 815823534 ref XP_012233084.1	68.81	19	2	2	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Linepithema humile]
7	8	gi 826475616 ref XP_012537040.1	68.81	19	2	2	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Monomorium pharaonis]
7	9	gi 752866064 ref XP_011269506.1	68.81	19	2	2	N	16860	PREDICTED: cofilin/actin-depolymerizing factor homolog [Camponotus floridanus]
7	14	gi 861649741 gb KMQ96964.1	68.81	19	2	2	N	16974	cofilin actin-depolymerizing factor-like protein [Lasius niger]
7	15	gi 307187751 gb EFN72723.1	68.81	17	2	2	N	19355	Cofilin/actin-depolymerizing factor-like protein [Camponotus floridanus]
7	16	gi 801383792 ref XP_012055075.1	68.81	15	2	2	N	20394	PREDICTED: cofilin/actin-depolymerizing factor homolog [Atta cephalotes]
7	17	gi 1009357994 gb KYM83255.1	68.81	15	2	2	N	20394	Cofilin/actin-depolymerizing factor like protein [Atta colombica]
7	18	gi 307205222 gb EFN83612.1	68.81	15	2	2	N	20514	Cofilin/actin-depolymerizing factor-like protein [Harpegnathos saltator]
7	19	gi 1012971901 gb KYQ46466.1	68.81	15	2	2	N	20722	Cofilin/actin-depolymerizing factor like protein [Trachymyrmex zeteki]
7	20	gi 1009394301 gb KYN15343.1	68.81	15	2	2	N	20708	Cofilin/actin-depolymerizing factor like protein [Trachymyrmex cornetzi]
7	21	gi 332016345 gb EGI57258.1	68.81	15	2	2	N	20654	Cofilin/actin-depolymerizing factor-like protein [Acromyrmex echinator]
7	22	gi 1009419754 gb KYN38297.1	68.81	15	2	2	N	20608	Cofilin/actin-depolymerizing factor like protein [Trachymyrmex septentrionalis]
42	60	gi 1009367592 gb KYM92576.1	67.11	8	1	1	N	20432	Muscle-specific protein 20 [Atta colombica]
42	61	gi 801385197 ref XP_012055851.1	67.11	8	1	1	N	20432	PREDICTED: muscle-specific protein 20 [Atta cephalotes]
42	62	gi 746847374 ref XP_011054061.1	67.11	8	1	1	N	20432	PREDICTED: muscle-specific protein 20 [Acromyrmex echinator]
9	27	gi 780722010 ref XP_011707181.1	65.54	15	1	1	Y	9507	PREDICTED: high mobility group protein D SP1-like [Wasmannia auropunctata]
9	35	gi 322797840 gb EFZ19748.1	65.54	6	1	1	Y	23944	hypothetical protein SINV_09636, partial [Solenopsis invicta]
9	36	gi 769835800 ref XP_011648020.1	65.54	5	1	1	Y	31220	PREDICTED: LOW QUALITY PROTEIN: high mobility group protein DSP1-like [Pogonomyrmex barbatus]
9	37	gi 826472171 ref XP_012536359.1	65.54	5	1	1	Y	31643	PREDICTED: high mobility group protein D SP1 [Monomorium pharaonis]
9	38	gi 801385599 ref XP_012056070.1	65.54	4	1	1	Y	34063	PREDICTED: high mobility group protein D SP1-like, partial [Atta cephalotes]
9	39	gi 307191141 gb EFN74839.1	65.54	4	1	1	Y	33754	High mobility group protein DSP1 [Camponotus floridanus]
9	40	gi 1009398537 gb KYN18849.1	65.54	4	1	1	Y	35426	High mobility group protein DSP1 [Trachymyrmex cornetzi]
9	41	gi 795117179 ref XP_011883309.1	65.54	3	1	1	Y	45172	PREDICTED: high mobility group protein B 2-like isoform X2 [Vollenhovia emeryi]
9	42	gi 1012977941 gb KYQ51975.1	65.54	3	1	1	Y	47943	High mobility group protein DSP1 [Trachymyrmex zeteki]
9	43	gi 1009422717 gb KYN41077.1	65.54	3	1	1	Y	48643	High mobility group protein DSP1 [Trachymyrmex septentrionalis]
9	44	gi 1009367538 gb KYM92522.1	65.54	3	1	1	Y	49134	High mobility group protein DSP1 [Atta colombica]
9	45	gi 746847190 ref XP_011053958.1	65.54	3	1	1	Y	49806	PREDICTED: LOW QUALITY PROTEIN: high mobility group protein DSP1-like [Acromyrmex echinator]
9	46	gi 1009374084 gb KYM97868.1	65.54	3	1	1	Y	49585	High mobility group protein DSP1 [Cyphomyrmex costatus]
9	47	gi 307192728 gb EFN75836.1	65.54	3	1	1	Y	49406	High mobility group protein DSP1 [Harpegnathos saltator]
9	48	gi 749797897 ref XP_011152427.1	65.54	3	1	1	Y	49406	PREDICTED: high mobility group protein D SP1-like isoform X2 [Harpegnathos saltator]
9	24	gi 759074236 ref XP_011346799.1	65.54	3	1	1	Y	50220	PREDICTED: high mobility group protein D SP1 isoform X2 [Cerapachys biroi]
9	49	gi 752860044 ref XP_011269235.1	65.54	3	1	1	Y	50773	PREDICTED: high mobility group protein D SP1-like isoform X2 [Camponotus floridanus]
9	50	gi 815788593 ref XP_012214819.1	65.54	3	1	1	Y	51010	PREDICTED: high mobility group protein D SP1 isoform X2 [Linepithema humile]
9	51	gi 951547836 ref XP_014474071.1	65.54	3	1	1	Y	50343	PREDICTED: high mobility group protein D SP1-like isoform X2 [Dinoponera quadricapsa]

total 88 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
9	52	gi 749797895 ref XP_011152426.1	65.54	3	1	1	Y	51272	PREDICTED: high mobility group protein D SP1-like isoform X1 [Harpegnathos saltator]
9	53	gi 861658474 gb KMR03599.1	65.54	3	1	1	Y	50924	high mobility group protein dsp1 [Lasius niger]
9	54	gi 751208925 ref XP_011157097.1	65.54	3	1	1	Y	51679	PREDICTED: high mobility group protein D SP1-like isoform X2 [Solenopsis invicta]
9	25	gi 607354697 gb EZA49312.1	65.54	3	1	1	Y	52109	High mobility group protein DSP1 [Cerapachys biroi]
9	26	gi 759074234 ref XP_011346798.1	65.54	3	1	1	Y	52109	PREDICTED: high mobility group protein D SP1 isoform X1 [Cerapachys biroi]
9	55	gi 752860042 ref XP_011269227.1	65.54	3	1	1	Y	52662	PREDICTED: high mobility group protein D SP1-like isoform X1 [Camponotus floridanus]
9	56	gi 815788591 ref XP_012214818.1	65.54	3	1	1	Y	52900	PREDICTED: high mobility group protein D SP1 isoform X1 [Linepithema humile]
9	57	gi 951547833 ref XP_014474070.1	65.54	3	1	1	Y	52209	PREDICTED: high mobility group protein D SP1-like isoform X1 [Dinoponera quadricapsa]
9	58	gi 795117166 ref XP_011883308.1	65.54	3	1	1	Y	52682	PREDICTED: high mobility group protein D SP1-like isoform X1 [Vollenhovia emeryi]
9	28	gi 780695557 ref XP_011700702.1	65.54	3	1	1	Y	52949	PREDICTED: high mobility group protein D SP1-like [Wasmannia auropunctata]
9	59	gi 751208923 ref XP_011157096.1	65.54	3	1	1	Y	53568	PREDICTED: high mobility group protein D SP1-like isoform X1 [Solenopsis invicta]
3	77	gi 1911819 gb AAB50883.1	63.62	10	1	1	Y	11819	Myr p I=allergenic polypeptide {N-termina l} [Myrmecia pilosula=jumper ants, venom, Peptide Partial, 112 aa]
3	78	gi 312284 emb CAA49760.1	63.62	10	1	1	Y	11849	major allergen [Myrmecia pilosula]
3	76	gi 730091 sp Q07932.1 MYR1_MYRPI	63.62	10	1	1	Y	11849	RecName: Full=Pilosulin-1; AltName: Full=Allergen Myr p I; AltName: Full=Major allergen Myr p 1; AltName: Allergen=Myr p 1; Contains: RecName: Full=Pilosulin-1; Contains: RecName: Full=Pilosulin-1 65->112; Contains: RecNa...
8	2647	gi 749746251 ref XP_011135199.1	60.76	5	1	1	N	24439	PREDICTED: ras-related protein Rab-11A isoform X2 [Harpegnathos saltator]
43	129	gi 815788969 ref XP_012215013.1	48.79	4	1	1	N	24433	PREDICTED: glutathione S-transferase 1-1-like isoform X3 [Linepithema humile]
43	130	gi 815788967 ref XP_012215012.1	48.79	4	1	1	N	24433	PREDICTED: glutathione S-transferase 1-1-like isoform X3 [Linepithema humile]
43	131	gi 815788957 ref XP_012215007.1	48.79	3	1	1	N	27668	PREDICTED: glutathione S-transferase 1-1-like isoform X1 [Linepithema humile]
43	133	gi 815788971 ref XP_012215015.1	48.79	2	1	1	N	44327	PREDICTED: glutathione S-transferase 1-1-like isoform X4 [Linepithema humile]
total 88 proteins									

Band # 8 Proteins

Summary

1. Notes

2. Result Statistics

Figure 1. False discovery rate (FDR) curve. X axis is the number of peptide-spectrum matches (PSM) being kept. Y axis is the corresponding FDR.

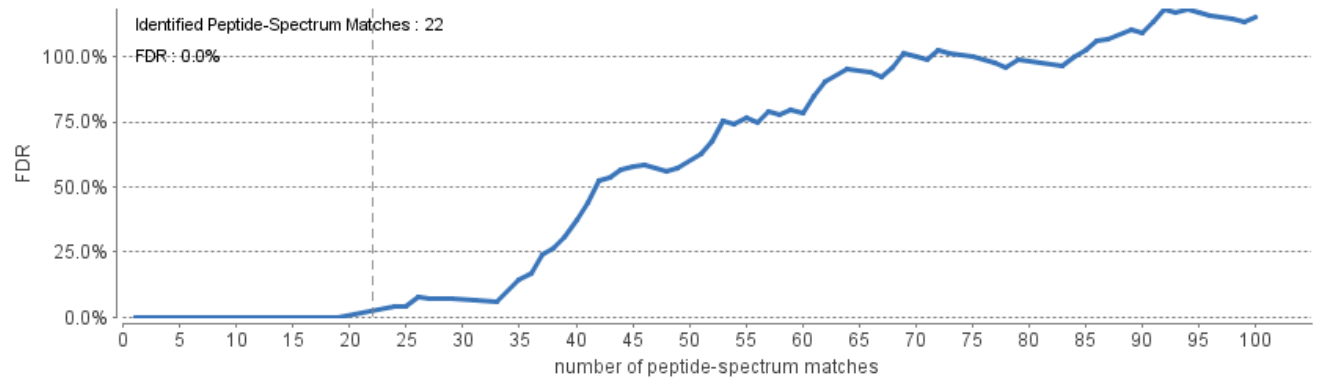


Figure 2. PSM score distribution. (a) Distribution of PEAKS peptide score; (b) Scatterplot of PEAKS peptide score versus precursor mass error.

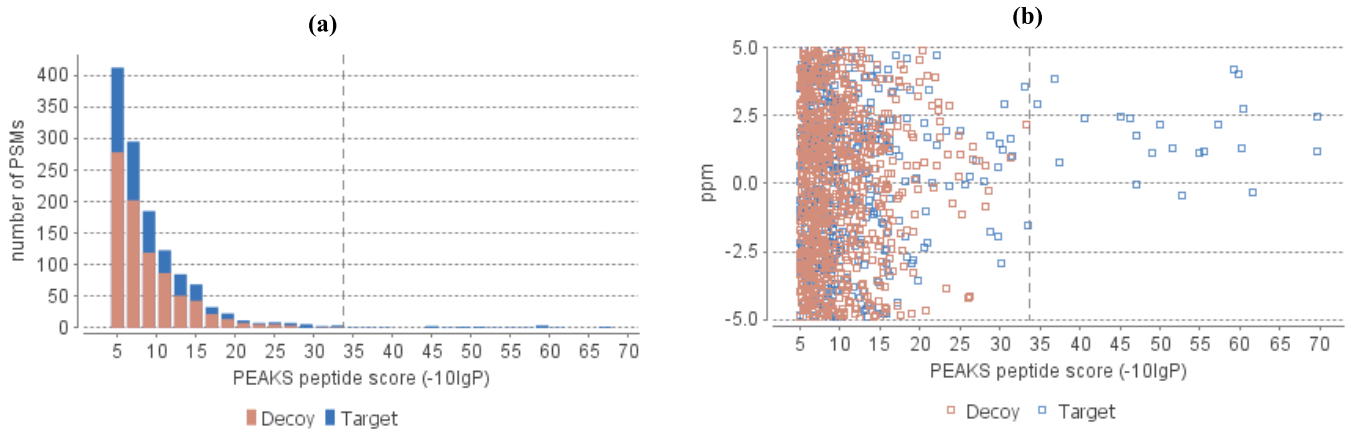


Figure 3. De novo result validation. Distribution of residue local confidence: (a) Residues in de novo sequences validated by confident database peptide assignment; (b) Residues in "de novo only" sequences.

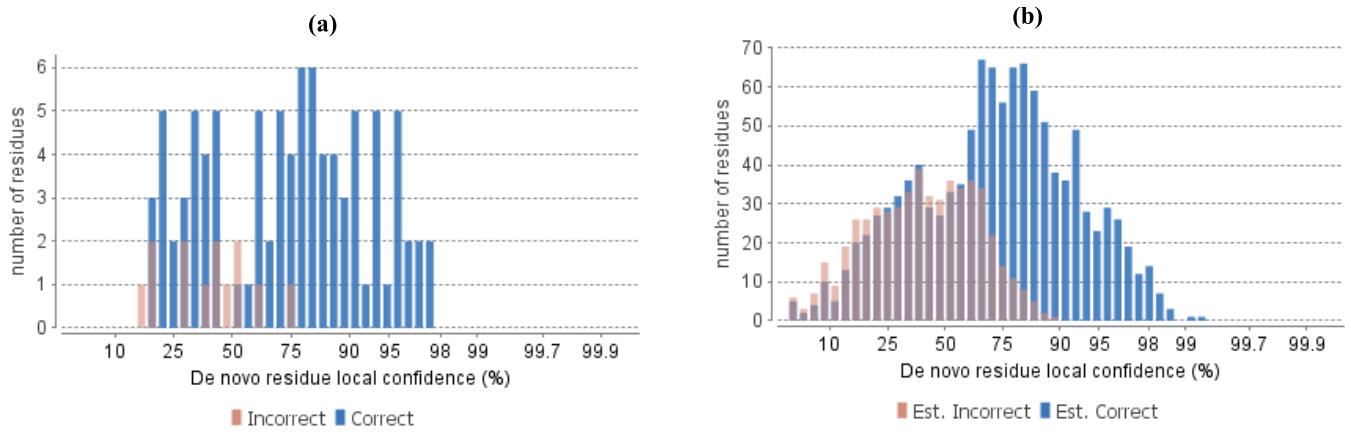


Table 1. Statistics of data.

# of MS Scans	1555
# of MS/MS Scans	3223

Table 4. PTM profile.

Name	Δ Mass	Position	#PSM	-10lgP	Area	AScore
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Table 2. Result filtration parameters.

Peptide -10lgP	≥33.8
Protein -10lgP	≥20
Proteins unique peptides	≥1
De novo ALC Score	≥50%

Table 3. Statistics of filtered result.

Peptide-Spectrum Matches	22
Peptide Sequences	20
Protein Groups	9
Proteins	46
Proteins (#Unique Peptides)	1 (>2); 2 (=2); 43 (=1);
FDR (Peptide-Spectrum Matches)	0.0%
FDR (Peptide Sequences)	0.0%
FDR (Protein)	0.0%
De Novo Only Spectra	144

3. Experiment Control

Figure 4. Precursor mass error of peptide-spectrum matches (PSM) in filtered result. (a) Distribution of precursor mass error in ppm; (b) Scatterplot of precursor m/z versus precursor mass error in ppm.

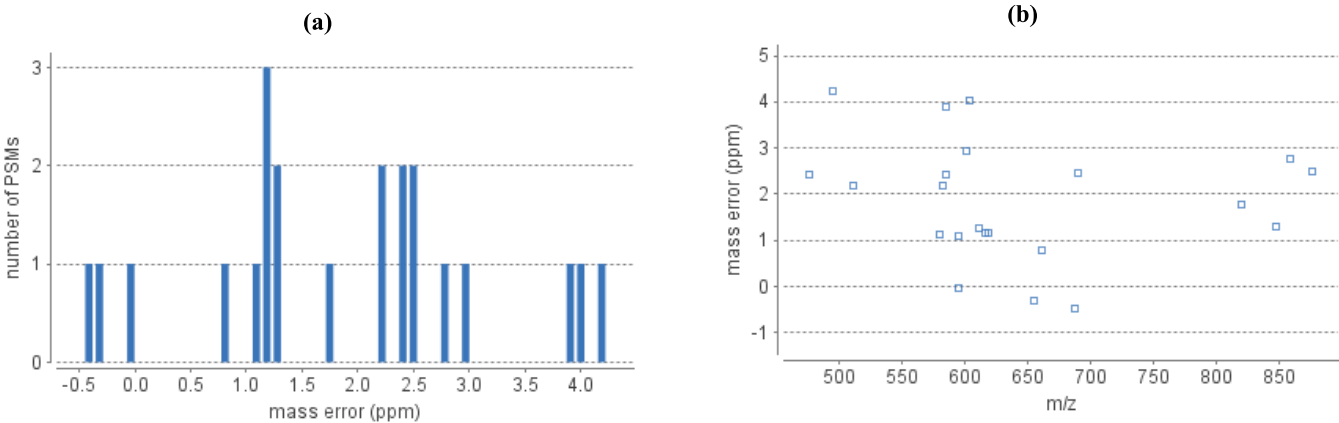


Table 5. Number of identified peptides in each sample by the number of missed cleavages

Missed Cleavages	0	1	2	3	4+
Sample 24	19	1	0	0	0

4. Other Information

Table 6. Search parameters.

Search Engine Name:	PEAKS
Parent Mass Error Tolerance:	5.0 ppm
Fragment Mass Error Tolerance:	0.5 Da
Precursor Mass Search Type:	monoisotopic
Enzyme:	Trypsin
Max Missed Cleavages:	3
Non-specific Cleavage:	one
Variable Modifications:	
Oxidation (M):	15.99
Max variable PTM per peptide:	3
Database:	Ant
Taxon:	All
Searched Entry:	473117
FDR Estimation:	Enabled
Merge Options:	no merge
Precursor Options:	corrected
Charge Options:	no correction

Table 7. Instrument parameters.

Fractions:	TW_8.raw
Ion Source:	ESI(nano-spray)
Fragmentation Mode:	CID, CAD(y and b ions)
MS Scan Mode:	FT-ICR/Orbitrap
MS/MS Scan Mode:	FT-ICR/Orbitrap

Filter Options: no filter
Process: true

Protein List

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
1	18120	gi 826414896 ref XP_012522151.1	158.09	31	7	7	N	28798	PREDICTED: phosphoglycerate mutase 1 [Monomorium pharaonis]
3	135	gi 815804483 ref XP_012222952.1	87.42	5	2	2	N	26367	PREDICTED: venom allergen 3-like [Linepit hema humile]
3	136	gi 815804481 ref XP_012222951.1	87.42	5	2	2	N	26367	PREDICTED: venom allergen 3-like [Linepit hema humile]
4	18139	gi 795066973 ref XP_011874524.1	82.61	5	1	1	N	26850	PREDICTED: 6-phosphogluconolactonase [Vollenhovia emeryi]
4	18140	gi 1009351227 gb KYM76708.1	82.61	5	1	1	N	26835	6-phosphogluconolactonase [Atta colombica]
4	18141	gi 746851252 ref XP_011056140.1	82.61	5	1	1	N	26864	PREDICTED: 6-phosphogluconolactonase [Acromyrmex echinator]
4	18142	gi 795066968 ref XP_011874523.1	82.61	5	1	1	N	26850	PREDICTED: 6-phosphogluconolactonase [Vollenhovia emeryi]
4	18143	gi 746851250 ref XP_011056139.1	82.61	5	1	1	N	26864	PREDICTED: 6-phosphogluconolactonase [Acromyrmex echinator]
4	18144	gi 801399955 ref XP_012060513.1	82.61	5	1	1	N	26835	PREDICTED: 6-phosphogluconolactonase [Atta cephalotes]
4	18145	gi 332024245 gb EGI64449.1	82.61	5	1	1	N	26864	6-phosphogluconolactonase [Acromyrmex echinator]
4	18146	gi 1012973224 gb KYQ47651.1	82.61	5	1	1	N	27086	6-phosphogluconolactonase [Trachymyrmex zeteki]
45	18174	gi 769832386 ref XP_011641963.1	69.63	4	1	1	N	36982	PREDICTED: renin receptor isoform X2 [Pogonomymex barbatus]
45	18175	gi 951552362 ref XP_014475836.1	69.63	4	1	1	N	37252	PREDICTED: renin receptor isoform X3 [Dinoponera quadriceps]
45	18176	gi 307206136 gb EFN84216.1	69.63	3	1	1	N	39566	Renin receptor [Harpegnathos saltator]
45	18177	gi 749754754 ref XP_011139827.1	69.63	3	1	1	N	39849	PREDICTED: renin receptor isoform X2 [Harpegnathos saltator]
45	18178	gi 951552359 ref XP_014475835.1	69.63	3	1	1	N	40234	PREDICTED: renin receptor isoform X2 [Dinoponera quadriceps]
45	18179	gi 769832384 ref XP_011641954.1	69.63	3	1	1	N	44236	PREDICTED: renin receptor isoform X1 [Pogonomymex barbatus]
45	18180	gi 749754752 ref XP_011139826.1	69.63	3	1	1	N	44445	PREDICTED: renin receptor isoform X1 [Harpegnathos saltator]
45	18181	gi 951552356 ref XP_014475834.1	69.63	3	1	1	N	44879	PREDICTED: renin receptor isoform X1 [Dinoponera quadriceps]
45	18182	gi 749754756 ref XP_011139828.1	69.63	3	1	1	N	47412	PREDICTED: uncharacterized protein LOC105183427 isoform X3 [Harpegnathos saltator]
5	18154	gi 332024226 gb EGI64430.1	66.37	9	2	1	N	25041	Peroxisredoxin-6 [Acromyrmex echinator]
5	18155	gi 826415424 ref XP_012522437.1	66.37	9	2	1	N	25214	PREDICTED: peroxiredoxin-6-like [Monomorium pharaonis]
5	18156	gi 1009358528 gb KYM83717.1	66.37	9	2	1	N	25067	Peroxisredoxin-6 [Atta colombica]
5	18157	gi 1012973206 gb KYQ47633.1	66.37	9	2	1	N	25042	Peroxisredoxin-6 [Trachymyrmex zeteki]
5	18158	gi 751209017 ref XP_011157150.1	66.37	9	2	1	N	25165	PREDICTED: peroxiredoxin-6-like [Solenopsis invicta]
5	18159	gi 801371409 ref XP_012062388.1	66.37	9	2	1	N	25094	PREDICTED: peroxiredoxin-6-like [Atta cephalotes]
5	18160	gi 746851185 ref XP_011056106.1	66.37	9	2	1	N	25041	PREDICTED: peroxiredoxin-6-like [Acromyrmex echinator]
5	18161	gi 780690201 ref XP_011699437.1	66.37	9	2	1	N	25114	PREDICTED: peroxiredoxin-6-like [Wasmannia auropunctata]
5	18162	gi 1009425993 gb KYN44124.1	66.37	9	2	1	N	25040	Peroxisredoxin-6 [Trachymyrmex septentrionalis]
5	18163	gi 322797657 gb EFZ19666.1	66.37	9	2	1	N	26460	hypothetical protein SINV_03768, partial [Solenopsis invicta]
46	18183	gi 1009377639 gb KYN00915.1	60.17	6	1	1	N	31070	Neural/ectodermal development factor IMP-L2 [Cyphomyrmex costatus]
46	18184	gi 1009413357 gb KYN32257.1	60.17	6	1	1	N	31145	Neural/ectodermal development factor IMP-L2 [Trachymyrmex septentrionalis]
46	18185	gi 746866235 ref XP_011064174.1	60.17	6	1	1	N	31386	PREDICTED: neural/ectodermal development factor IMP-L2 [Acromyrmex echinator]
46	18186	gi 746866231 ref XP_011064172.1	60.17	6	1	1	N	31386	PREDICTED: neural/ectodermal development factor IMP-L2 [Acromyrmex echinator]
46	18187	gi 746866233 ref XP_011064173.1	60.17	6	1	1	N	31386	PREDICTED: neural/ectodermal development factor IMP-L2 [Acromyrmex echinator]
46	18188	gi 769861060 ref XP_011642289.1	60.17	6	1	1	N	31662	PREDICTED: neural/ectodermal development factor IMP-L2 isoform X2 [Pogonomymex barbatus]

total 46 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
46	18189	gi 769861058 ref XP_011642288.1	60.17	6	1	1	N	32004	PREDICTED: neural/ectodermal development factor IMP-L2 isoform X1 [Pogonomyrmex barbatus]
46	18190	gi 332018952 gb EGI59498.1	60.17	5	1	1	N	33783	Neural/ectodermal development factor IMP-L2 [Acromyrmex echinator]
46	18191	gi 1009365340 gb KYM90371.1	60.17	2	1	1	N	89447	Neural/ectodermal development factor IMP-L2 [Atta colombica]
46	18192	gi 1012987417 gb KYQ60792.1	60.17	2	1	1	N	95226	Neural/ectodermal development factor IMP-L2, partial [Trachymyrmex zeteki]
46	18193	gi 1009394077 gb KYN15150.1	60.17	2	1	1	N	103587	Neural/ectodermal development factor IMP-L2, partial [Trachymyrmex cornetzi]
2	77	gi 1911819 gb AAB50883.1	59.75	10	1	1	Y	11819	Myr p I=allergenic polypeptide {N-termina l} [Myrmecia pilosula=jumper ants, venom, Peptide Partial, 112 aa]
2	78	gi 312284 emb CAA49760.1	59.75	10	1	1	Y	11849	major allergen [Myrmecia pilosula]
2	76	gi 730091 sp Q07932.1 MYR1_MYRPI	59.75	10	1	1	Y	11849	RecName: Full=Pilosulin-1; AltName: Full=Allergen Myr p I; AltName: Full=Major allergen Myr p I; AltName: Allergen=Myr p I; Contains: RecName: Full=Pilosulin-1; Contains: RecName: Full=Pilosulin-1 65->112; Contains: RecNa...
9	5563	gi 815812192 ref XP_012227043.1	46.97	11	1	1	N	15487	PREDICTED: LOW QUALITY PROTEIN: superoxide dismutase [Cu-Zn]-like [Linepithema humile]
47	182	gi 780703760 ref XP_011702702.1	40.61	3	1	1	N	25807	PREDICTED: venom allergen 3-like [Wasmannia auropunctata]
total 46 proteins									

Prepared with PEAKS™ (bioinformatics.com)

Band # 9 Proteins

Summary

1. Notes

2. Result Statistics

Figure 1. False discovery rate (FDR) curve. X axis is the number of peptide-spectrum matches (PSM) being kept. Y axis is the corresponding FDR.

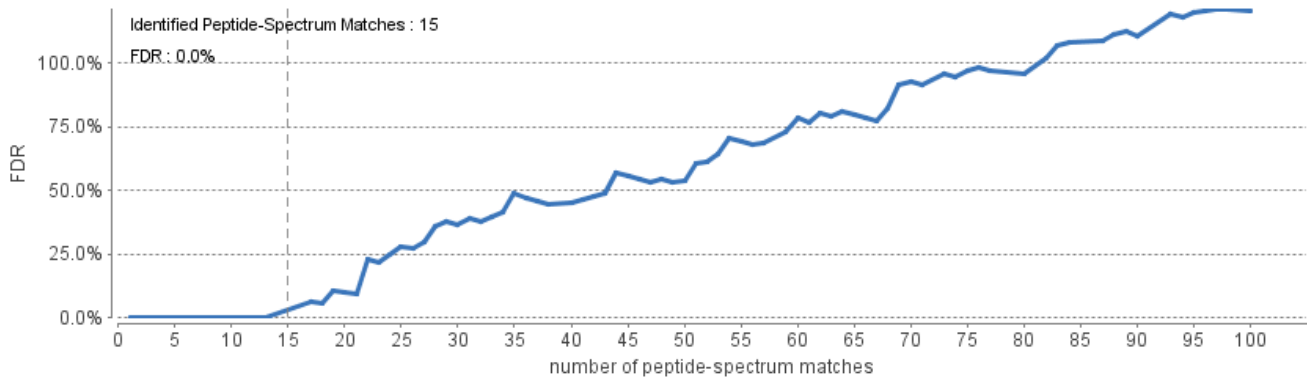


Figure 2. PSM score distribution. (a) Distribution of PEAKS peptide score; (b) Scatterplot of PEAKS peptide score versus precursor mass error.

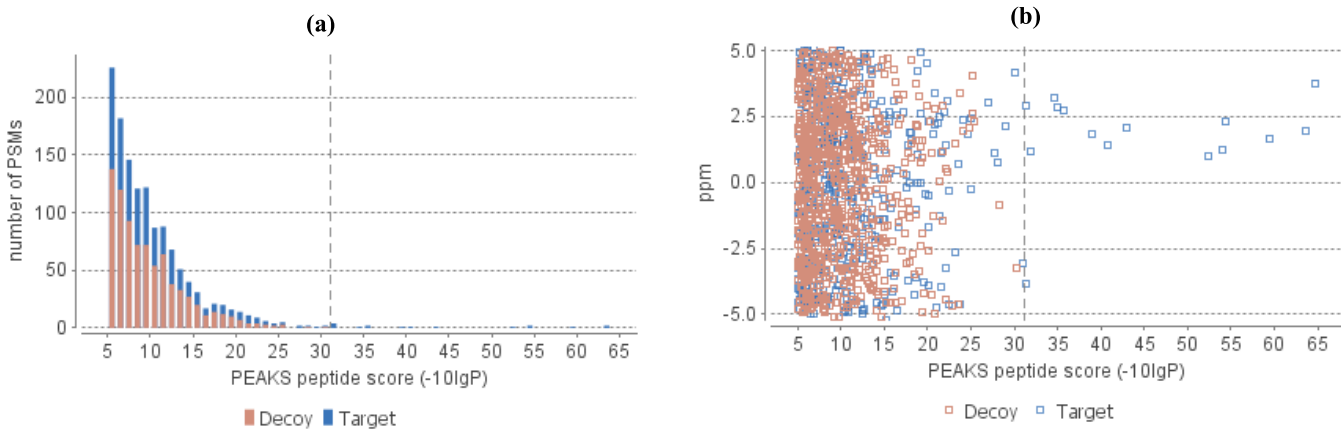


Figure 3. De novo result validation. Distribution of residue local confidence: (a) Residues in de novo sequences validated by confident database peptide assignment; (b) Residues in "de novo only" sequences.

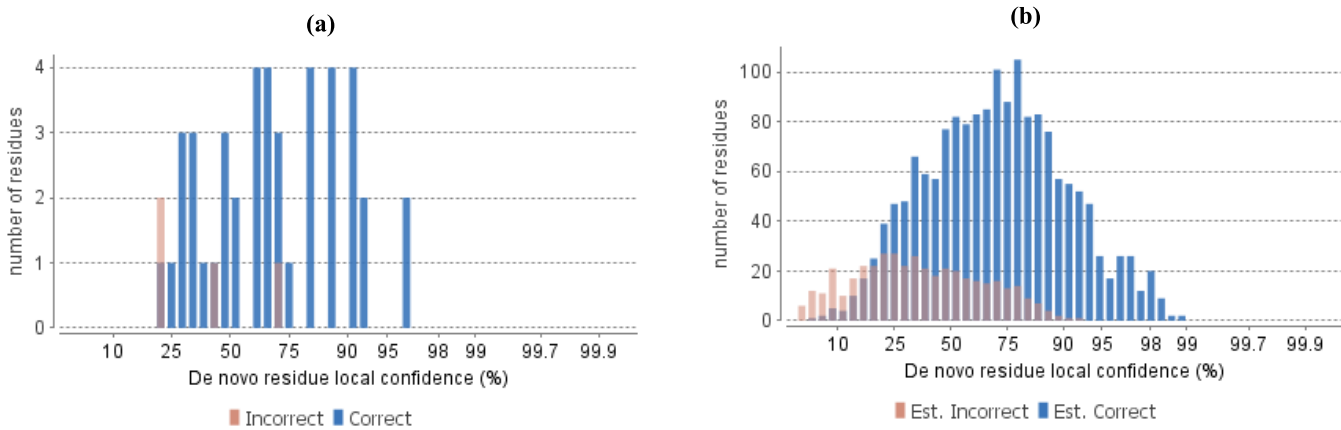


Table 1. Statistics of data.

# of MS Scans	1575
# of MS/MS Scans	3212

Table 4. PTM profile.

Name	Δ Mass	Position	#PSM	-10lgP	Area	AScore
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Table 2. Result filtration parameters.

Peptide -10lgP	≥31.1
Protein -10lgP	≥20
Proteins unique peptides	≥1
De novo ALC Score	≥50%

Table 3. Statistics of filtered result.

Peptide-Spectrum Matches	15
Peptide Sequences	13
Protein Groups	10
Proteins	55
Proteins (#Unique Peptides)	0 (>2); 2 (=2); 53 (=1);
FDR (Peptide-Spectrum Matches)	0.0%
FDR (Peptide Sequences)	0.0%
FDR (Protein)	0.0%
De Novo Only Spectra	192

3. Experiment Control

Figure 4. Precursor mass error of peptide-spectrum matches (PSM) in filtered result. **(a)** Distribution of precursor mass error in ppm; **(b)** Scatterplot of precursor m/z versus precursor mass error in ppm. ?

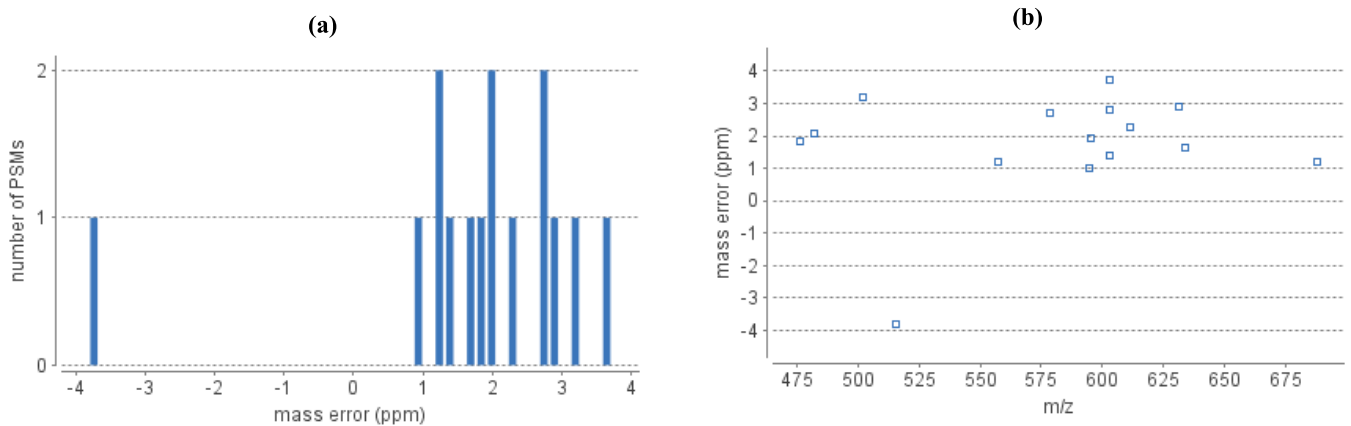


Table 5. Number of identified peptides in each sample by the number of missed cleavages

Missed Cleavages	0	1	2	3	4+
Sample 2	10	3	0	0	0

4. Other Information

Table 6. Search parameters.

Search Engine Name:	PEAKS
Parent Mass Error Tolerance:	5.0 ppm
Fragment Mass Error Tolerance:	0.5 Da
Precursor Mass Search Type:	monoisotopic
Enzyme:	Trypsin
Max Missed Cleavages:	3
Non-specific Cleavage:	one
Variable Modifications:	
Oxidation (M):	15.99
Max variable PTM per peptide:	3
Database:	Ant
Taxon:	All
Searched Entry:	473117
FDR Estimation:	Enabled
Merge Options:	no merge
Precursor Options:	corrected
Charge Options:	no correction

Table 7. Instrument parameters.

Fractions:	TW_9.raw
Ion Source:	ESI(nano-spray)
Fragmentation Mode:	CID, CAD(y and b ions)
MS Scan Mode:	FT-ICR/Orbitrap
MS/MS Scan Mode:	FT-ICR/Orbitrap

Filter Options: no filter

Process: true

Protein List

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
3	135	gi 815804483 ref XP_012222952.1	90.63	5	2	2	N	26367	PREDICTED: venom allergen 3-like [Linepithema humile]
3	136	gi 815804481 ref XP_012222951.1	90.63	5	2	2	N	26367	PREDICTED: venom allergen 3-like [Linepithema humile]
1	77	gi 1911819 gb AAB50883.1	64.73	10	1	1	Y	11819	Myr p I=allergenic polypeptide {N-termina l} [Myrmecia pilosula=jumper ants, veno m, Peptide Partial, 112 aa]
1	78	gi 312284 emb CAA49760.1	64.73	10	1	1	Y	11849	major allergen [Myrmecia pilosula]
1	76	gi 730091 sp Q07932.1 MYR1_MYRPI	64.73	10	1	1	Y	11849	RecName: Full=Pilosulin-1; AltName: Full=Allergen Myr p I; AltName: Full=Major allergen Myr p 1; AltName: Allergen=Myr p 1; Contains: RecName: Full=Pilosulin-1; Contains: RecName: Full=Pilosulin-1 65->112; Contains: RecNa...
13	23	gi 769852441 ref XP_011637689.1	59.53	4	1	1	N	30700	PREDICTED: apolipoprotein D-like [Pogonomyrmex barbatus]
13	100	gi 795018679 ref XP_011859302.1	59.53	4	1	1	N	29980	PREDICTED: apolipoprotein D-like [Vollenhovia emeryi]
13	101	gi 795018681 ref XP_011859303.1	59.53	4	1	1	N	29980	PREDICTED: apolipoprotein D-like [Vollenhovia emeryi]
13	102	gi 1009391833 gb KYN13116.1	59.53	4	1	1	N	30178	Apolipoprotein D [Trachymyrmex cornetzi]
13	103	gi 780637946 ref XP_011687250.1	59.53	4	1	1	N	30230	PREDICTED: apolipoprotein D-like isoform X2 [Wasmannia auropunctata]
13	104	gi 780637954 ref XP_011687252.1	59.53	4	1	1	N	30230	PREDICTED: apolipoprotein D-like isoform X2 [Wasmannia auropunctata]
13	105	gi 780637950 ref XP_011687251.1	59.53	4	1	1	N	30230	PREDICTED: apolipoprotein D-like isoform X2 [Wasmannia auropunctata]
13	106	gi 1009415883 gb KYN34685.1	59.53	4	1	1	N	30226	Apolipoprotein D [Trachymyrmex septentrionalis]
13	107	gi 780637958 ref XP_011687253.1	59.53	4	1	1	N	30230	PREDICTED: apolipoprotein D-like isoform X2 [Wasmannia auropunctata]
13	108	gi 815798630 ref XP_012219934.1	59.53	4	1	1	N	30263	PREDICTED: apolipoprotein D-like isoform X2 [Linepithema humile]
13	111	gi 752883266 ref XP_011259329.1	59.53	4	1	1	N	30560	PREDICTED: apolipoprotein D-like [Campo notus floridanus]
13	112	gi 1009378593 gb KYN01799.1	59.53	4	1	1	N	30380	Apolipoprotein D [Cyphomyrmex costatus]
13	109	gi 861652739 gb KMQ98491.1	59.53	4	1	1	N	30507	apolipoprotein d [Lasius niger]
13	110	gi 307177066 gb EFN66334.1	59.53	4	1	1	N	30560	Apolipoprotein D [Camponotus floridanus]
13	113	gi 1009357318 gb KYM82590.1	59.53	4	1	1	N	30536	Apolipoprotein D [Atta colombica]
13	114	gi 951576767 ref XP_014486317.1	59.53	4	1	1	N	30843	PREDICTED: apolipoprotein D-like [Dinoponera quadricaps]
13	115	gi 951576769 ref XP_014486318.1	59.53	4	1	1	N	30843	PREDICTED: apolipoprotein D-like [Dinoponera quadricaps]
13	116	gi 307202431 gb EFN81851.1	59.53	4	1	1	N	30652	Apolipoprotein D [Harpegnathos saltator]
13	117	gi 749777656 ref XP_011143638.1	59.53	4	1	1	N	30652	PREDICTED: apolipoprotein D-like [Harpegnathos saltator]
13	118	gi 749777659 ref XP_011143639.1	59.53	4	1	1	N	30652	PREDICTED: apolipoprotein D-like [Harpegnathos saltator]
13	119	gi 780637941 ref XP_011687249.1	59.53	4	1	1	N	31633	PREDICTED: apolipoprotein D-like isoform X1 [Wasmannia auropunctata]
13	120	gi 746846016 ref XP_011053314.1	59.53	4	1	1	N	31633	PREDICTED: apolipoprotein D-like isoform X4 [Acromyrmex echinator]
13	121	gi 815798628 ref XP_012219933.1	59.53	4	1	1	N	31568	PREDICTED: apolipoprotein D-like isoform X1 [Linepithema humile]
13	122	gi 746846014 ref XP_011053313.1	59.53	3	1	1	N	32009	PREDICTED: apolipoprotein D-like isoform X3 [Acromyrmex echinator]
13	123	gi 746846012 ref XP_011053312.1	59.53	3	1	1	N	32879	PREDICTED: apolipoprotein D-like isoform X2 [Acromyrmex echinator]
13	124	gi 332025852 gb EGI66008.1	59.53	3	1	1	N	35048	Apolipoprotein D [Acromyrmex echinator]
13	125	gi 1012977673 gb KYQ51728.1	59.53	3	1	1	N	35324	Apolipoprotein D, partial [Trachymyrmex zeteki]
13	126	gi 746846010 ref XP_011053311.1	59.53	3	1	1	N	35655	PREDICTED: apolipoprotein D-like isoform X1 [Acromyrmex echinator]
13	127	gi 801374597 ref XP_012063028.1	59.53	3	1	1	N	35743	PREDICTED: LOW QUALITY PROTEIN: apolipoprotein D-like [Atta cephalotes]
43	183	gi 749792410 ref XP_011149448.1	43.02	2	1	1	N	42356	PREDICTED: quinone oxidoreductase-like protein 2 isoform X3 [Harpegnathos saltator]
43	4121	gi 951547983 ref XP_014474129.1	43.02	2	1	1	N	45182	PREDICTED: quinone oxidoreductase-like protein 2 isoform X5 [Dinoponera quadricaps]

total 55 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
43	185	gi 307196260 gb EFN77906.1	43.02	2	1	1	N	45335	Quinone oxidoreductase-like protein 2 [Harpegnathos saltator]
43	184	gi 749792408 ref XP_011149447.1	43.02	2	1	1	N	45335	PREDICTED: quinone oxidoreductase-like protein 2 isoform X2 [Harpegnathos saltator]
43	4122	gi 951547980 ref XP_014474128.1	43.02	2	1	1	N	45683	PREDICTED: quinone oxidoreductase-like protein 2 isoform X4 [Dinoponera quadricaps]
43	186	gi 749792406 ref XP_011149446.1	43.02	2	1	1	N	45929	PREDICTED: quinone oxidoreductase-like protein 2 isoform X1 [Harpegnathos saltator]
43	4123	gi 951547977 ref XP_014474126.1	43.02	2	1	1	N	46074	PREDICTED: quinone oxidoreductase-like protein 2 isoform X3 [Dinoponera quadricaps]
43	4124	gi 815799876 ref XP_012220584.1	43.02	2	1	1	N	45429	PREDICTED: quinone oxidoreductase-like protein 2 [Linepithema humile]
43	187	gi 951547974 ref XP_014474125.1	43.02	2	1	1	N	46587	PREDICTED: quinone oxidoreductase-like protein 2 isoform X2 [Dinoponera quadricaps]
43	4125	gi 951547971 ref XP_014474124.1	43.02	2	1	1	N	46979	PREDICTED: quinone oxidoreductase-like protein 2 isoform X1 [Dinoponera quadricaps]
8	182	gi 780703760 ref XP_011702702.1	39.03	3	1	1	N	25807	PREDICTED: venom allergen 3-like [Wasmannia auropunctata]
44	194	gi 826418112 ref XP_012523875.1	35.74	1	1	1	N	94279	PREDICTED: DNA ligase 1-like [Monomorium pharaonis]
45	143	gi 307184709 gb EFN71038.1	34.70	4	1	1	N	22151	hypothetical protein EAG_09928 [Camponotus floridanus]
45	4127	gi 861653549 gb KMQ99191.1	34.70	1	1	1	N	108034	dynammin-like mitochondrial protein [Lasius niger]
45	195	gi 801397101 ref XP_012058936.1	34.70	1	1	1	N	113731	PREDICTED: dynammin-like 120 kDa protein, mitochondrial isoform X3 [Atta cephalotes]
45	4128	gi 801397099 ref XP_012058935.1	34.70	1	1	1	N	113933	PREDICTED: dynammin-like 120 kDa protein, mitochondrial isoform X2 [Atta cephalotes]
45	4129	gi 801397097 ref XP_012058934.1	34.70	1	1	1	N	114004	PREDICTED: dynammin-like 120 kDa protein, mitochondrial isoform X1 [Atta cephalotes]
46	193	gi 752890834 ref XP_011263428.1	31.92	1	1	1	N	102130	PREDICTED: LOW QUALITY PROTEIN: transient receptor potential channel pyrexia-like [Camponotus floridanus]
47	189	gi 332019958 gb EGI60418.1	31.39	4	1	1	N	33825	hypothetical protein G5I_11398 [Acromyrmex echinator]
47	190	gi 1009394013 gb KYN15086.1	31.39	2	1	1	N	59014	Carbonyl reductase [NADPH] 1 [Trachymyrmex cornetzi]
48	191	gi 815813158 ref XP_012227562.1	31.36	3	1	1	N	34640	PREDICTED: coiled-coil domain-containing protein 186-like isoform X3 [Linepithema humile]
total 55 proteins									

Band # 10 Proteins

Summary

1. Notes

2. Result Statistics

Figure 1. False discovery rate (FDR) curve. X axis is the number of peptide-spectrum matches (PSM) being kept. Y axis is the corresponding FDR.

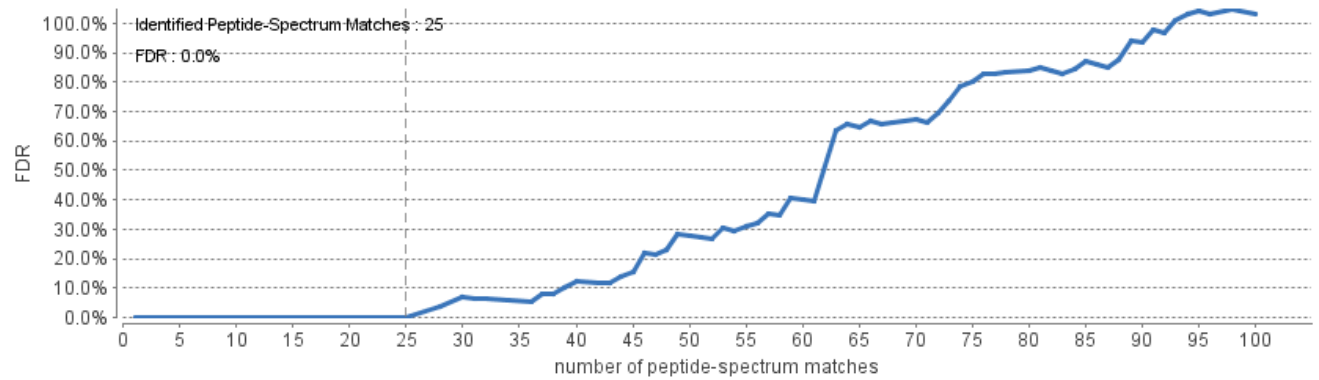


Figure 2. PSM score distribution. (a) Distribution of PEAKS peptide score; (b) Scatterplot of PEAKS peptide score versus precursor mass error.

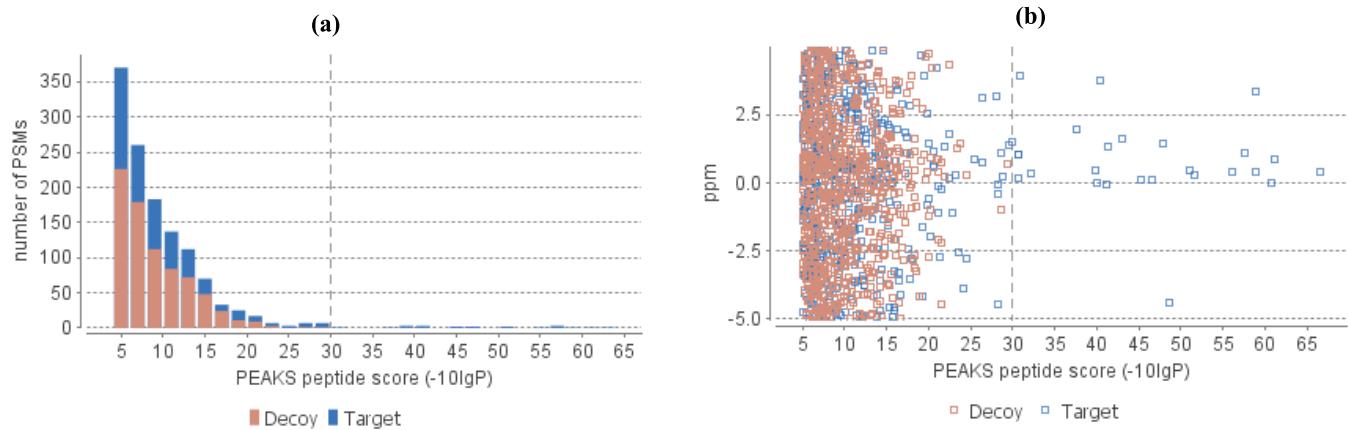


Figure 3. De novo result validation. Distribution of residue local confidence: (a) Residues in de novo sequences validated by confident database peptide assignment; (b) Residues in "de novo only" sequences.

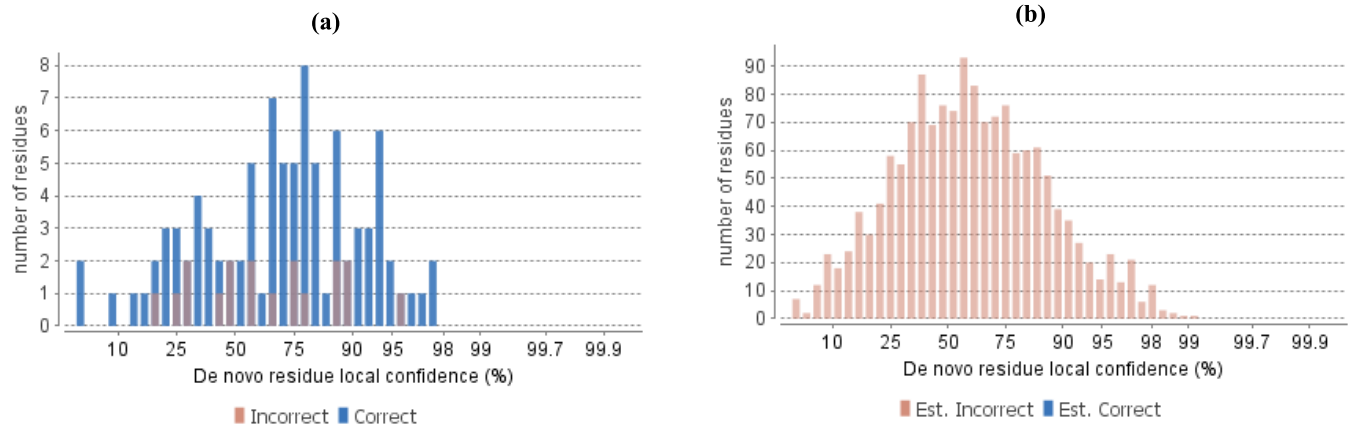


Table 1. Statistics of data.

# of MS Scans	1632
# of MS/MS Scans	3117

Table 4. PTM profile.

Name	Δ Mass	Position	#PSM	-10lgP	Area	AScore
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Table 2. Result filtration parameters.

Peptide -10lgP	≥29.9
Protein -10lgP	≥20
Proteins unique peptides	≥1
De novo ALC Score	≥50%

Table 3. Statistics of filtered result.

Peptide-Spectrum Matches	25
Peptide Sequences	23
Protein Groups	12
Proteins	69
Proteins (#Unique Peptides)	12 (>2); 8 (=2); 49 (=1);
FDR (Peptide-Spectrum Matches)	0.0%
FDR (Peptide Sequences)	0.0%
FDR (Protein)	0.0%
De Novo Only Spectra	140

3. Experiment Control

Figure 4. Precursor mass error of peptide-spectrum matches (PSM) in filtered result. **(a)** Distribution of precursor mass error in ppm; **(b)** Scatterplot of precursor m/z versus precursor mass error in ppm. 

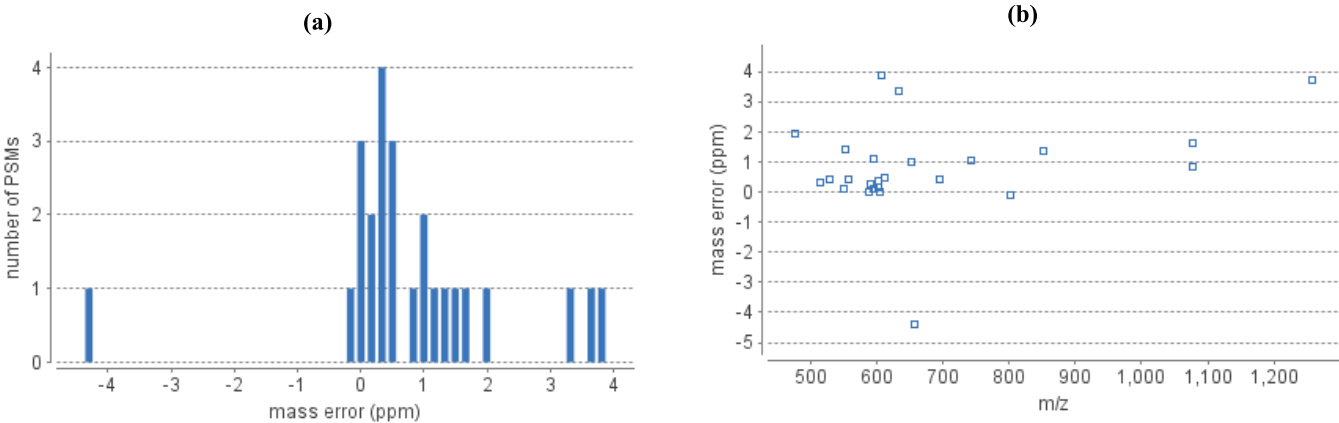


Table 5. Number of identified peptides in each sample by the number of missed cleavages

Missed Cleavages	0	1	2	3	4+
Sample 4	20	3	0	0	0

4. Other Information

Table 6. Search parameters.

Search Engine Name:	PEAKS
Parent Mass Error Tolerance:	5.0 ppm
Fragment Mass Error Tolerance:	0.5 Da
Precursor Mass Search Type:	monoisotopic
Enzyme:	Trypsin
Max Missed Cleavages:	3
Non-specific Cleavage:	one
Variable Modifications:	
Oxidation (M):	15.99
Max variable PTM per peptide:	3
Database:	Ant
Taxon:	All
Searched Entry:	473117
FDR Estimation:	Enabled
Merge Options:	no merge
Precursor Options:	corrected
Charge Options:	no correction

Table 7. Instrument parameters.

Fractions:	TW_10.raw
Ion Source:	ESI(nano-spray)
Fragmentation Mode:	CID, CAD(y and b ions)
MS Scan Mode:	FT-ICR/Orbitrap
MS/MS Scan Mode:	FT-ICR/Orbitrap

Filter Options: no filter

Process: true

Protein List

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
4	6778	gi 752876495 ref XP_011255648.1	115.93	12	4	4	N	36097	PREDICTED: annexin B9 [Camponotus floridanus]
4	6779	gi 795018427 ref XP_011859208.1	115.93	12	4	4	N	36100	PREDICTED: annexin B9-like [Vollenhovia emeryi]
4	6780	gi 826409661 ref XP_012534131.1	115.93	12	4	4	N	36188	PREDICTED: annexin B9 [Monomorium pharaonis]
4	6781	gi 751234091 ref XP_011170758.1	115.93	12	4	4	N	36221	PREDICTED: annexin B9-like [Solenopsis invicta]
4	6782	gi 826409659 ref XP_012534123.1	115.93	12	4	4	N	36188	PREDICTED: annexin B9 [Monomorium pharaonis]
4	6783	gi 795018424 ref XP_011859205.1	115.93	12	4	4	N	36100	PREDICTED: annexin B9-like [Vollenhovia emeryi]
4	6784	gi 795018430 ref XP_011859209.1	115.93	12	4	4	N	36100	PREDICTED: annexin B9-like [Vollenhovia emeryi]
4	6785	gi 951561054 ref XP_014479495.1	115.93	12	4	4	N	36092	PREDICTED: annexin B9 isoform X1 [Dinoponera quadricaps]
4	6786	gi 322783201 gb EFZ10787.1	115.93	12	4	4	N	36221	hypothetical protein SINV_01089, partial [Solenopsis invicta]
4	6787	gi 815820705 ref XP_012231575.1	115.93	12	4	4	N	36000	PREDICTED: annexin B9 [Linepithema humile]
4	6788	gi 307181035 gb EFN68809.1	115.93	12	4	4	N	36097	Annexin-B9 [Camponotus floridanus]
1	23	gi 769852441 ref XP_011637689.1	106.83	15	3	2	N	30700	PREDICTED: apolipoprotein D-like [Pogonomyrmex barbatus]
5	6789	gi 752887596 ref XP_011261677.1	95.20	17	4	4	N	33334	PREDICTED: LOW QUALITY PROTEIN: glyoxalase domain-containing protein 4-like [Camponotus floridanus]
9	100	gi 795018679 ref XP_011859302.1	74.21	7	2	1	N	29980	PREDICTED: apolipoprotein D-like [Vollenhovia emeryi]
9	101	gi 795018681 ref XP_011859303.1	74.21	7	2	1	N	29980	PREDICTED: apolipoprotein D-like [Vollenhovia emeryi]
9	108	gi 815798630 ref XP_012219934.1	74.21	7	2	1	N	30263	PREDICTED: apolipoprotein D-like isoform X2 [Linepithema humile]
9	109	gi 861652739 gb KMQ98491.1	74.21	7	2	1	N	30507	apolipoprotein d [Lasius niger]
9	121	gi 815798628 ref XP_012219933.1	74.21	7	2	1	N	31568	PREDICTED: apolipoprotein D-like isoform X1 [Linepithema humile]
55	6835	gi 332018065 gb EGI58681.1	66.58	7	1	1	N	18253	Lipase member H [Acromyrmex echinatior]
55	6836	gi 1009351219 gb KYM76701.1	66.58	5	1	1	N	25318	Pancreatic triacylglycerol lipase [Atta colombica]
55	6837	gi 1009395873 gb KYN16656.1	66.58	5	1	1	N	25477	Pancreatic triacylglycerol lipase [Trachymyrmex cornetzi]
55	6838	gi 1009420770 gb KYN39257.1	66.58	5	1	1	N	25376	Lipase member H-A [Trachymyrmex septentrionalis]
55	6839	gi 746868512 ref XP_011065387.1	66.58	4	1	1	N	32848	PREDICTED: pancreatic triacylglycerol lipase-like [Acromyrmex echinatior]
55	6840	gi 801398640 ref XP_012059785.1	66.58	4	1	1	N	36144	PREDICTED: phospholipase A1 member A-like [Atta cephalotes]
7	135	gi 815804483 ref XP_012222952.1	59.40	4	1	1	N	26367	PREDICTED: venom allergen 3-like [Linepithema humile]
7	136	gi 815804481 ref XP_012222951.1	59.40	4	1	1	N	26367	PREDICTED: venom allergen 3-like [Linepithema humile]
3	77	gi 1911819 gb AAB50883.1	58.94	10	1	1	Y	11819	Myr p I=allergenic polypeptide {N-terminus [Myrmecia pilosula=jumper ants, venom, Peptide Partial, 112 aa]}
3	78	gi 312284 emb CAA49760.1	58.94	10	1	1	Y	11849	major allergen [Myrmecia pilosula]
3	76	gi 730091 sp Q07932.1 MYR1_MYRPI	58.94	10	1	1	Y	11849	RecName: Full=Pilosulin-1; AltName: Full=Allergen Myr p I; AltName: Full=Major allergen Myr p 1; AltName: Allergen=Myr p 1; Contains: RecName: Full=Pilosulin-1; Contains: RecName: Full=Pilosulin-1 65->112; Contains: RecName...
10	6823	gi 951518524 ref XP_014473490.1	55.44	8	2	2	N	35925	PREDICTED: malate dehydrogenase, mitochondrial [Dinoponera quadricaps]
10	6824	gi 307180366 gb EFN68392.1	55.44	8	2	2	N	35963	Malate dehydrogenase, mitochondrial [Camponotus floridanus]
10	6825	gi 815825824 ref XP_012234288.1	55.44	8	2	2	N	35771	PREDICTED: LOW QUALITY PROTEIN: malate dehydrogenase, mitochondrial [Linepithema humile]
10	6826	gi 861642979 gb KMQ94145.1	55.44	8	2	2	N	35869	malate mitochondrial [Lasius niger]
10	6827	gi 607363491 gb EZA57723.1	55.44	8	2	2	N	35754	Malate dehydrogenase, mitochondrial [Cerapachys biroi]
10	6828	gi 759048415 ref XP_011333248.1	55.44	8	2	2	N	35754	PREDICTED: malate dehydrogenase, mitochondrial [Cerapachys biroi]
total 69 proteins									

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
10	6829	gi 752877346 ref XP_011256104.1	55.44	8	2	2	N	35963	PREDICTED: malate dehydrogenase, mitochondrial [Camponotus floridanus]
56	64	gi 751219056 ref XP_011162596.1	51.57	5	1	1	N	25498	PREDICTED: acidic phospholipase A2 PA4 isoform X2 [Solenopsis invicta]
56	79	gi 752883275 ref XP_011259333.1	51.57	5	1	1	N	25675	PREDICTED: acidic phospholipase A2 PA4 isoform X2 [Camponotus floridanus]
56	81	gi 752883277 ref XP_011259334.1	51.57	5	1	1	N	25675	PREDICTED: acidic phospholipase A2 PA4 isoform X2 [Camponotus floridanus]
56	82	gi 795027450 ref XP_011862285.1	51.57	5	1	1	N	25771	PREDICTED: acidic phospholipase A2 PA4 [Vollenhovia emeryi]
56	83	gi 795027459 ref XP_011862288.1	51.57	5	1	1	N	25771	PREDICTED: acidic phospholipase A2 PA4 [Vollenhovia emeryi]
56	65	gi 769852445 ref XP_011637691.1	51.57	5	1	1	N	25718	PREDICTED: acidic phospholipase A2 PA4 isoform X2 [Pogonomyrmex barbatus]
56	84	gi 795027456 ref XP_011862287.1	51.57	5	1	1	N	25771	PREDICTED: acidic phospholipase A2 PA4 [Vollenhovia emeryi]
56	85	gi 795027453 ref XP_011862286.1	51.57	5	1	1	N	25771	PREDICTED: acidic phospholipase A2 PA4 [Vollenhovia emeryi]
56	66	gi 607361739 gb EZA56014.1	51.57	5	1	1	N	25661	Group 3 secretory phospholipase A2 [Cera-pachys biroii]
56	86	gi 746846018 ref XP_011053315.1	51.57	5	1	1	N	25913	PREDICTED: acidic phospholipase A2 PA4-like isoform X1 [Acromyrmex echinator]
56	87	gi 801374599 ref XP_012063030.1	51.57	5	1	1	N	25985	PREDICTED: acidic phospholipase A2 PA4-like [Atta cephalotes]
56	67	gi 780637978 ref XP_011687259.1	51.57	5	1	1	N	26007	PREDICTED: phospholipase A2 isozymes P A3A/PA3B/PA5 isoform X2 [Wasmannia auropunctata]
56	68	gi 769852443 ref XP_011637690.1	51.57	5	1	1	N	27251	PREDICTED: acidic phospholipase A2 PA4 isoform X1 [Pogonomyrmex barbatus]
56	88	gi 749777653 ref XP_011143637.1	51.57	4	1	1	N	27531	PREDICTED: acidic phospholipase A2 PA4 isoform X6 [Harpegnathos saltator]
56	89	gi 749777651 ref XP_011143636.1	51.57	4	1	1	N	27947	PREDICTED: phospholipase A2 isoform X5 [Harpegnathos saltator]
56	69	gi 751219054 ref XP_011162595.1	51.57	4	1	1	N	28045	PREDICTED: uncharacterized protein LOC105197765 isoform X1 [Solenopsis invicta]
56	70	gi 759054210 ref XP_011336300.1	51.57	4	1	1	N	28030	PREDICTED: uncharacterized protein LOC105278712 isoform X3 [Cera-pachys biroii]
56	90	gi 752883273 ref XP_011259332.1	51.57	4	1	1	N	28503	PREDICTED: acidic phospholipase A2 PA4 isoform X1 [Camponotus floridanus]
56	91	gi 749777649 ref XP_011143635.1	51.57	4	1	1	N	28548	PREDICTED: acidic phospholipase A2 PA4 isoform X4 [Harpegnathos saltator]
56	71	gi 759054208 ref XP_011336299.1	51.57	4	1	1	N	28800	PREDICTED: uncharacterized protein LOC105278712 isoform X2 [Cera-pachys biroii]
56	73	gi 780637966 ref XP_011687254.1	51.57	4	1	1	N	28793	PREDICTED: uncharacterized protein LOC105449644 isoform X1 [Wasmannia auropunctata]
56	72	gi 780637974 ref XP_011687258.1	51.57	4	1	1	N	28793	PREDICTED: uncharacterized protein LOC105449644 isoform X1 [Wasmannia auropunctata]
56	74	gi 780637970 ref XP_011687255.1	51.57	4	1	1	N	28793	PREDICTED: uncharacterized protein LOC105449644 isoform X1 [Wasmannia auropunctata]
56	93	gi 749777645 ref XP_011143633.1	51.57	4	1	1	N	29891	PREDICTED: uncharacterized protein LOC105185668 isoform X3 [Harpegnathos saltator]
56	94	gi 749777647 ref XP_011143634.1	51.57	4	1	1	N	29891	PREDICTED: uncharacterized protein LOC105185668 isoform X3 [Harpegnathos saltator]
56	92	gi 749777643 ref XP_011143632.1	51.57	4	1	1	N	29891	PREDICTED: uncharacterized protein LOC105185668 isoform X3 [Harpegnathos saltator]
56	95	gi 749777640 ref XP_011143631.1	51.57	4	1	1	N	30593	PREDICTED: uncharacterized protein LOC105185668 isoform X2 [Harpegnathos saltator]
56	75	gi 759054206 ref XP_011336298.1	51.57	4	1	1	N	31169	PREDICTED: uncharacterized protein LOC105278712 isoform X1 [Cera-pachys biroii]
56	96	gi 749777637 ref XP_011143630.1	51.57	4	1	1	N	31610	PREDICTED: uncharacterized protein LOC105185668 isoform X1 [Harpegnathos saltator]
56	99	gi 815798632 ref XP_012219935.1	51.57	1	1	1	N	148213	PREDICTED: uncharacterized protein LOC105670791 [Linepithema humile]
57	6846	gi 749750028 ref XP_011137253.1	40.46	4	1	1	N	71477	PREDICTED: heat shock 70 kDa protein cognate 4 [Harpegnathos saltator]
58	182	gi 780703760 ref XP_011702702.1	37.51	3	1	1	N	25807	PREDICTED: venom allergen 3-like [Wasmannia auropunctata]
59	215	gi 1009385602 gb KYN07954.1	30.63	1	1	1	N	124955	hypothetical protein ALC62_01070 [Cyphomyrmex costatus]
total 69 proteins									

Band # 11 Proteins

Summary

1. Notes

2. Result Statistics

Figure 1. False discovery rate (FDR) curve. X axis is the number of peptide-spectrum matches (PSM) being kept. Y axis is the corresponding FDR.

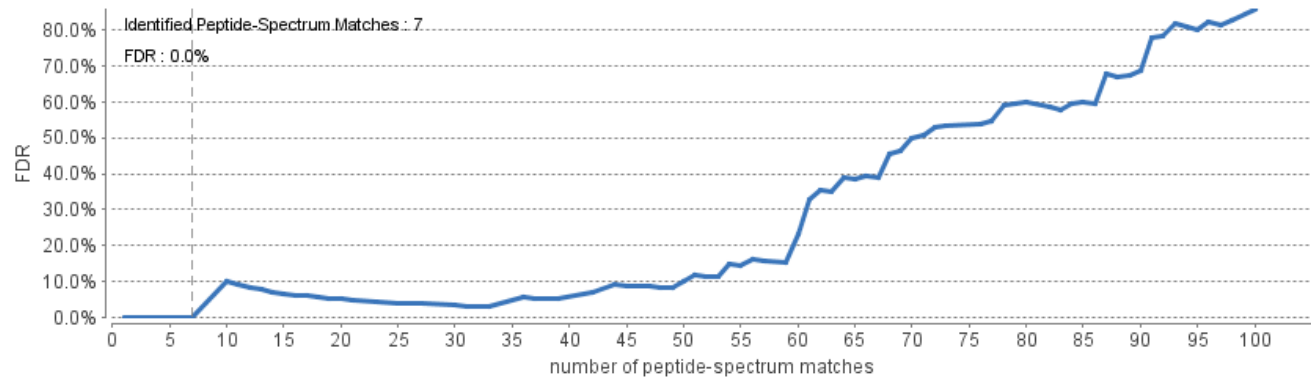


Figure 2. PSM score distribution. (a) Distribution of PEAKS peptide score; (b) Scatterplot of PEAKS peptide score versus precursor mass error.

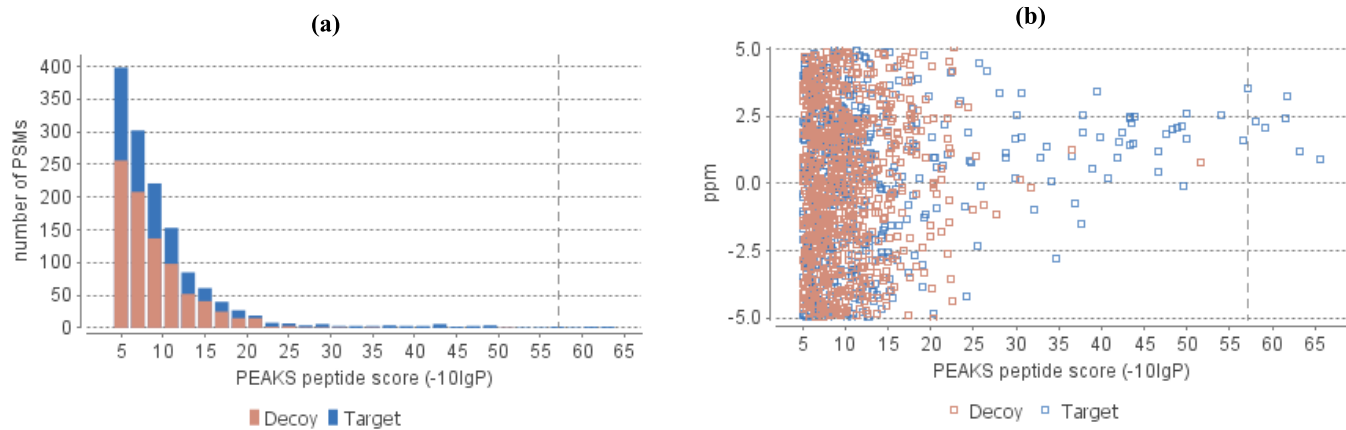


Figure 3. De novo result validation. Distribution of residue local confidence: (a) Residues in de novo sequences validated by confident database peptide assignment; (b) Residues in "de novo only" sequences.

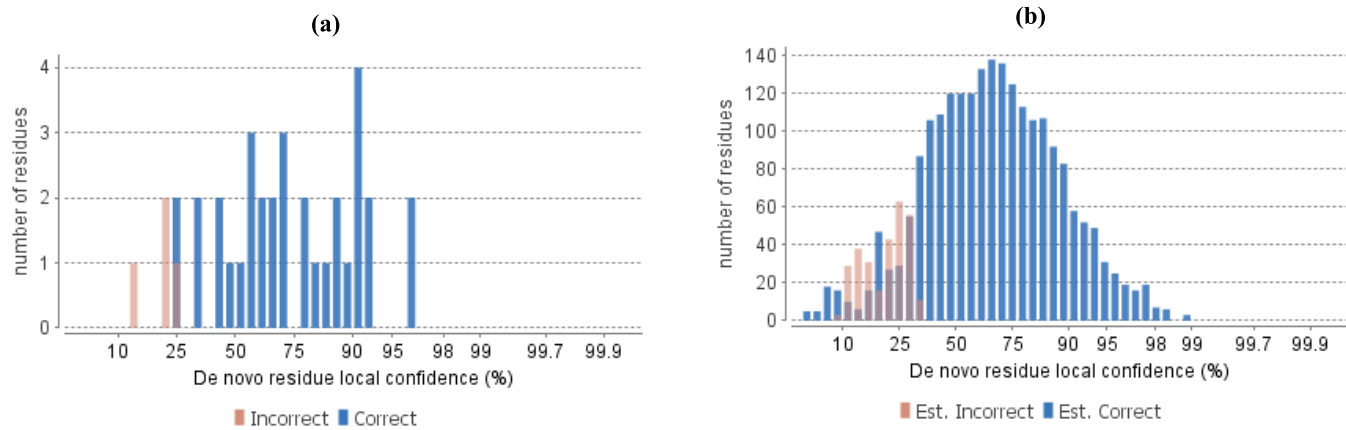


Table 1. Statistics of data.

# of MS Scans	1590
# of MS/MS Scans	3424

Table 4. PTM profile.

Name	Δ Mass	Position	#PSM	-10lgP	Area	AScore
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Table 2. Result filtration parameters.

Peptide -10lgP	≥57.1
Protein -10lgP	≥20
Proteins unique peptides	≥1
De novo ALC Score	≥50%

Table 3. Statistics of filtered result.

Peptide-Spectrum Matches	7
Peptide Sequences	6
Protein Groups	3
Proteins	5
Proteins (#Unique Peptides)	0 (>2); 0 (=2); 5 (=1);
FDR (Peptide-Spectrum Matches)	0.0%
FDR (Peptide Sequences)	0.0%
FDR (Protein)	0.0%
De Novo Only Spectra	250

3. Experiment Control

Figure 4. Precursor mass error of peptide-spectrum matches (PSM) in filtered result. **(a)** Distribution of precursor mass error in ppm; **(b)** Scatterplot of precursor m/z versus precursor mass error in ppm. 

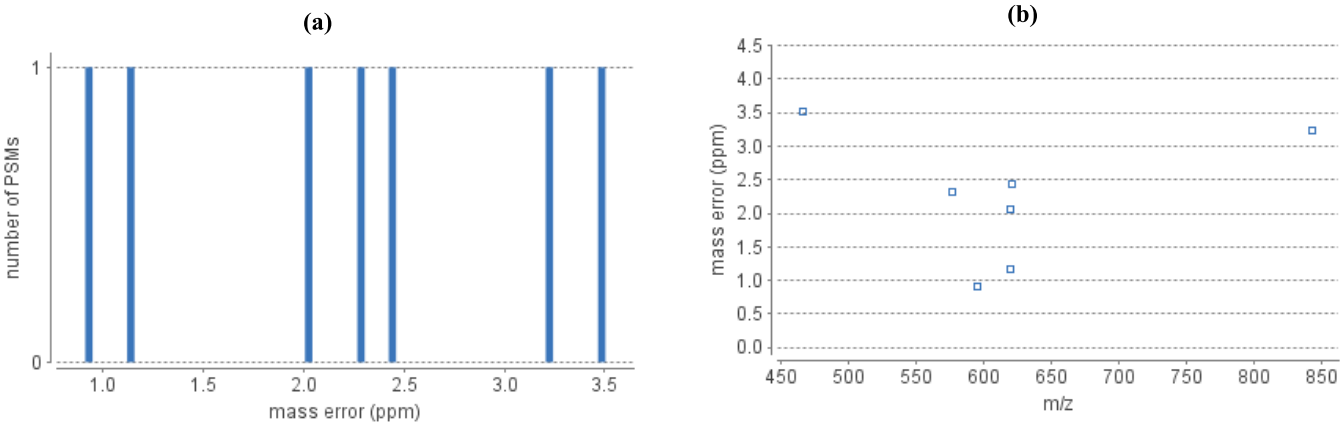


Table 5. Number of identified peptides in each sample by the number of missed cleavages

Missed Cleavages	0	1	2	3	4+
Sample 5	2	3	1	0	0

4. Other Information

Table 6. Search parameters.

Search Engine Name:	PEAKS
Parent Mass Error Tolerance:	5.0 ppm
Fragment Mass Error Tolerance:	0.5 Da
Precursor Mass Search Type:	monoisotopic
Enzyme:	Trypsin
Max Missed Cleavages:	3
Non-specific Cleavage:	one
Variable Modifications:	
Oxidation (M):	15.99
Max variable PTM per peptide:	3
Database:	Ant
Taxon:	All
Searched Entry:	473117
FDR Estimation:	Enabled
Merge Options:	no merge
Precursor Options:	corrected
Charge Options:	no correction

Table 7. Instrument parameters.

Fractions:	TW_11.raw
Ion Source:	ESI(nano-spray)
Fragmentation Mode:	CID, CAD(y and b ions)
MS Scan Mode:	FT-ICR/Orbitrap
MS/MS Scan Mode:	FT-ICR/Orbitrap

Filter Options: no filter
Process: true

Protein List

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
1	8258	gi 861652016 gb KMQ98097.1	155.90	3	3	1	N	82006	glycylpeptide n-tetradecanoyltransferase 1-like protein [Lasius niger]
4	8257	gi 826428058 ref XP_012527752.1	143.76	5	2	1	N	41397	PREDICTED: hyaluronidase-like [Monomorium pharaonis]
8	77	gi 1911819 gb AAB50883.1	65.59	10	1	1	N	11819	Myr p I=allergenic polypeptide {N-terminal} [Myrmecia pilosula=jumper ants, venom, Peptide Partial, 112 aa]
8	78	gi 312284 emb CAA49760.1	65.59	10	1	1	N	11849	major allergen [Myrmecia pilosula]
8	76	gi 730091 sp Q07932.1 MYR1_MYRPI	65.59	10	1	1	N	11849	RecName: Full=Pilosulin-1; AltName: Full=Allergen Myr p I; AltName: Full=Major allergen Myr p 1; AltName: Allergen=Myr p 1; Contains: RecName: Full=Pilosulin-1; Contains: RecName: Full=Pilosulin-1 65->112; Contains: RecNa...
total 5 proteins									

Band # 12 Proteins

Summary

1. Notes

2. Result Statistics

Figure 1. False discovery rate (FDR) curve. X axis is the number of peptide-spectrum matches (PSM) being kept. Y axis is the corresponding FDR.

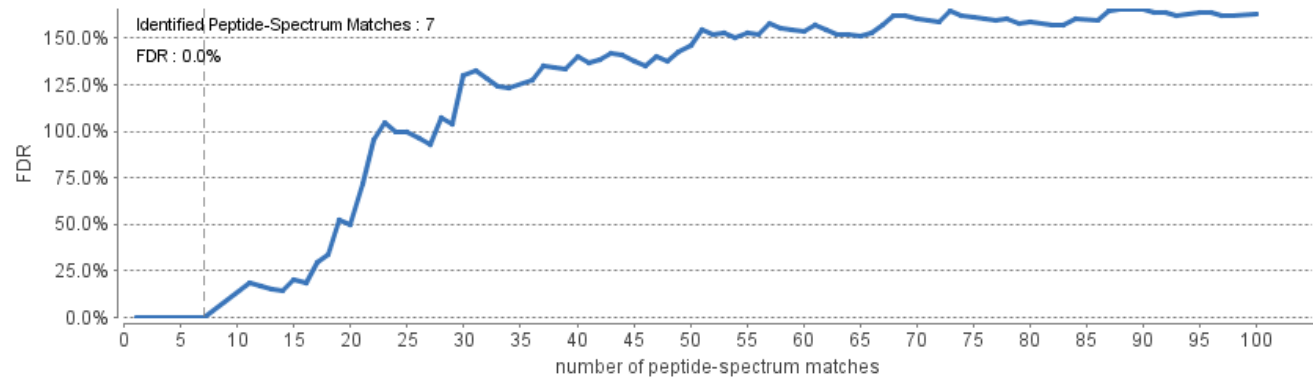


Figure 2. PSM score distribution. (a) Distribution of PEAKS peptide score; (b) Scatterplot of PEAKS peptide score versus precursor mass error.

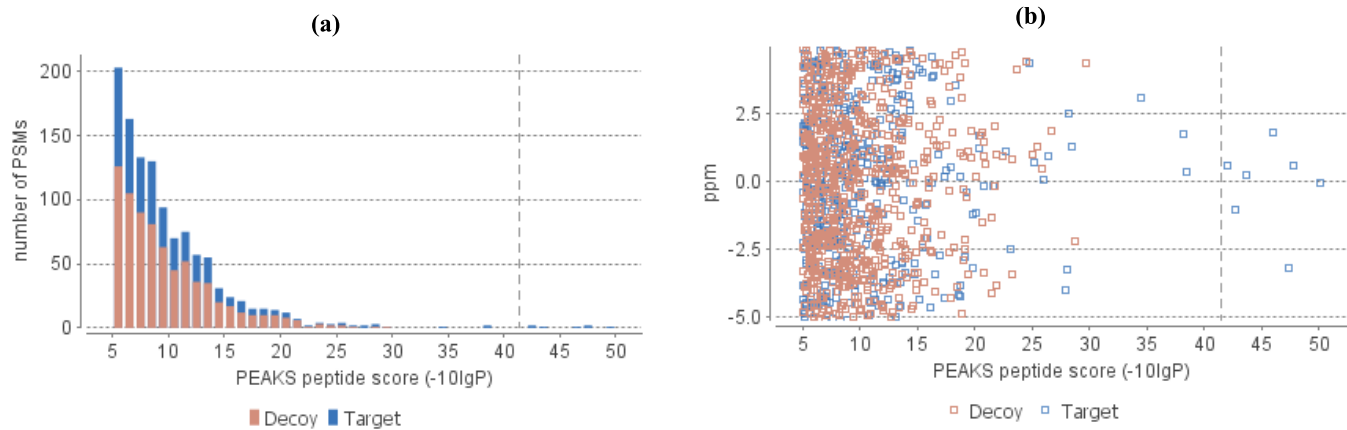


Figure 3. De novo result validation. Distribution of residue local confidence: (a) Residues in de novo sequences validated by confident database peptide assignment; (b) Residues in "de novo only" sequences.

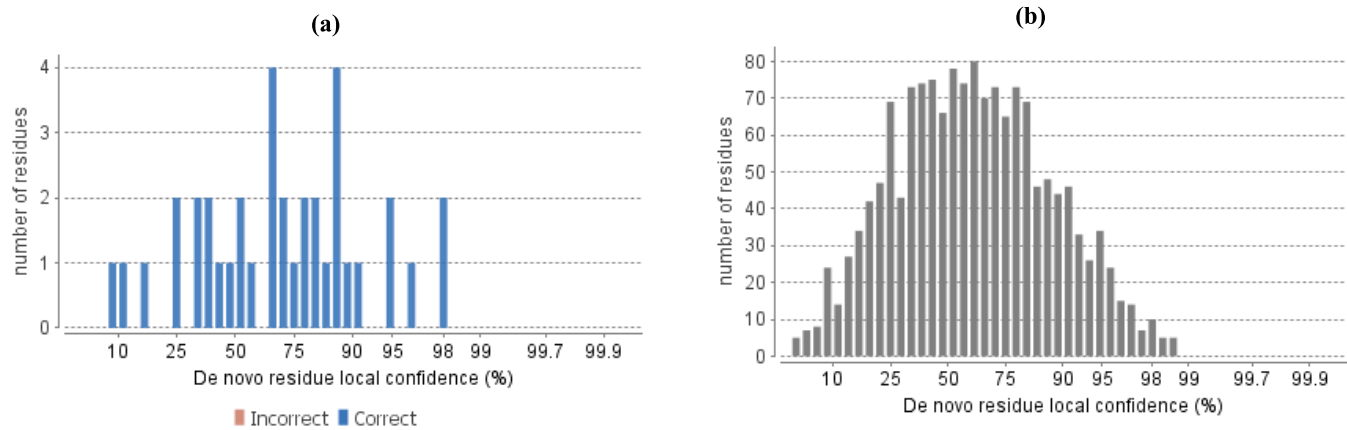


Table 1. Statistics of data.

# of MS Scans	1692
# of MS/MS Scans	3083

Table 4. PTM profile.

Name	Δ Mass	Position	#PSM	-10lgP	Area	AScore
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Table 2. Result filtration parameters.

Peptide -10lgP	≥41.4
Protein -10lgP	≥20
Proteins unique peptides	≥1
De novo ALC Score	≥50%

Table 3. Statistics of filtered result.

Peptide-Spectrum Matches	7
Peptide Sequences	6
Protein Groups	3
Proteins	52
Proteins (#Unique Peptides)	26 (>2); 0 (=2); 26 (=1);
FDR (Peptide-Spectrum Matches)	0.0%
FDR (Peptide Sequences)	0.0%
FDR (Protein)	0.0%
De Novo Only Spectra	145

3. Experiment Control

Figure 4. Precursor mass error of peptide-spectrum matches (PSM) in filtered result. **(a)** Distribution of precursor mass error in ppm; **(b)** Scatterplot of precursor m/z versus precursor mass error in ppm.

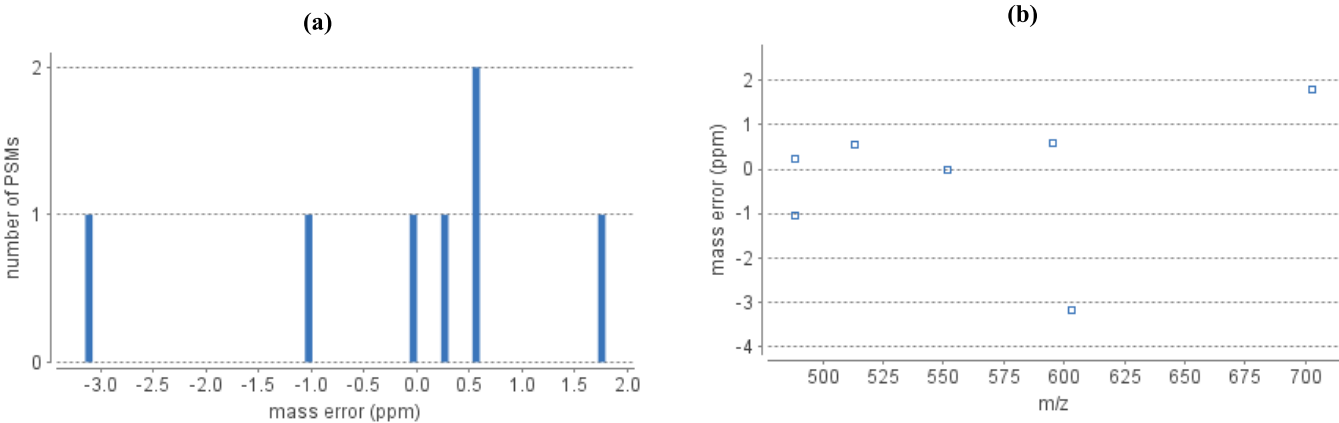


Table 5. Number of identified peptides in each sample by the number of missed cleavages

Missed Cleavages	0	1	2	3	4+
Sample 6	6	0	0	0	0

4. Other Information

Table 6. Search parameters.

Search Engine Name:	PEAKS
Parent Mass Error Tolerance:	5.0 ppm
Fragment Mass Error Tolerance:	0.5 Da
Precursor Mass Search Type:	monoisotopic
Enzyme:	Trypsin
Max Missed Cleavages:	3
Non-specific Cleavage:	one
Variable Modifications:	
Oxidation (M):	15.99
Max variable PTM per peptide:	3
Database:	Ant
Taxon:	All
Searched Entry:	473117
FDR Estimation:	Enabled
Merge Options:	no merge
Precursor Options:	corrected
Charge Options:	no correction

Table 7. Instrument parameters.

Fractions:	TW_12.raw
Ion Source:	ESI(nano-spray)
Fragmentation Mode:	CID, CAD(y and b ions)
MS Scan Mode:	FT-ICR/Orbitrap
MS/MS Scan Mode:	FT-ICR/Orbitrap

Filter Options: no filter

Process: true

Protein List

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
1	9817	gi 795085211 ref XP_011878235.1	81.87	7	3	3	N	50249	PREDICTED: elongation factor 1-alpha [Vollenhovia emeryi]
1	9818	gi 382930741 gb AFG30247.1	81.87	16	3	3	N	21061	elongation factor 1-alpha, partial [Camponotus claviscapus occultus]
1	9819	gi 54289426 gb AAV31963.1	81.87	14	3	3	N	23400	elongation factor 1-alpha, partial [Pogonomyrmex snellingi]
1	9820	gi 307715730 gb ABK54616.2	81.87	9	3	3	N	39176	elongation factor 1-alpha, partial [Forelius pruinus]
1	9821	gi 307715722 gb ABK54576.2	81.87	9	3	3	N	39152	elongation factor 1-alpha, partial [Anonychomyrma gilberti]
1	9822	gi 307715720 gb ABK54574.2	81.87	9	3	3	N	39178	elongation factor 1-alpha, partial [Aneuretus simoni]
1	9823	gi 307715738 gb ABK54632.2	81.87	9	3	3	N	39179	elongation factor 1-alpha, partial [Liometopum apiculatum]
1	9824	gi 307715732 gb ABK54628.2	81.87	9	3	3	N	39162	elongation factor 1-alpha, partial [Leptomyrmex sp. AUS01]
1	9825	gi 307715750 gb ABK54674.2	81.87	9	3	3	N	39152	elongation factor 1-alpha, partial [Philidris cordata]
1	9826	gi 307715744 gb ABK54646.2	81.87	9	3	3	N	39162	elongation factor 1-alpha, partial [Myrmecia pyriformis Smith, 1858]
1	9827	gi 307715748 gb ABK54668.2	81.87	9	3	3	N	39152	elongation factor 1-alpha, partial [Papyrus nitidus]
1	9828	gi 307715746 gb ABK54658.2	81.87	9	3	3	N	39162	elongation factor 1-alpha, partial [Nothomyrmecia macrops]
1	9829	gi 307715762 gb ABK54719.2	81.87	9	3	3	N	39152	elongation factor 1-alpha, partial [Turneria bidentata]
1	9830	gi 307715734 gb ABK54629.2	81.87	9	3	3	N	39162	elongation factor 1-alpha, partial [Leptomyrmex erythrocephalus]
1	9831	gi 307715726 gb ABK54608.2	81.87	9	3	3	N	39150	elongation factor 1-alpha, partial [Dolichoderus scabridus]
1	9832	gi 307715724 gb ABK54585.2	81.87	9	3	3	N	39162	elongation factor 1-alpha, partial [Azteca ovaticeps]
1	9833	gi 307715728 gb ABK54611.2	81.87	9	3	3	N	39162	elongation factor 1-alpha, partial [Dorymyrmex bicolor]
1	9834	gi 307715740 gb ABK54633.2	81.87	9	3	3	N	39179	elongation factor 1-alpha, partial [Liometopum occidentale]
1	9835	gi 307715754 gb ABK54707.2	81.87	9	3	3	N	39189	elongation factor 1-alpha, partial [Tapinoma sessile]
1	9836	gi 307715758 gb ABK54710.2	81.87	9	3	3	N	39179	elongation factor 1-alpha, partial [Technomyrmex sp. MAD05]
1	9837	gi 307715736 gb ABK54631.2	81.87	9	3	3	N	39162	elongation factor 1-alpha, partial [Linepithema humile]
1	9838	gi 307715752 gb ABK54697.2	81.87	9	3	3	N	39162	elongation factor 1-alpha, partial [Rhytidoponera chalybaea]
1	9839	gi 307715756 gb ABK54709.2	81.87	9	3	3	N	39189	elongation factor 1-alpha, partial [Technomyrmex difficilis]
1	9840	gi 307715760 gb ABK54716.2	81.87	9	3	3	N	39148	elongation factor 1-alpha, partial [Tetraponera rufonigra]
1	9841	gi 307715742 gb ABK54635.2	81.87	9	3	3	N	39162	elongation factor 1-alpha, partial [Manica bradleyi]
1	9842	gi 861617680 gb KM086643.1	81.87	7	3	3	N	50551	elongation factor 1-alpha isoform x1 [Lasius niger]
9	9843	gi 607368229 gb EZA62343.1	50.09	2	1	1	N	49146	putative citrate synthase 2, mitochondrial, partial [Cerapachys biroi]
9	1892	gi 307202019 gb EFN81583.1	50.09	2	1	1	N	49233	Probable citrate synthase 1, mitochondrial, partial [Harpegnathos saltator]
9	9844	gi 861640908 gb KM093360.1	50.09	2	1	1	N	49807	putative citrate synthase mitochondrial-like protein, partial [Lasius niger]
9	9845	gi 307170202 gb EFN62588.1	50.09	2	1	1	N	49842	Probable citrate synthase 2, mitochondrial, partial [Camponotus floridanus]
9	9846	gi 759034446 ref XP_011333847.1	50.09	2	1	1	N	50132	PREDICTED: probable citrate synthase 2, mitochondrial isoform X3 [Cerapachys biroi]
9	9847	gi 759034442 ref XP_011333831.1	50.09	2	1	1	N	51583	PREDICTED: probable citrate synthase 2, mitochondrial isoform X1 [Cerapachys biroi]
9	9848	gi 759034444 ref XP_011333839.1	50.09	2	1	1	N	51485	PREDICTED: probable citrate synthase 2, mitochondrial isoform X2 [Cerapachys biroi]
9	9849	gi 769861993 ref XP_011642787.1	50.09	2	1	1	N	51552	PREDICTED: probable citrate synthase 2, mitochondrial [Pogonomyrmex barbatus]
9	3240	gi 749778816 ref XP_011144055.1	50.09	2	1	1	N	51484	PREDICTED: probable citrate synthase 2, mitochondrial [Harpegnathos saltator]

total 52 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
9	9850	gi 752893067 ref XP_011264652.1	50.09	2	1	1	N	51748	PREDICTED: probable citrate synthase 2, mitochondrial [Camponotus floridanus]
9	9859	gi 322780854 gb EFZ10083.1	50.09	3	1	1	N	34209	hypothetical protein SINV_14511, partial [Solenopsis invicta]
9	9860	gi 1009356053 gb KYM81351.1	50.09	3	1	1	N	44053	putative citrate synthase 2, mitochondrial [Atta colombica]
9	9861	gi 1009408454 gb KYN27791.1	50.09	3	1	1	N	43962	putative citrate synthase 2, mitochondrial [Trachymyrmex cornetzi]
9	9862	gi 1009369545 gb KYM94163.1	50.09	3	1	1	N	43985	putative citrate synthase 2, mitochondrial [Cyphomyrmex costatus]
9	9863	gi 332029591 gb EGI69480.1	50.09	2	1	1	N	49078	Putative citrate synthase 1, mitochondrial, partial [Acromyrmex echinator]
9	9864	gi 1012982305 gb KYQ56115.1	50.09	2	1	1	N	50420	putative citrate synthase 2, mitochondrial, partial [Trachymyrmex zeteki]
9	9865	gi 780690656 ref XP_011699551.1	50.09	2	1	1	N	51496	PREDICTED: probable citrate synthase 2, mitochondrial [Wasmannia auropunctata]
9	9866	gi 746835345 ref XP_011068363.1	50.09	2	1	1	N	51485	PREDICTED: probable citrate synthase 2, mitochondrial [Acromyrmex echinator]
9	9867	gi 751236216 ref XP_011171933.1	50.09	2	1	1	N	51499	PREDICTED: probable citrate synthase 2, mitochondrial [Solenopsis invicta]
9	9868	gi 815792923 ref XP_012217071.1	50.09	2	1	1	N	51445	PREDICTED: probable citrate synthase 2, mitochondrial [Linepithema humile]
9	9869	gi 795050045 ref XP_011869746.1	50.09	2	1	1	N	51552	PREDICTED: probable citrate synthase 2, mitochondrial [Vollenhovia emeryi]
9	9870	gi 801392694 ref XP_012057948.1	50.09	2	1	1	N	51711	PREDICTED: probable citrate synthase 2, mitochondrial [Atta cephalotes]
9	9871	gi 826409340 ref XP_012532069.1	50.09	2	1	1	N	52359	PREDICTED: probable citrate synthase 2, mitochondrial, partial [Monomorium pharaonis]
2	77	gi 1911819 gb AAB50883.1	47.81	10	1	1	Y	11819	Myr p I=allergenic polypeptide {N-terminal} [Myrmecia pilosula=jumper ants, venom, Peptide Partial, 112 aa]
2	78	gi 312284 emb CAA49760.1	47.81	10	1	1	Y	11849	major allergen [Myrmecia pilosula]
2	76	gi 730091 sp Q07932.1 MYR1_MYRPI	47.81	10	1	1	Y	11849	RecName: Full=Pilosulin-1; AltName: Full=Allergen Myr p I; AltName: Full=Major allergen Myr p 1; AltName: Allergen=Myr p 1; Contains: RecName: Full=Pilosulin-1; Contains: RecName: Full=Pilosulin-1 65->112; Contains: RecNa...
total 52 proteins									

Band # 13 Proteins

Summary

1. Notes

2. Result Statistics

Figure 1. False discovery rate (FDR) curve. X axis is the number of peptide-spectrum matches (PSM) being kept. Y axis is the corresponding FDR.

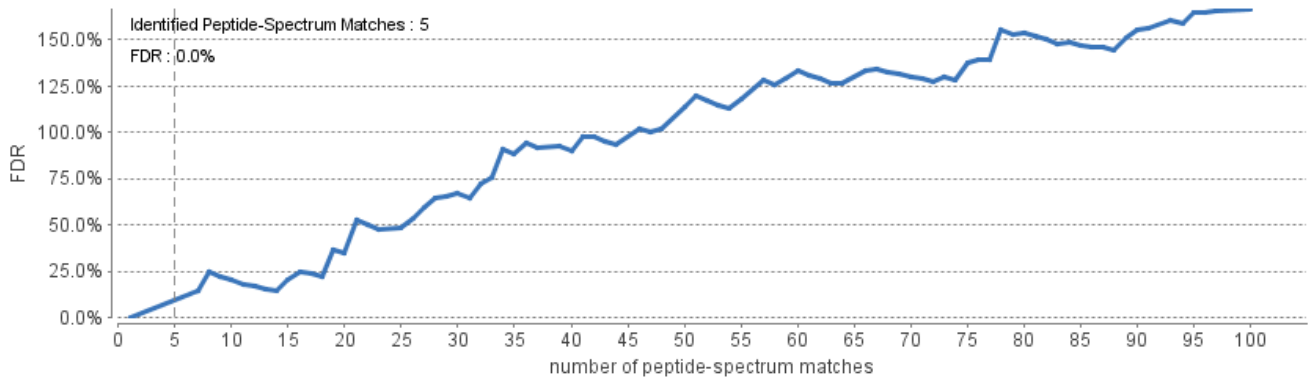


Figure 2. PSM score distribution. (a) Distribution of PEAKS peptide score; (b) Scatterplot of PEAKS peptide score versus precursor mass error.

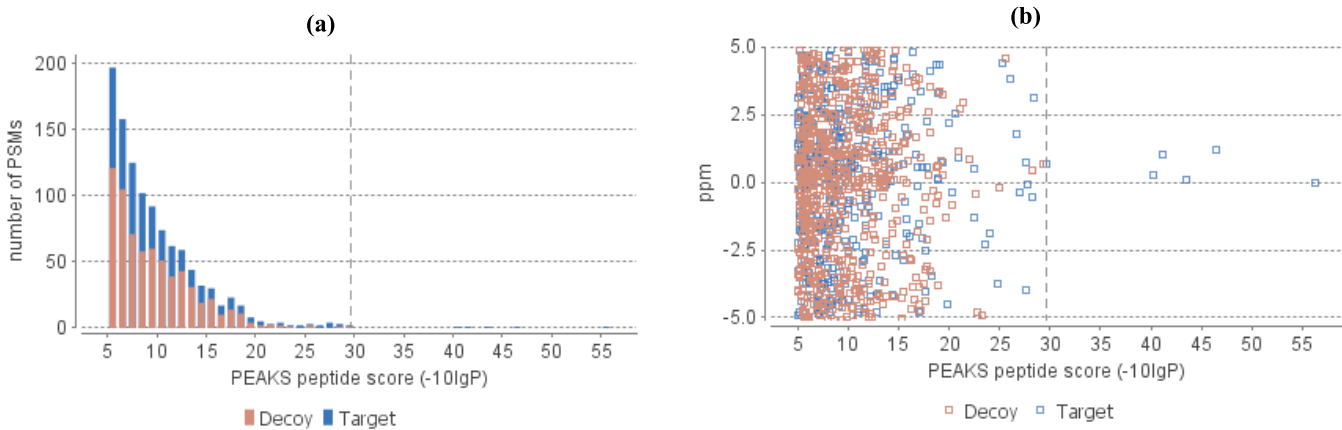


Figure 3. De novo result validation. Distribution of residue local confidence: (a) Residues in de novo sequences validated by confident database peptide assignment; (b) Residues in "de novo only" sequences.

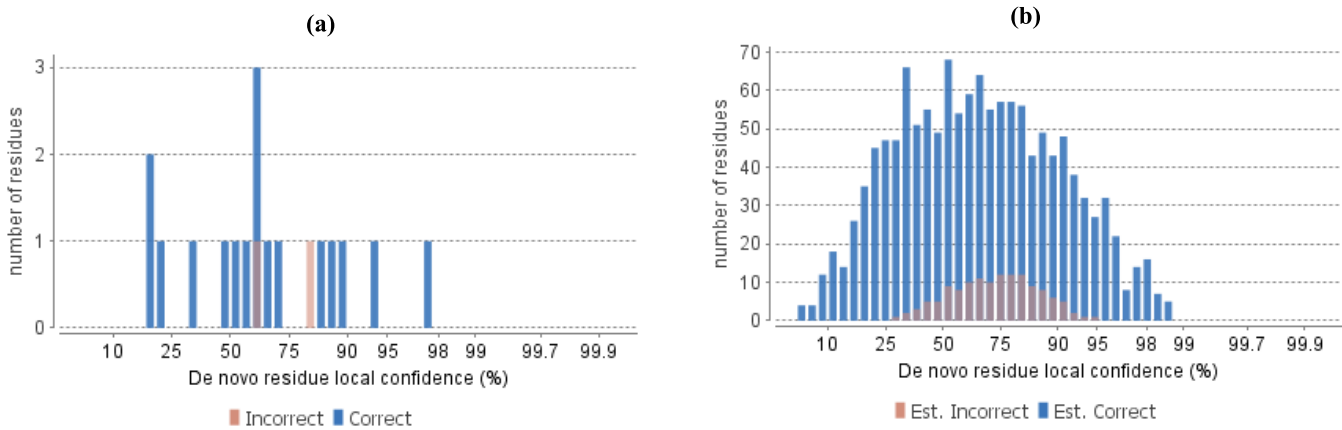


Table 1. Statistics of data.

# of MS Scans	1688
# of MS/MS Scans	3036

Table 4. PTM profile.

Name	Δ Mass	Position	#PSM	-10lgP	Area	AScore
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Table 2. Result filtration parameters.

Peptide -10lgP	≥29.7
Protein -10lgP	≥20
Proteins unique peptides	≥1
De novo ALC Score	≥50%

Table 3. Statistics of filtered result.

Peptide-Spectrum Matches	5
Peptide Sequences	5
Protein Groups	2
Proteins	33
Proteins (#Unique Peptides)	0 (>2); 30 (=2); 3 (=1);
FDR (Peptide-Spectrum Matches)	0.0%
FDR (Peptide Sequences)	0.0%
FDR (Protein)	0.0%
De Novo Only Spectra	137

3. Experiment Control

Figure 4. Precursor mass error of peptide-spectrum matches (PSM) in filtered result. (a) Distribution of precursor mass error in ppm; (b) Scatterplot of precursor m/z versus precursor mass error in ppm.

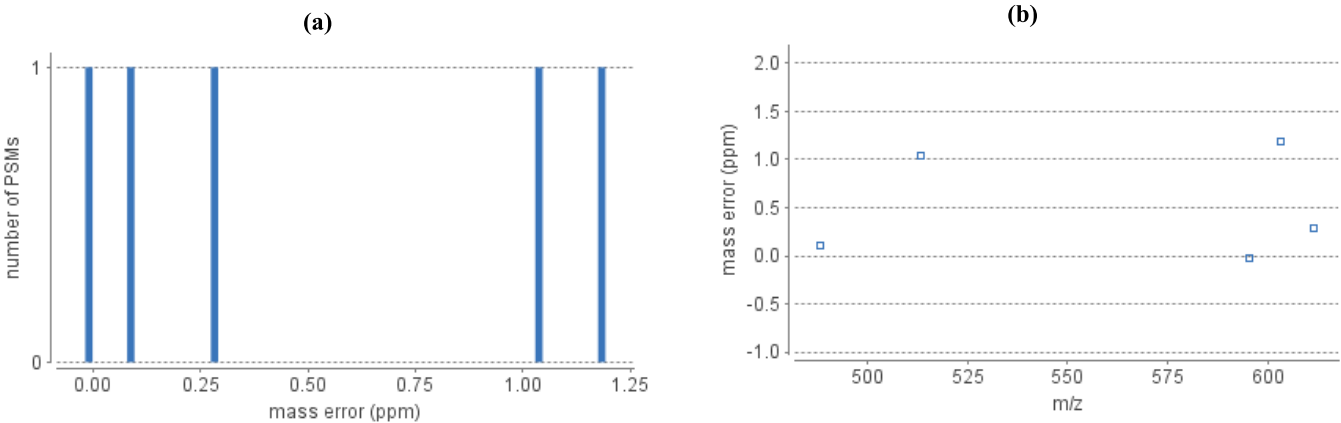


Table 5. Number of identified peptides in each sample by the number of missed cleavages

Missed Cleavages	0	1	2	3	4+
Sample 7	5	0	0	0	0

4. Other Information

Table 6. Search parameters.

Search Engine Name:	PEAKS
Parent Mass Error Tolerance:	5.0 ppm
Fragment Mass Error Tolerance:	0.5 Da
Precursor Mass Search Type:	monoisotopic
Enzyme:	Trypsin
Max Missed Cleavages:	3
Non-specific Cleavage:	one
Variable Modifications:	
Oxidation (M):	15.99
Max variable PTM per peptide:	3
Database:	Ant
Taxon:	All
Searched Entry:	473117
FDR Estimation:	Enabled
Merge Options:	no merge
Precursor Options:	corrected
Charge Options:	no correction

Table 7. Instrument parameters.

Fractions:	TW_13.raw
Ion Source:	ESI(nano-spray)
Fragmentation Mode:	CID, CAD(y and b ions)
MS Scan Mode:	FT-ICR/Orbitrap
MS/MS Scan Mode:	FT-ICR/Orbitrap

Filter Options: no filter

Process: true

Protein List

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
4	9851	gi 407021090 gb AFS65405.1	63.99	16	2	2	N	13104	elongation factor 1-alpha, partial [Pseudolaius typhlops]
4	9852	gi 407021072 gb AFS65396.1	63.99	7	2	2	N	28137	elongation factor 1-alpha, partial [Paraparatrechina sp. PHL02]
4	9853	gi 407021088 gb AFS65404.1	63.99	7	2	2	N	28137	elongation factor 1-alpha, partial [Pseudolaius sp. PHL01]
4	9854	gi 407021093 gb AFS65407.1	63.99	7	2	2	N	28137	elongation factor 1-alpha, partial [Zatania cisipa]
4	9855	gi 407021076 gb AFS65398.1	63.99	7	2	2	N	28075	elongation factor 1-alpha, partial [Paratrechina longicornis]
4	9856	gi 460422929 gb AGH12537.1	63.99	7	2	2	N	28137	elongation factor 1-alpha F1, partial [Nylanderia fulva]
4	9857	gi 407021097 gb AFS65409.1	63.99	7	2	2	N	28137	elongation factor 1-alpha, partial [Zatania gloriosa]
4	9858	gi 407021082 gb AFS65401.1	63.99	7	2	2	N	28137	elongation factor 1-alpha, partial [Prenolepis sp. PHL02]
4	9820	gi 307715730 gb ABK54616.2	63.99	5	2	2	N	39176	elongation factor 1-alpha, partial [Forelius pruinus]
4	9821	gi 307715722 gb ABK54576.2	63.99	5	2	2	N	39152	elongation factor 1-alpha, partial [Anonymomyrma gilberti]
4	9822	gi 307715720 gb ABK54574.2	63.99	5	2	2	N	39178	elongation factor 1-alpha, partial [Aneuretus simoni]
4	9823	gi 307715738 gb ABK54632.2	63.99	5	2	2	N	39179	elongation factor 1-alpha, partial [Liometopum apiculatum]
4	9824	gi 307715732 gb ABK54628.2	63.99	5	2	2	N	39162	elongation factor 1-alpha, partial [Leptomyrmex sp. AUS01]
4	9825	gi 307715750 gb ABK54674.2	63.99	5	2	2	N	39152	elongation factor 1-alpha, partial [Philidris cordata]
4	9826	gi 307715744 gb ABK54646.2	63.99	5	2	2	N	39162	elongation factor 1-alpha, partial [Myrmecia pyriformis Smith, 1858]
4	9827	gi 307715748 gb ABK54668.2	63.99	5	2	2	N	39152	elongation factor 1-alpha, partial [Papyrus nitidus]
4	9828	gi 307715746 gb ABK54658.2	63.99	5	2	2	N	39162	elongation factor 1-alpha, partial [Nothomyrmecia macrops]
4	9829	gi 307715762 gb ABK54719.2	63.99	5	2	2	N	39152	elongation factor 1-alpha, partial [Turneria bidentata]
4	9830	gi 307715734 gb ABK54629.2	63.99	5	2	2	N	39162	elongation factor 1-alpha, partial [Leptomyrmex erythrocephalus]
4	9831	gi 307715726 gb ABK54608.2	63.99	5	2	2	N	39150	elongation factor 1-alpha, partial [Dolichoderus scabridus]
4	9832	gi 307715724 gb ABK54585.2	63.99	5	2	2	N	39162	elongation factor 1-alpha, partial [Azteca ovaticeps]
4	9833	gi 307715728 gb ABK54611.2	63.99	5	2	2	N	39162	elongation factor 1-alpha, partial [Dorymyrmex bicolor]
4	9834	gi 307715740 gb ABK54633.2	63.99	5	2	2	N	39179	elongation factor 1-alpha, partial [Liometopum occidentale]
4	9835	gi 307715754 gb ABK54707.2	63.99	5	2	2	N	39189	elongation factor 1-alpha, partial [Tapinoma sessile]
4	9836	gi 307715758 gb ABK54710.2	63.99	5	2	2	N	39179	elongation factor 1-alpha, partial [Technomyrmex sp. MAD05]
4	9837	gi 307715736 gb ABK54631.2	63.99	5	2	2	N	39162	elongation factor 1-alpha, partial [Linepithema humile]
4	9838	gi 307715752 gb ABK54697.2	63.99	5	2	2	N	39162	elongation factor 1-alpha, partial [Rhytidoponera chalybaea]
4	9839	gi 307715756 gb ABK54709.2	63.99	5	2	2	N	39189	elongation factor 1-alpha, partial [Technomyrmex difficilis]
4	9840	gi 307715760 gb ABK54716.2	63.99	5	2	2	N	39148	elongation factor 1-alpha, partial [Tetraponera rufonigra]
4	9841	gi 307715742 gb ABK54635.2	63.99	5	2	2	N	39162	elongation factor 1-alpha, partial [Manica bradleyi]
1	77	gi 1911819 gb AAB50883.1	56.25	10	1	1	Y	11819	Myr p I=allergenic polypeptide {N-terminal} [Myrmecia pilosula=jumper ants, venom, Peptide Partial, 112 aa]
1	78	gi 312284 emb CAA49760.1	56.25	10	1	1	Y	11849	major allergen [Myrmecia pilosula]
1	76	gi 730091 sp Q07932.1 MYR1_MYRPI	56.25	10	1	1	Y	11849	RecName: Full=Pilosulin-1; AltName: Full=Allergen Myr p I; AltName: Full=Major allergen Myr p I; AltName: Allergen=Myr p I; Contains: RecName: Full=Pilosulin-1; Contains: RecName: Full=Pilosulin-1 65->112; Contains: RecNa...
total 33 proteins									

Band # 14 Proteins

Summary

1. Notes

2. Result Statistics

Figure 1. False discovery rate (FDR) curve. X axis is the number of peptide-spectrum matches (PSM) being kept. Y axis is the corresponding FDR.

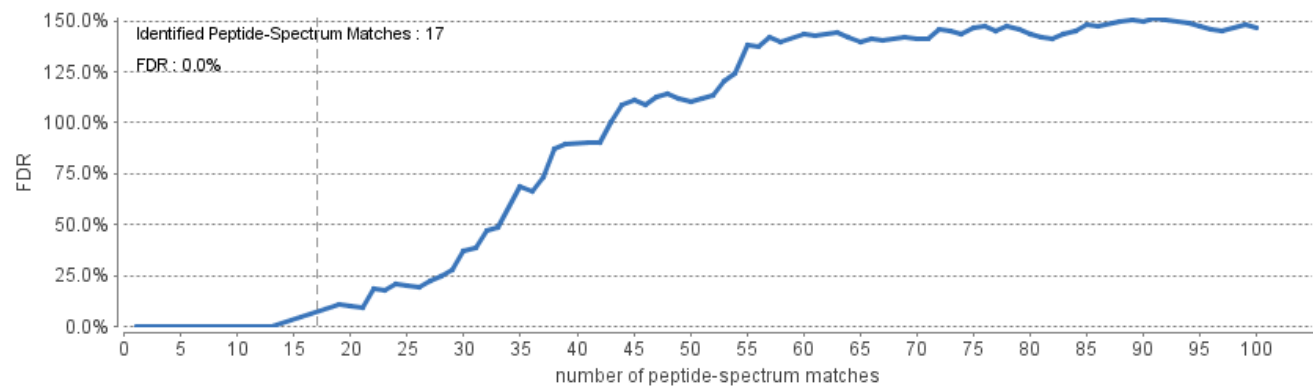


Figure 2. PSM score distribution. (a) Distribution of PEAKS peptide score; (b) Scatterplot of PEAKS peptide score versus precursor mass error.

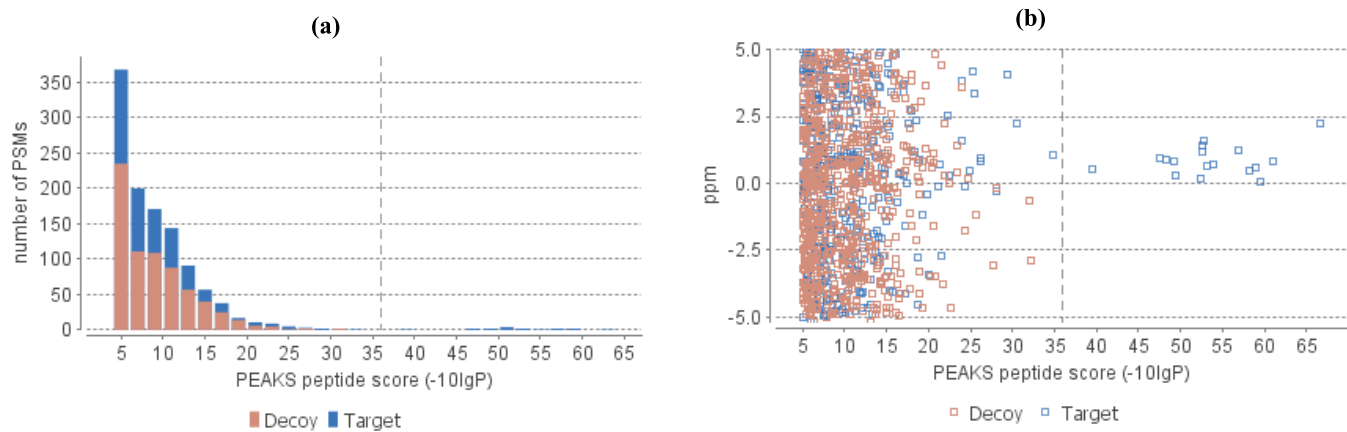


Figure 3. De novo result validation. Distribution of residue local confidence: (a) Residues in de novo sequences validated by confident database peptide assignment; (b) Residues in "de novo only" sequences.

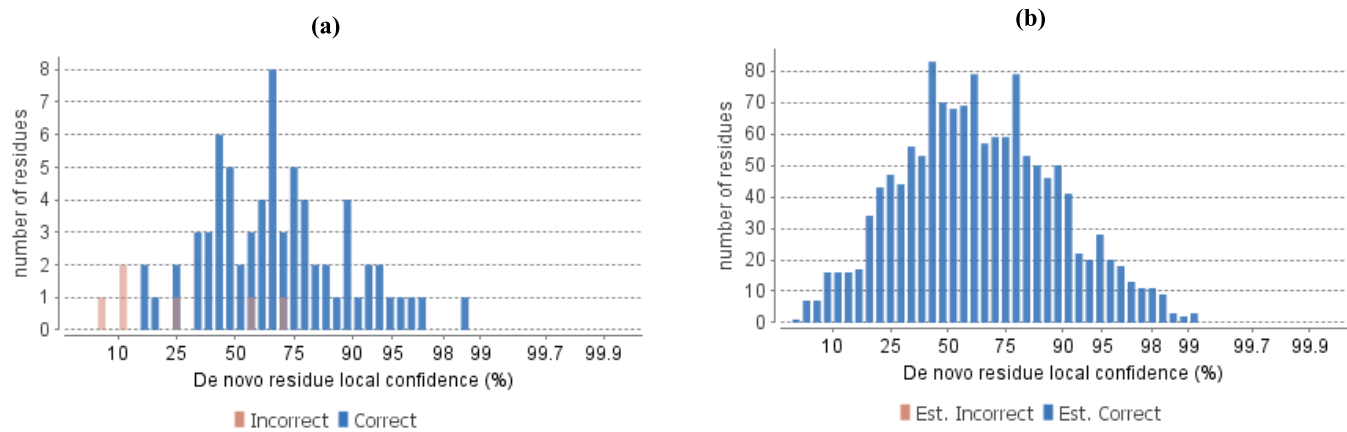


Table 1. Statistics of data.

# of MS Scans	1683
# of MS/MS Scans	3024

Table 4. PTM profile.

Name	Δ Mass	Position	#PSM	-10lgP	Area	AScore
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Table 2. Result filtration parameters.

Peptide -10lgP	≥35.9
Protein -10lgP	≥20
Proteins unique peptides	≥1
De novo ALC Score	≥50%

Table 3. Statistics of filtered result.

Peptide-Spectrum Matches	17
Peptide Sequences	17
Protein Groups	7
Proteins	66
Proteins (#Unique Peptides)	13 (>2); 0 (=2); 53 (=1);
FDR (Peptide-Spectrum Matches)	0.0%
FDR (Peptide Sequences)	0.0%
FDR (Protein)	0.0%
De Novo Only Spectra	131

3. Experiment Control

Figure 4. Precursor mass error of peptide-spectrum matches (PSM) in filtered result. **(a)** Distribution of precursor mass error in ppm; **(b)** Scatterplot of precursor m/z versus precursor mass error in ppm. 

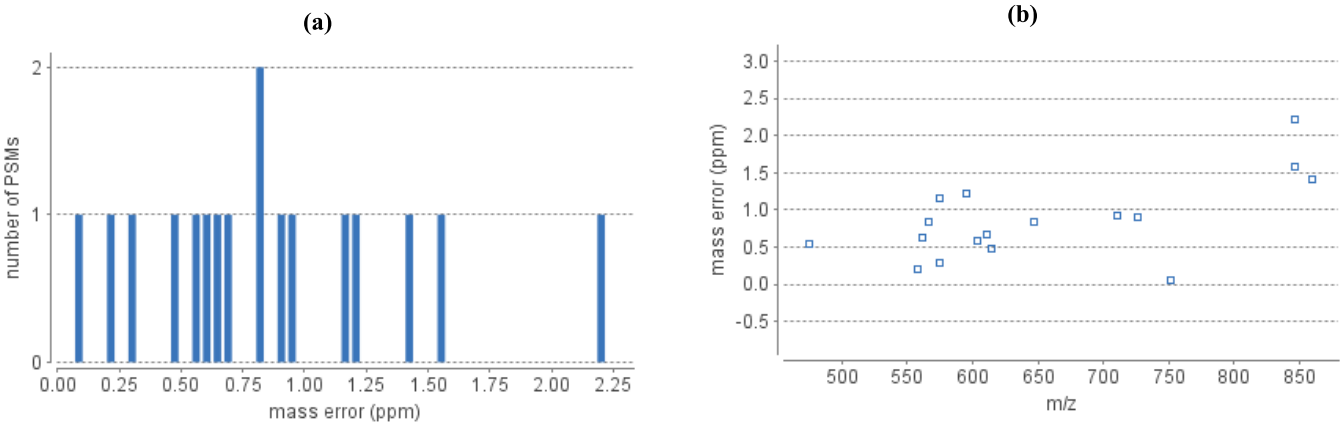


Table 5. Number of identified peptides in each sample by the number of missed cleavages

Missed Cleavages	0	1	2	3	4+
Sample 8	16	1	0	0	0

4. Other Information

Table 6. Search parameters.

Search Engine Name:	PEAKS
Parent Mass Error Tolerance:	5.0 ppm
Fragment Mass Error Tolerance:	0.5 Da
Precursor Mass Search Type:	monoisotopic
Enzyme:	Trypsin
Max Missed Cleavages:	3
Non-specific Cleavage:	one
Variable Modifications:	
Oxidation (M):	15.99
Max variable PTM per peptide:	3
Database:	Ant
Taxon:	All
Searched Entry:	473117
FDR Estimation:	Enabled
Merge Options:	no merge
Precursor Options:	corrected
Charge Options:	no correction

Table 7. Instrument parameters.

Fractions:	TW_14.raw
Ion Source:	ESI(nano-spray)
Fragmentation Mode:	CID, CAD(y and b ions)
MS Scan Mode:	FT-ICR/Orbitrap
MS/MS Scan Mode:	FT-ICR/Orbitrap

Filter Options: no filter

Process: true

Protein List

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
2	20915	gi 751230077 ref XP_011168531.1	138.61	10	5	5	Y	71166	PREDICTED: heat shock 70 kDa protein cognate 4 [Solenopsis invicta]
2	20916	gi 815771288 ref XP_012235802.1	138.61	10	5	5	Y	71165	PREDICTED: heat shock 70 kDa protein cognate 4 [Linepithema humile]
2	20917	gi 780624956 ref XP_011708184.1	138.61	10	5	5	Y	71152	PREDICTED: heat shock 70 kDa protein cognate 4 [Wasmannia auropunctata]
2	20918	gi 795030306 ref XP_011863236.1	138.61	10	5	5	Y	71179	PREDICTED: heat shock 70 kDa protein cognate 4 [Vollenhovia emeryi]
2	20171	gi 826471967 ref XP_012536319.1	138.61	10	5	5	Y	70909	PREDICTED: LOW QUALITY PROTEIN: heat shock 70 kDa protein cognate 4-like [Monomorium pharaonis]
2	20919	gi 769842700 ref XP_011632552.1	138.61	10	5	5	Y	71223	PREDICTED: heat shock 70 kDa protein cognate 4 [Pogonomyrmex barbatus]
2	20920	gi 861623393 gb KMQ87979.1	138.61	10	5	5	Y	71308	heat shock 70 kda protein cognate 4 [Lasius niger]
2	20921	gi 752884487 ref XP_011259986.1	138.61	10	5	5	Y	71368	PREDICTED: heat shock 70 kDa protein cognate 4 [Camponotus floridanus]
2	20922	gi 451173139 gb AGF33487.1	138.61	10	5	5	Y	71424	heat shock cognate 70 [Polyrhachis vicina]
2	20923	gi 307176326 gb EFN65945.1	138.61	10	5	5	Y	71368	Heat shock 70 kDa protein cognate 4 [Camponotus floridanus]
1	20912	gi 951526129 ref XP_014467326.1	133.36	16	5	5	N	39712	PREDICTED: arginine kinase isoform X2 [Dinoponera quadricaps]
1	20913	gi 951526126 ref XP_014467325.1	133.36	16	5	5	N	39712	PREDICTED: arginine kinase isoform X2 [Dinoponera quadricaps]
1	20914	gi 951526124 ref XP_014467324.1	133.36	16	5	5	N	41640	PREDICTED: arginine kinase isoform X1 [Dinoponera quadricaps]
3	77	gi 1911819 gb AAB50883.1	58.96	10	1	1	Y	11819	Myr p I=allergenic polypeptide {N-termina l} [Myrmecia pilosula=jumper ants, venom, Peptide Partial, 112 aa]
3	78	gi 312284 emb CAA49760.1	58.96	10	1	1	Y	11849	major allergen [Myrmecia pilosula]
3	76	gi 730091 sp Q07932.1 MYR1_MYRPI	58.96	10	1	1	Y	11849	RecName: Full=Pilosulin-1; AltName: Full=Allergen Myr p I; AltName: Full=Major allergen Myr p I; AltName: Allergen=Myr p I; Contains: RecName: Full=Pilosulin-1; Contains: RecName: Full=Pilosulin-1 65->112; Contains: RecNa...
36	21037	gi 780633339 ref XP_011686024.1	49.33	3	1	1	N	38487	PREDICTED: aldose 1-epimerase isoform X2 [Wasmannia auropunctata]
36	21038	gi 780633331 ref XP_011686022.1	49.33	3	1	1	N	38487	PREDICTED: aldose 1-epimerase isoform X2 [Wasmannia auropunctata]
36	21039	gi 780633335 ref XP_011686023.1	49.33	3	1	1	N	38487	PREDICTED: aldose 1-epimerase isoform X2 [Wasmannia auropunctata]
36	21040	gi 780633327 ref XP_011686021.1	49.33	3	1	1	N	38487	PREDICTED: aldose 1-epimerase isoform X2 [Wasmannia auropunctata]
36	21041	gi 780633322 ref XP_011686020.1	49.33	3	1	1	N	40448	PREDICTED: aldose 1-epimerase isoform X1 [Wasmannia auropunctata]
37	11323	gi 746830005 ref XP_011060669.1	49.18	5	1	1	N	21366	PREDICTED: actin-5, muscle-specific-like, partial [Acromyrmex echinator]
37	11160	gi 759032952 ref XP_011334617.1	49.18	3	1	1	N	41770	PREDICTED: actin, clone 205 [Ceraopachys biro]
37	5591	gi 751239306 ref XP_011173634.1	49.18	3	1	1	N	41783	PREDICTED: actin-5, muscle-specific [Solenopsis invicta]
37	5565	gi 749754572 ref XP_011139727.1	49.18	3	1	1	N	41822	PREDICTED: actin-5C [Harpegnathos saltator]
37	5593	gi 752898359 ref XP_011267531.1	49.18	3	1	1	N	41783	PREDICTED: actin-5, muscle-specific [Camponotus floridanus]
37	5566	gi 751198952 ref XP_011173672.1	49.18	3	1	1	N	41822	PREDICTED: actin-5C [Solenopsis invicta]
37	5594	gi 752898361 ref XP_011267532.1	49.18	3	1	1	N	41783	PREDICTED: actin-5, muscle-specific [Camponotus floridanus]
37	11161	gi 752898367 ref XP_011267535.1	49.18	3	1	1	N	41756	PREDICTED: actin, muscle [Camponotus floridanus]
37	5567	gi 752879620 ref XP_011257343.1	49.18	3	1	1	N	41822	PREDICTED: actin-5C [Camponotus floridanus]
37	5595	gi 749790975 ref XP_011148680.1	49.18	3	1	1	N	41783	PREDICTED: actin-5, muscle-specific [Harpegnathos saltator]
37	5568	gi 746842703 ref XP_011051576.1	49.18	3	1	1	N	41822	PREDICTED: actin-5C [Acromyrmex echinator]
37	5596	gi 607368824 gb EZA62930.1	49.18	3	1	1	N	41774	Actin, muscle [Ceraopachys biro]
37	5569	gi 260401142 gb ACX37099.1	49.18	3	1	1	N	41792	beta actin [Polyrhachis vicina]
37	5598	gi 751239318 ref XP_011173641.1	49.18	3	1	1	N	41783	PREDICTED: actin-5, muscle-specific [Solenopsis invicta]

total 66 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
37	5599	gi 607368821 gb EZA62927.1	49.18	3	1	1	N	41770	Actin, clone [Ceropachys biroï]
37	5600	gi 327387361 gb AEA72282.1	49.18	3	1	1	N	41783	actin-87E isoform 1 [Solenopsis invicta]
37	5570	gi 607362215 gb EZA56475.1	49.18	3	1	1	N	41822	Actin-5C [Ceropachys biroï]
37	11162	gi 752898365 ref XP_011267534.1	49.18	3	1	1	N	41756	PREDICTED: actin, muscle [Camponotus fl oridanus]
37	5602	gi 746849933 ref XP_011055428.1	49.18	3	1	1	N	41745	PREDICTED: actin-5, muscle-specific-like [Acromyrmex echinator]
37	5603	gi 751239316 ref XP_011173639.1	49.18	3	1	1	N	41758	PREDICTED: actin, muscle [Solenopsis invi cta]
37	5604	gi 746849931 ref XP_011055426.1	49.18	3	1	1	N	41684	PREDICTED: actin-5, muscle-specific [Acro myrmex echinator]
37	5571	gi 746842701 ref XP_011051575.1	49.18	3	1	1	N	41822	PREDICTED: actin-5C [Acromyrmex echina tior]
37	5636	gi 749793865 ref XP_011150241.1	49.18	3	1	1	N	41890	PREDICTED: actin-5C-like [Harpegnathos s altator]
37	5572	gi 751198954 ref XP_011173741.1	49.18	3	1	1	N	41822	PREDICTED: actin-5C [Solenopsis invicta]
37	5573	gi 752879618 ref XP_011257342.1	49.18	3	1	1	N	41822	PREDICTED: actin-5C [Camponotus florida nus]
37	5605	gi 752898363 ref XP_011267533.1	49.18	3	1	1	N	41783	PREDICTED: actin-5, muscle-specific [Cam ponotus floridanus]
37	11179	gi 759032950 ref XP_011334490.1	49.18	3	1	1	N	41774	PREDICTED: actin, muscle [Ceropachys bir oi]
37	5574	gi 749754574 ref XP_011139728.1	49.18	3	1	1	N	41822	PREDICTED: actin-5C [Harpegnathos saltat or]
37	5606	gi 749790980 ref XP_011148681.1	49.18	3	1	1	N	41783	PREDICTED: actin-5, muscle-specific [Harp egnathos saltator]
37	5607	gi 607368823 gb EZA62929.1	49.18	3	1	1	N	43729	Actin, muscle [Ceropachys biroï]
4	64	gi 751219056 ref XP_011162596.1	47.61	6	1	1	N	25498	PREDICTED: acidic phospholipase A2 PA4 i soform X2 [Solenopsis invicta]
4	65	gi 769852445 ref XP_011637691.1	47.61	6	1	1	N	25718	PREDICTED: acidic phospholipase A2 PA4 i soform X2 [Pogonomyrmex barbatus]
4	66	gi 607361739 gb EZA56014.1	47.61	6	1	1	N	25661	Group 3 secretory phospholipase A2 [Cera pachys biroï]
4	67	gi 780637978 ref XP_011687259.1	47.61	6	1	1	N	26007	PREDICTED: phospholipase A2 isozymes P A3A/PA3B/PA5 isoform X2 [Wasmannia aur opunctata]
4	68	gi 769852443 ref XP_011637690.1	47.61	6	1	1	N	27251	PREDICTED: acidic phospholipase A2 PA4 i soform X1 [Pogonomyrmex barbatus]
4	69	gi 751219054 ref XP_011162595.1	47.61	6	1	1	N	28045	PREDICTED: uncharacterized protein LOC1 05197765 isoform X1 [Solenopsis invicta]
4	70	gi 759054210 ref XP_011336300.1	47.61	6	1	1	N	28030	PREDICTED: uncharacterized protein LOC1 05278712 isoform X3 [Ceropachys biroï]
4	71	gi 759054208 ref XP_011336299.1	47.61	5	1	1	N	28800	PREDICTED: uncharacterized protein LOC1 05278712 isoform X2 [Ceropachys biroï]
4	73	gi 780637966 ref XP_011687254.1	47.61	5	1	1	N	28793	PREDICTED: uncharacterized protein LOC1 05449644 isoform X1 [Wasmannia auropu nctata]
4	72	gi 780637974 ref XP_011687258.1	47.61	5	1	1	N	28793	PREDICTED: uncharacterized protein LOC1 05449644 isoform X1 [Wasmannia auropu nctata]
4	74	gi 780637970 ref XP_011687255.1	47.61	5	1	1	N	28793	PREDICTED: uncharacterized protein LOC1 05449644 isoform X1 [Wasmannia auropu nctata]
4	75	gi 759054206 ref XP_011336298.1	47.61	5	1	1	N	31169	PREDICTED: uncharacterized protein LOC1 05278712 isoform X1 [Ceropachys biroï]
38	21043	gi 307170284 gb EFN62639.1	39.41	2	1	1	N	42176	Serine protease easter [Camponotus florid anus]
38	21044	gi 861649233 gb KMQ96720.1	39.41	2	1	1	N	42943	serine protease easter [Lasius niger]
38	21045	gi 752892972 ref XP_011264599.1	39.41	1	1	1	N	122343	PREDICTED: transmembrane protease seri ne 9-like [Camponotus floridanus]
total 66 proteins									

Band # 15 Proteins

Summary

1. Notes

2. Result Statistics

Figure 1. False discovery rate (FDR) curve. X axis is the number of peptide-spectrum matches (PSM) being kept. Y axis is the corresponding FDR.

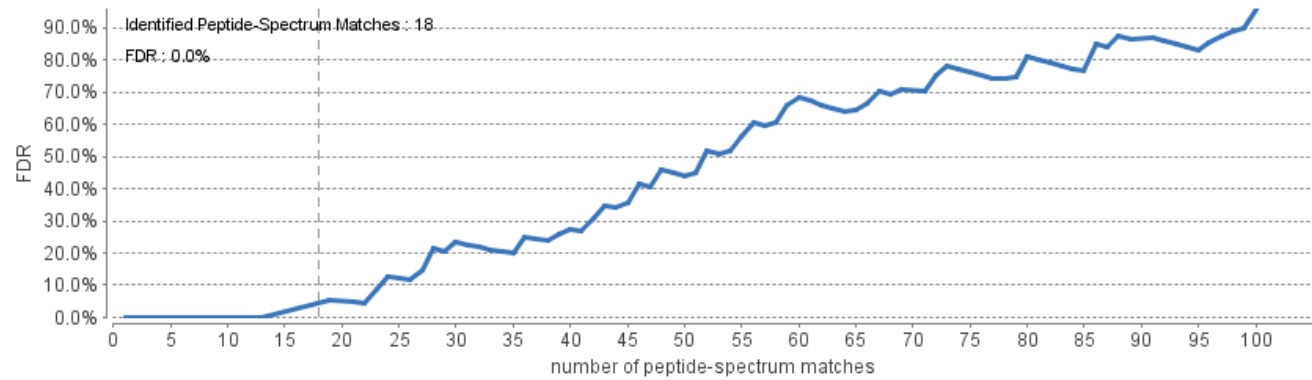


Figure 2. PSM score distribution. (a) Distribution of PEAKS peptide score; (b) Scatterplot of PEAKS peptide score versus precursor mass error.

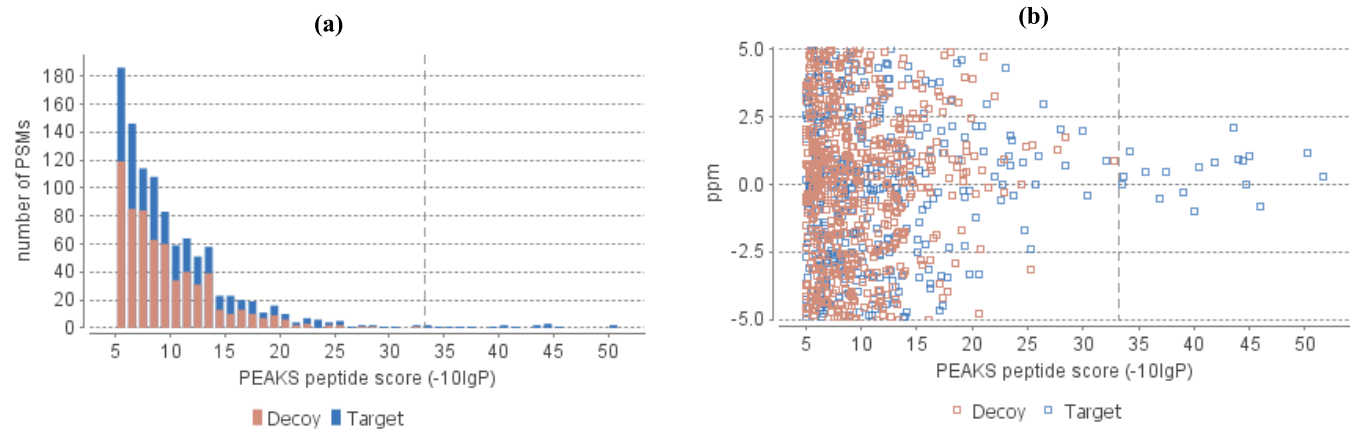


Figure 3. De novo result validation. Distribution of residue local confidence: (a) Residues in de novo sequences validated by confident database peptide assignment; (b) Residues in "de novo only" sequences.

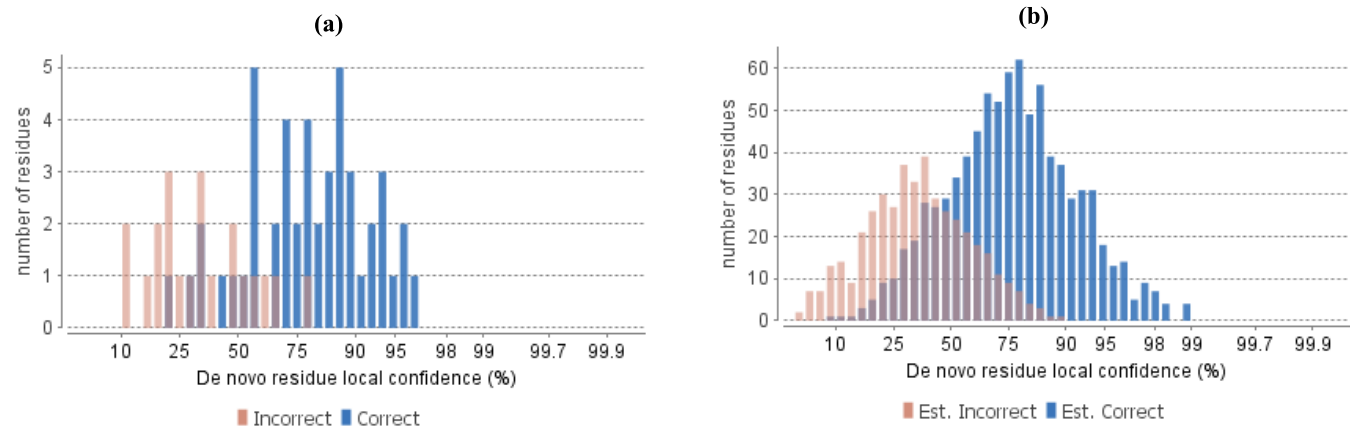


Table 1. Statistics of data.

# of MS Scans	1752
# of MS/MS Scans	2671

Table 4. PTM profile.

Name	Δ Mass	Position	#PSM	-10lgP	Area	AScore
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Table 2. Result filtration parameters.

Peptide -10lgP	≥33.2
Protein -10lgP	≥20
Proteins unique peptides	≥1
De novo ALC Score	≥50%

Table 3. Statistics of filtered result.

Peptide-Spectrum Matches	18
Peptide Sequences	18
Protein Groups	9
Proteins	72
Proteins (#Unique Peptides)	49 (>2); 5 (=2); 18 (=1);
FDR (Peptide-Spectrum Matches)	0.0%
FDR (Peptide Sequences)	0.0%
FDR (Protein)	0.0%
De Novo Only Spectra	119

3. Experiment Control

Figure 4. Precursor mass error of peptide-spectrum matches (PSM) in filtered result. **(a)** Distribution of precursor mass error in ppm; **(b)** Scatterplot of precursor m/z versus precursor mass error in ppm.

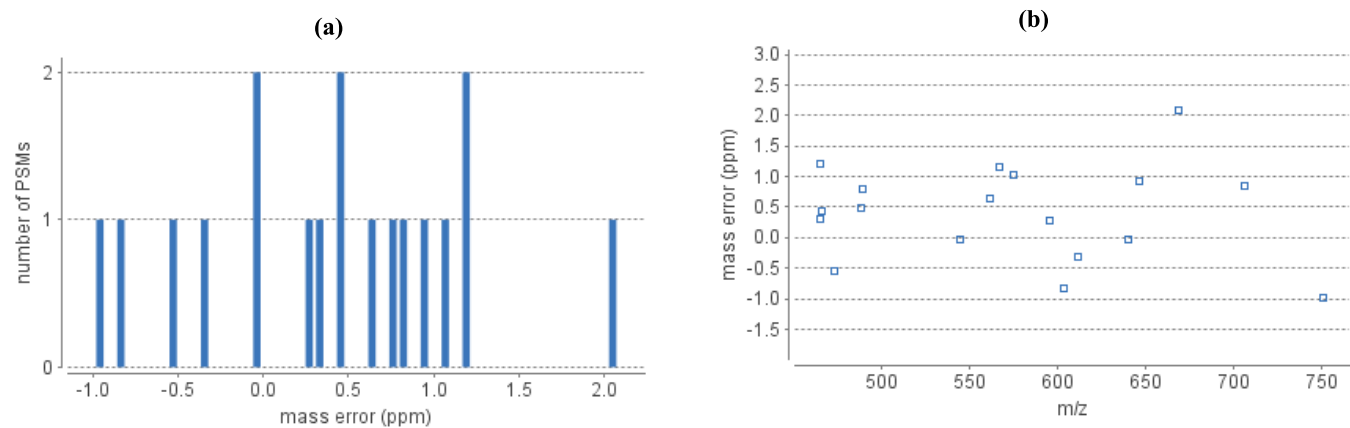


Table 5. Number of identified peptides in each sample by the number of missed cleavages

Missed Cleavages	0	1	2	3	4+
Sample 9	17	1	0	0	0

4. Other Information

Table 6. Search parameters.

Search Engine Name:	PEAKS
Parent Mass Error Tolerance:	5.0 ppm
Fragment Mass Error Tolerance:	0.5 Da
Precursor Mass Search Type:	monoisotopic
Enzyme:	Trypsin
Max Missed Cleavages:	3
Non-specific Cleavage:	one
Variable Modifications:	
Oxidation (M):	15.99
Max variable PTM per peptide:	3
Database:	Ant
Taxon:	All
Searched Entry:	473117
FDR Estimation:	Enabled
Merge Options:	no merge
Precursor Options:	corrected
Charge Options:	no correction

Table 7. Instrument parameters.

Fractions:	TW_15.raw
Ion Source:	ESI(nano-spray)
Fragmentation Mode:	CID, CAD(y and b ions)
MS Scan Mode:	FT-ICR/Orbitrap
MS/MS Scan Mode:	FT-ICR/Orbitrap

Filter Options: no filter

Process: true

Protein List

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
1	22345	gi 769857915 ref XP_011640613.1	104.06	12	5	1	N	44960	PREDICTED: phosphoglycerate kinase [Pogonormyrmex barbatus]
1	22346	gi 861651854 gb KMQ98019.1	104.06	12	5	1	N	44890	phosphoglycerate kinase [Lasius niger]
1	22347	gi 322791271 gb EFZ15795.1	104.06	10	5	1	N	51542	hypothetical protein SINV_08663, partial [Solenopsis invicta]
1	22348	gi 751220516 ref XP_011163392.1	104.06	10	5	1	N	53682	PREDICTED: phosphoglycerate kinase [Solenopsis invicta]
1	22349	gi 1012983603 gb KYQ57292.1	104.06	10	5	1	N	54088	Phosphoglycerate kinase [Trachymyrmex zeteki]
2	22355	gi 1009426647 gb KYN44725.1	99.78	9	5	1	N	54299	Phosphoglycerate kinase [Trachymyrmex septentrionalis]
4	11160	gi 759032952 ref XP_011334617.1	89.36	8	3	3	N	41770	PREDICTED: actin, clone 205 [Ceraopachys biro]
4	5591	gi 751239306 ref XP_011173634.1	89.36	8	3	3	N	41783	PREDICTED: actin-5, muscle-specific [Solenopsis invicta]
4	22364	gi 1009381508 gb KYN04384.1	89.36	8	3	3	N	41822	Actin-5C [Cyphomyrmex costatus]
4	5565	gi 749754572 ref XP_011139727.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Harpegnathos saltator]
4	5593	gi 752898359 ref XP_011267531.1	89.36	8	3	3	N	41783	PREDICTED: actin-5, muscle-specific [Camponotus floridanus]
4	22365	gi 861646675 gb KMQ95606.1	89.36	8	3	3	N	41822	actin-4 [Lasius niger]
4	5566	gi 751198952 ref XP_011173672.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Solenopsis invicta]
4	22366	gi 826414678 ref XP_012522032.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Monomorium pharaonis]
4	22367	gi 1009427183 gb KYN45235.1	89.36	8	3	3	N	41822	Actin-5C [Trachymyrmex septentrionalis]
4	22368	gi 815788473 ref XP_012214760.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Linepithema humile]
4	22369	gi 1009408868 gb KYN28144.1	89.36	8	3	3	N	41822	Actin-5C [Trachymyrmex cornetzi]
4	5594	gi 752898361 ref XP_011267532.1	89.36	8	3	3	N	41783	PREDICTED: actin-5, muscle-specific [Camponotus floridanus]
4	11161	gi 752898367 ref XP_011267535.1	89.36	8	3	3	N	41756	PREDICTED: actin, muscle [Camponotus floridanus]
4	22370	gi 951573454 ref XP_014484761.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Dinoponera quadriceps]
4	22371	gi 801405939 ref XP_012062192.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Atta cephalotes]
4	5567	gi 752879620 ref XP_011257343.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Camponotus floridanus]
4	5595	gi 749790975 ref XP_011148680.1	89.36	8	3	3	N	41783	PREDICTED: actin-5, muscle-specific [Harpegnathos saltator]
4	5568	gi 746842703 ref XP_011051576.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Acromyrmex echinator]
4	5596	gi 607368824 gb EZA62930.1	89.36	8	3	3	N	41774	Actin, muscle [Ceraopachys biro]
4	22372	gi 826414676 ref XP_012522031.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Monomorium pharaonis]
4	5569	gi 260401142 gb ACX37099.1	89.36	8	3	3	N	41792	beta actin [Polyrhachis vicina]
4	5598	gi 751239318 ref XP_011173641.1	89.36	8	3	3	N	41783	PREDICTED: actin-5, muscle-specific [Solenopsis invicta]
4	5599	gi 607368821 gb EZA62927.1	89.36	8	3	3	N	41770	Actin, clone [Ceraopachys biro]
4	5600	gi 327387361 gb AEA72282.1	89.36	8	3	3	N	41783	actin-87E isoform 1 [Solenopsis invicta]
4	22373	gi 769855685 ref XP_011639413.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Pogonormyrmex barbatus]
4	22374	gi 1012983438 gb KYQ57141.1	89.36	8	3	3	N	41822	Actin-5C [Trachymyrmex zeteki]
4	5570	gi 607362215 gb EZA56475.1	89.36	8	3	3	N	41822	Actin-5C [Ceraopachys biro]
4	11162	gi 752898365 ref XP_011267534.1	89.36	8	3	3	N	41756	PREDICTED: actin, muscle [Camponotus floridanus]
4	5602	gi 746849933 ref XP_011055428.1	89.36	8	3	3	N	41745	PREDICTED: actin-5, muscle-specific-like [Acromyrmex echinator]
4	22375	gi 780708250 ref XP_011703767.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Wasmannia auropunctata]
4	22376	gi 1009354281 gb KYM79637.1	89.36	8	3	3	N	41822	Actin-5C [Atta colombica]
4	22377	gi 795061729 ref XP_011873597.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Vollenhovia emeryi]
4	22378	gi 795061726 ref XP_011873596.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Vollenhovia emeryi]
4	5603	gi 751239316 ref XP_011173639.1	89.36	8	3	3	N	41758	PREDICTED: actin, muscle [Solenopsis invicta]
4	22379	gi 815788475 ref XP_012214761.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Linepithema humile]
4	5604	gi 746849931 ref XP_011055426.1	89.36	8	3	3	N	41684	PREDICTED: actin-5, muscle-specific [Acromyrmex echinator]

total 72 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
4	5571	gi 746842701 ref XP_011051575.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Acromyrmex echinator]
4	5572	gi 751198954 ref XP_011173741.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Solenopsis invicta]
4	22380	gi 780708254 ref XP_011703768.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Wasmannia auropunctata]
4	5573	gi 752879618 ref XP_011257342.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Camponotus floridanus]
4	5605	gi 752898363 ref XP_011267533.1	89.36	8	3	3	N	41783	PREDICTED: actin-5, muscle-specific [Camponotus floridanus]
4	11179	gi 759032950 ref XP_011334490.1	89.36	8	3	3	N	41774	PREDICTED: actin, muscle [Ceraopachys biroij]
4	22381	gi 759053316 ref XP_011335820.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Ceraopachys biroij]
4	5574	gi 749754574 ref XP_011139728.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Harpegnathos saltator]
4	22382	gi 769855687 ref XP_011639414.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Pogonomyrmex barbatus]
4	22383	gi 759053314 ref XP_011335819.1	89.36	8	3	3	N	41822	PREDICTED: actin-5C [Ceraopachys biroij]
4	5606	gi 749790980 ref XP_011148681.1	89.36	8	3	3	N	41783	PREDICTED: actin-5, muscle-specific [Harpegnathos saltator]
4	5607	gi 607368823 gb EZA62929.1	89.36	7	3	3	N	43729	Actin, muscle [Ceraopachys biroij]
4	5636	gi 749793865 ref XP_011150241.1	89.36	8	3	3	N	41890	PREDICTED: actin-5C-like [Harpegnathos saltator]
6	20912	gi 951526129 ref XP_014467326.1	74.19	6	2	2	N	39712	PREDICTED: arginine kinase isoform X2 [Dinoponera quadriceps]
6	20913	gi 951526126 ref XP_014467325.1	74.19	6	2	2	N	39712	PREDICTED: arginine kinase isoform X2 [Dinoponera quadriceps]
6	1687	gi 746868095 ref XP_011065164.1	74.19	6	2	2	N	39772	PREDICTED: arginine kinase isoform X1 [Acromyrmex echinator]
6	20924	gi 746868097 ref XP_011065165.1	74.19	6	2	2	N	41700	PREDICTED: arginine kinase isoform X2 [Acromyrmex echinator]
6	20914	gi 951526124 ref XP_014467324.1	74.19	6	2	2	N	41640	PREDICTED: arginine kinase isoform X1 [Dinoponera quadriceps]
5	77	gi 1911819 gb AAB50883.1	51.64	10	1	1	Y	11819	Myr p I=allergenic polypeptide {N-terminal}-[Myrmecia pilosula=jumper ants, venom, Peptide Partial, 112 aa]
5	78	gi 312284 emb CAA49760.1	51.64	10	1	1	Y	11849	major allergen [Myrmecia pilosula]
5	76	gi 730091 sp Q07932.1 MYR1_MYRPI	51.64	10	1	1	Y	11849	RecName: Full=Pilosulin-1; AltName: Full=Allergen Myr p I; AltName: Full=Major allergen Myr p I; AltName: Allergen=Myr p I; Contains: RecName: Full=Pilosulin-1; Contains: RecName: Full=Pilosulin-1 65->112; Contains: RecNa...
8	22386	gi 731904326 gb AIZ67278.1	48.43	4	1	1	N	24162	elongation factor 1-alpha, partial [Pheidole sp. NC02]
8	22387	gi 1012978961 gb KYQ52948.1	48.43	2	1	1	N	49246	Elongation factor 1-alpha [Trachymyrmex zetekii]
28	21037	gi 780633339 ref XP_011686024.1	44.95	3	1	1	N	38487	PREDICTED: aldose 1-epimerase isoform X2 [Wasmannia auropunctata]
28	21038	gi 780633331 ref XP_011686022.1	44.95	3	1	1	N	38487	PREDICTED: aldose 1-epimerase isoform X2 [Wasmannia auropunctata]
28	21039	gi 780633335 ref XP_011686023.1	44.95	3	1	1	N	38487	PREDICTED: aldose 1-epimerase isoform X2 [Wasmannia auropunctata]
28	21040	gi 780633327 ref XP_011686021.1	44.95	3	1	1	N	38487	PREDICTED: aldose 1-epimerase isoform X2 [Wasmannia auropunctata]
28	21041	gi 780633322 ref XP_011686020.1	44.95	3	1	1	N	40448	PREDICTED: aldose 1-epimerase isoform X1 [Wasmannia auropunctata]
29	22388	gi 861659444 gb KMR04484.1	44.41	4	1	1	N	40700	glyceraldehyde-3-phosphate dehydrogenase 1-like protein [Lasius niger]
30	6846	gi 749750028 ref XP_011137253.1	40.05	2	1	1	N	71477	PREDICTED: heat shock 70 kDa protein cognate 4 [Harpegnathos saltator]
total 72 proteins									

Band # 16 Proteins

Summary

1. Notes

2. Result Statistics

Figure 1. False discovery rate (FDR) curve. X axis is the number of peptide-spectrum matches (PSM) being kept. Y axis is the corresponding FDR.

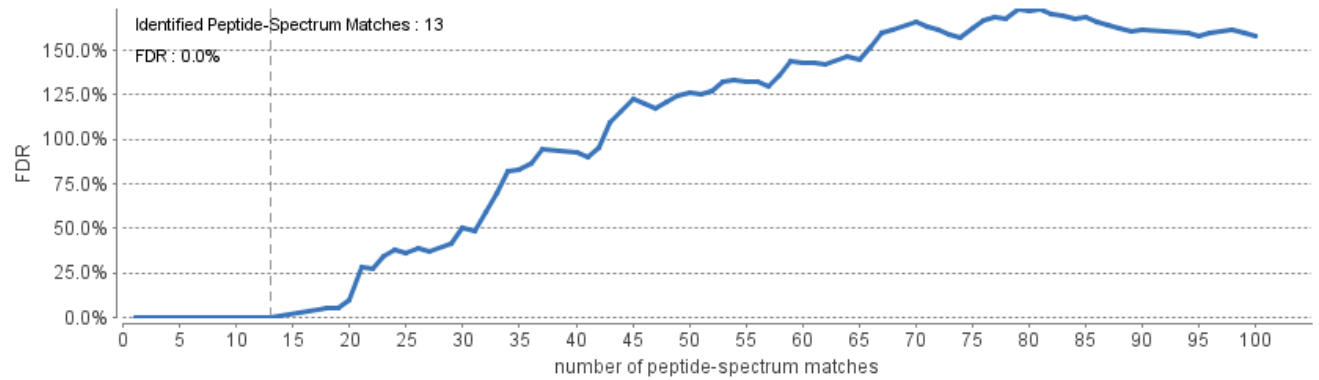


Figure 2. PSM score distribution. (a) Distribution of PEAKS peptide score; (b) Scatterplot of PEAKS peptide score versus precursor mass error.

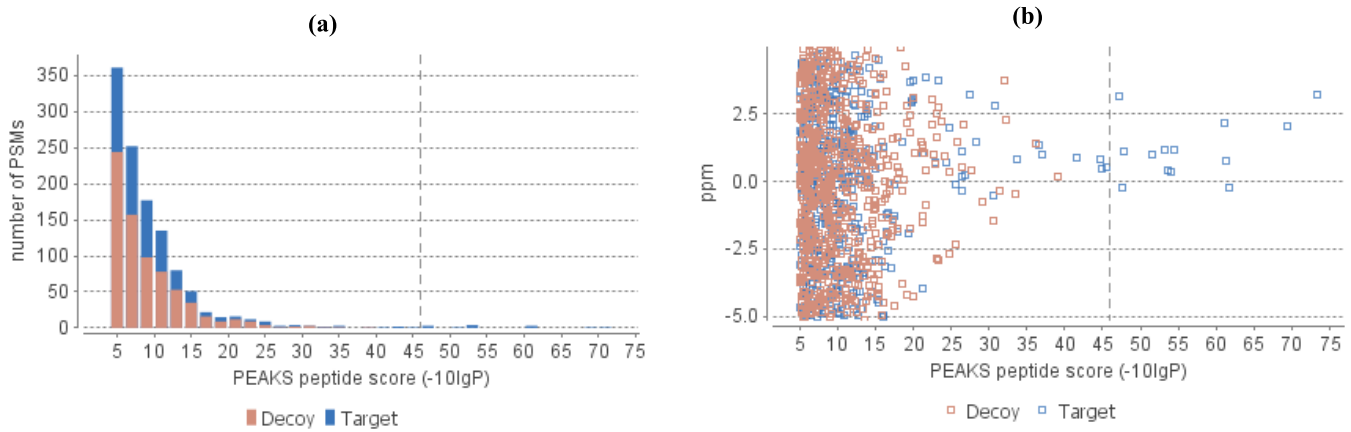


Figure 3. De novo result validation. Distribution of residue local confidence: (a) Residues in de novo sequences validated by confident database peptide assignment; (b) Residues in "de novo only" sequences.

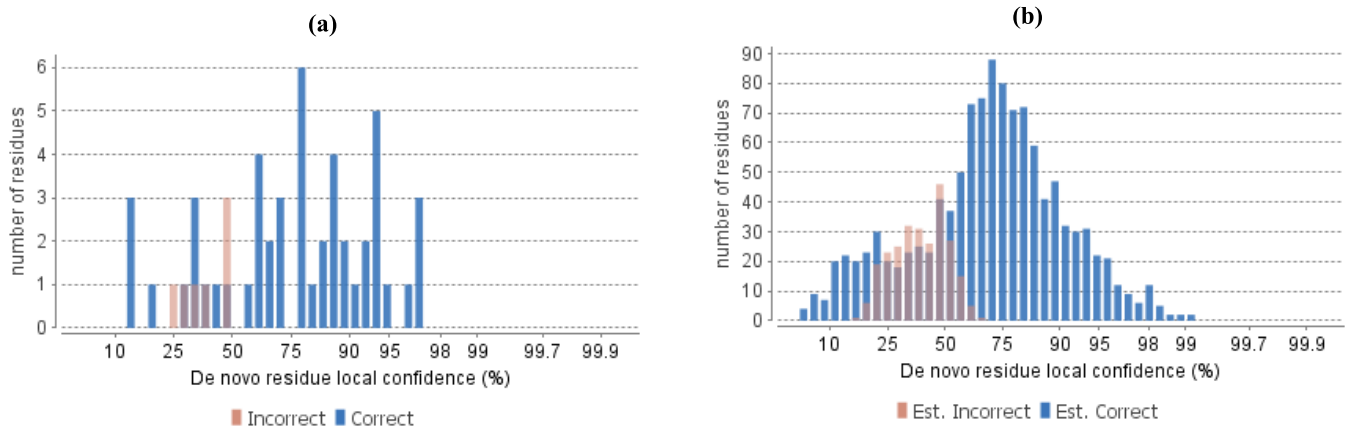


Table 1. Statistics of data.

# of MS Scans	1692
# of MS/MS Scans	2888

Table 4. PTM profile.

Name	Δ Mass	Position	#PSM	-10lgP	Area	AScore
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Table 2. Result filtration parameters.

Peptide -10lgP	≥46
Protein -10lgP	≥20
Proteins unique peptides	≥1
De novo ALC Score	≥50%

Table 3. Statistics of filtered result.

Peptide-Spectrum Matches	13
Peptide Sequences	12
Protein Groups	8
Proteins	142
Proteins (#Unique Peptides)	0 (>2); 50 (=2); 92 (=1);
FDR (Peptide-Spectrum Matches)	0.0%
FDR (Peptide Sequences)	0.0%
FDR (Protein)	0.0%
De Novo Only Spectra	134

3. Experiment Control

Figure 4. Precursor mass error of peptide-spectrum matches (PSM) in filtered result. **(a)** Distribution of precursor mass error in ppm; **(b)** Scatterplot of precursor m/z versus precursor mass error in ppm. 

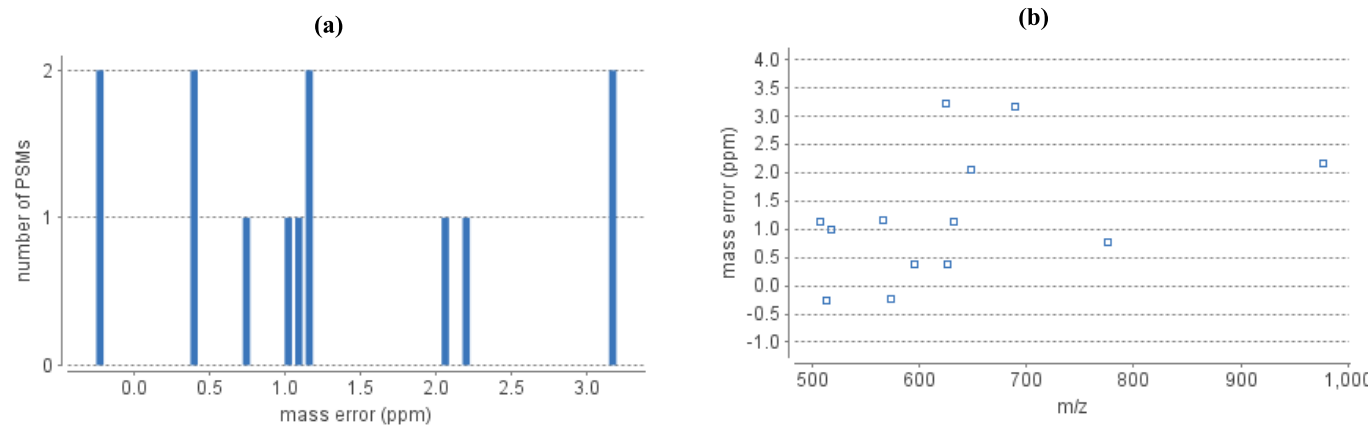


Table 5. Number of identified peptides in each sample by the number of missed cleavages

Missed Cleavages	0	1	2	3	4+
Sample 10	11	1	0	0	0

4. Other Information

Table 6. Search parameters.

Search Engine Name:	PEAKS
Parent Mass Error Tolerance:	5.0 ppm
Fragment Mass Error Tolerance:	0.5 Da
Precursor Mass Search Type:	monoisotopic
Enzyme:	Trypsin
Max Missed Cleavages:	3
Non-specific Cleavage:	one
Variable Modifications:	
Oxidation (M):	15.99
Max variable PTM per peptide:	3
Database:	Ant
Taxon:	All
Searched Entry:	473117
FDR Estimation:	Enabled
Merge Options:	no merge
Precursor Options:	corrected
Charge Options:	no correction

Table 7. Instrument parameters.

Fractions:	TW_16.raw
Ion Source:	ESI(nano-spray)
Fragmentation Mode:	CID, CAD(y and b ions)
MS Scan Mode:	FT-ICR/Orbitrap
MS/MS Scan Mode:	FT-ICR/Orbitrap

Filter Options: no filter

Process: true

Protein List

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
2	23704	gi 861647540 gb KMQ95962.1	131.28	7	3	1	N	62716	esterase fe4-like protein [<i>Lasius niger</i>]
1	23703	gi 780651505 ref XP_011690504.1	131.16	7	3	1	N	63173	PREDICTED: esterase FE4-like [<i>Wasmannia auropunctata</i>]
3	23707	gi 751222706 ref XP_011164602.1	108.18	7	3	1	N	62771	PREDICTED: esterase FE4-like [<i>Solenopsis invicta</i>]
4	11160	gi 759032952 ref XP_011334617.1	107.02	7	2	2	N	41770	PREDICTED: actin, clone 205 [<i>Cerapachys biroi</i>]
4	5591	gi 751239306 ref XP_011173634.1	107.02	7	2	2	N	41783	PREDICTED: actin-5, muscle-specific [<i>Solenopsis invicta</i>]
4	22364	gi 1009381508 gb KYN04384.1	107.02	7	2	2	N	41822	Actin-5C [<i>Cyphomyrmex costatus</i>]
4	5565	gi 749754572 ref XP_011139727.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [<i>Harpegnathos saltator</i>]
4	23708	gi 307179404 gb EFN67734.1	107.02	7	2	2	N	41822	Actin-5C [<i>Camponotus floridanus</i>]
4	5593	gi 752898359 ref XP_011267531.1	107.02	7	2	2	N	41783	PREDICTED: actin-5, muscle-specific [<i>Camponotus floridanus</i>]
4	22365	gi 861646675 gb KMQ95606.1	107.02	7	2	2	N	41822	actin-4 [<i>Lasius niger</i>]
4	5566	gi 751198952 ref XP_011173672.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [<i>Solenopsis invicta</i>]
4	23709	gi 307166491 gb EFN60576.1	107.02	7	2	2	N	41756	Actin, muscle [<i>Camponotus floridanus</i>]
4	22366	gi 826414678 ref XP_012522032.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [<i>Monomorium pharaonis</i>]
4	22367	gi 1009427183 gb KYN45235.1	107.02	7	2	2	N	41822	Actin-5C [<i>Trachymyrmex septentrionalis</i>]
4	22368	gi 815788473 ref XP_012214760.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [<i>Linepithema humile</i>]
4	22369	gi 1009408868 gb KYN28144.1	107.02	7	2	2	N	41822	Actin-5C [<i>Trachymyrmex cornetzi</i>]
4	5594	gi 752898361 ref XP_011267532.1	107.02	7	2	2	N	41783	PREDICTED: actin-5, muscle-specific [<i>Camponotus floridanus</i>]
4	11161	gi 752898367 ref XP_011267535.1	107.02	7	2	2	N	41756	PREDICTED: actin, muscle [<i>Camponotus floridanus</i>]
4	22370	gi 951573454 ref XP_014484761.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [<i>Dinoponera quadripes</i>]
4	22371	gi 801405939 ref XP_012062192.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [<i>Atta cephalotes</i>]
4	5567	gi 752879620 ref XP_011257343.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [<i>Camponotus floridanus</i>]
4	5595	gi 749790975 ref XP_011148680.1	107.02	7	2	2	N	41783	PREDICTED: actin-5, muscle-specific [<i>Harpegnathos saltator</i>]
4	5568	gi 746842703 ref XP_011051576.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [<i>Acromyrmex echinator</i>]
4	5596	gi 607368824 gb EZA62930.1	107.02	7	2	2	N	41774	Actin, muscle [<i>Cerapachys biroi</i>]
4	22372	gi 826414676 ref XP_012522031.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [<i>Monomorium pharaonis</i>]
4	5569	gi 260401142 gb ACX37099.1	107.02	7	2	2	N	41792	beta actin [<i>Polyrhachis vicina</i>]
4	5598	gi 751239318 ref XP_011173641.1	107.02	7	2	2	N	41783	PREDICTED: actin-5, muscle-specific [<i>Solenopsis invicta</i>]
4	5599	gi 607368821 gb EZA62927.1	107.02	7	2	2	N	41770	Actin, clone [<i>Cerapachys biroi</i>]
4	5600	gi 327387361 gb AEA72282.1	107.02	7	2	2	N	41783	actin-87E isoform 1 [<i>Solenopsis invicta</i>]
4	22373	gi 769855685 ref XP_011639413.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [<i>Pogonomyrmex barbatus</i>]
4	22374	gi 1012983438 gb KYQ57141.1	107.02	7	2	2	N	41822	Actin-5C [<i>Trachymyrmex zeteki</i>]
4	5570	gi 607362215 gb EZA56475.1	107.02	7	2	2	N	41822	Actin-5C [<i>Cerapachys biroi</i>]
4	11162	gi 752898365 ref XP_011267534.1	107.02	7	2	2	N	41756	PREDICTED: actin, muscle [<i>Camponotus floridanus</i>]
4	5602	gi 746849933 ref XP_011055428.1	107.02	7	2	2	N	41745	PREDICTED: actin-5, muscle-specific-like [<i>Acromyrmex echinator</i>]
4	22375	gi 780708250 ref XP_011703767.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [<i>Wasmannia auropunctata</i>]
4	22376	gi 1009354281 gb KYM79637.1	107.02	7	2	2	N	41822	Actin-5C [<i>Atta colombica</i>]
4	22377	gi 795061729 ref XP_011873597.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [<i>Vollenhovia emeryi</i>]
4	22378	gi 795061726 ref XP_011873596.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [<i>Vollenhovia emeryi</i>]
4	5603	gi 751239316 ref XP_011173639.1	107.02	7	2	2	N	41758	PREDICTED: actin, muscle [<i>Solenopsis invicta</i>]
4	22379	gi 815788475 ref XP_012214761.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [<i>Linepithema humile</i>]
4	5604	gi 746849931 ref XP_011055426.1	107.02	7	2	2	N	41684	PREDICTED: actin-5, muscle-specific [<i>Acromyrmex echinator</i>]
4	5571	gi 746842701 ref XP_011051575.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [<i>Acromyrmex echinator</i>]
4	5572	gi 751198954 ref XP_011173741.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [<i>Solenopsis invicta</i>]
4	22380	gi 780708254 ref XP_011703768.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [<i>Wasmannia auropunctata</i>]

total 142 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
4	5573	gi 752879618 ref XP_011257342.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [Camponotus floridanus]
4	5605	gi 752898363 ref XP_011267533.1	107.02	7	2	2	N	41783	PREDICTED: actin-5, muscle-specific [Camponotus floridanus]
4	11179	gi 759032950 ref XP_011334490.1	107.02	7	2	2	N	41774	PREDICTED: actin, muscle [Ceraupachys biroii]
4	22381	gi 759053316 ref XP_011335820.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [Ceraupachys biroii]
4	5574	gi 749754574 ref XP_011139728.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [Harpegnathos saltator]
4	22382	gi 769855687 ref XP_011639414.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [Pogonomyrmex barbatus]
4	22383	gi 759053314 ref XP_011335819.1	107.02	7	2	2	N	41822	PREDICTED: actin-5C [Ceraupachys biroii]
4	5606	gi 749790980 ref XP_011148681.1	107.02	7	2	2	N	41783	PREDICTED: actin-5, muscle-specific [Harpegnathos saltator]
4	5607	gi 607368823 gb EZA62929.1	107.02	7	2	2	N	43729	Actin, muscle [Ceraupachys biroii]
7	19641	gi 780651208 ref XP_011690427.1	70.06	4	1	1	N	32936	PREDICTED: ATP synthase subunit beta, mitochondrial-like [Wasmannia auropunctata]
7	23728	gi 322787386 gb EFZ13476.1	70.06	4	1	1	N	32750	hypothetical protein SINVA_10078, partial [Solenopsis invicta]
7	23729	gi 751227187 ref XP_011167061.1	70.06	4	1	1	N	33369	PREDICTED: ATP synthase subunit beta, mitochondrial [Solenopsis invicta]
7	23730	gi 746870197 ref XP_011066278.1	70.06	3	1	1	N	51466	PREDICTED: ATP synthase subunit beta, mitochondrial-like [Acromyrmex echinator]
7	23731	gi 1012972782 gb KYQ47240.1	70.06	2	1	1	N	51701	ATP synthase subunit beta, mitochondrial, partial [Trachymyrmex zeteki]
7	23732	gi 1009358283 gb KYM83491.1	70.06	2	1	1	N	52030	ATP synthase subunit beta, mitochondrial, partial [Atta colombica]
7	23733	gi 332017324 gb EGI58074.1	70.06	2	1	1	N	52533	ATP synthase subunit beta, mitochondrial [Acromyrmex echinator]
7	23734	gi 307181472 gb EFN69064.1	70.06	2	1	1	N	55105	ATP synthase subunit beta, mitochondrial [Camponotus floridanus]
7	23735	gi 759037183 ref XP_011348310.1	70.06	2	1	1	N	55118	PREDICTED: ATP synthase subunit beta, mitochondrial [Ceraupachys biroii]
7	23736	gi 607367456 gb EZA61603.1	70.06	2	1	1	N	55118	ATP synthase subunit beta, mitochondrial [Ceraupachys biroii]
7	23737	gi 752875614 ref XP_011255166.1	70.06	2	1	1	N	55237	PREDICTED: ATP synthase subunit beta, mitochondrial [Camponotus floridanus]
7	23738	gi 1009368702 gb KYM93547.1	70.06	2	1	1	N	55391	ATP synthase subunit beta, mitochondrial [Cypomyrmex costatus]
7	23739	gi 795019357 ref XP_011859549.1	70.06	2	1	1	N	55371	PREDICTED: ATP synthase subunit beta, mitochondrial [Vollenhovia emeryi]
7	23740	gi 749793843 ref XP_011150231.1	70.06	2	1	1	N	55258	PREDICTED: ATP synthase subunit beta, mitochondrial [Harpegnathos saltator]
7	23741	gi 307195440 gb EFN77326.1	70.06	2	1	1	N	55258	ATP synthase subunit beta, mitochondrial [Harpegnathos saltator]
7	23742	gi 951517399 ref XP_014467370.1	70.06	2	1	1	N	55411	PREDICTED: ATP synthase subunit beta, mitochondrial [Dinoponera quadricipes]
7	23743	gi 826431387 ref XP_012528411.1	70.06	2	1	1	N	55578	PREDICTED: ATP synthase subunit beta, mitochondrial [Monomorium pharaonis]
7	23744	gi 815790072 ref XP_012215594.1	70.06	2	1	1	N	55454	PREDICTED: ATP synthase subunit beta, mitochondrial [Linepithema humile]
7	23745	gi 1009415237 gb KYN34049.1	70.06	2	1	1	N	55636	ATP synthase subunit beta, mitochondrial [Trachymyrmex septentrionalis]
7	23746	gi 861639608 gb KMQ92914.1	70.06	2	1	1	N	55523	atp synthase subunit mitochondrial-like protein [Lasius niger]
7	23747	gi 769846449 ref XP_011634528.1	70.06	2	1	1	N	55586	PREDICTED: ATP synthase subunit beta, mitochondrial [Pogonomyrmex barbatus]
7	23748	gi 801394789 ref XP_012058285.1	70.06	2	1	1	N	55644	PREDICTED: ATP synthase subunit beta, mitochondrial [Atta cephalotes]
6	9851	gi 407021090 gb AFS65405.1	68.36	9	1	1	N	13104	elongation factor 1-alpha, partial [Pseudolasius typhlops]
6	23724	gi 1043379953 gb ANS53834.1	68.36	6	1	1	N	21162	translation elongation factor 1-alpha, partial [Camponotus maculatus]
6	23725	gi 342316952 gb AEL22340.1	68.36	5	1	1	N	24739	elongation factor 1 alpha, partial [Mycocepurus smithii]
6	9852	gi 407021072 gb AFS65396.1	68.36	4	1	1	N	28137	elongation factor 1-alpha, partial [Paraparatchina sp. PHL02]
6	9853	gi 407021088 gb AFS65404.1	68.36	4	1	1	N	28137	elongation factor 1-alpha, partial [Pseudolasius sp. PHL01]
6	9854	gi 407021093 gb AFS65407.1	68.36	4	1	1	N	28137	elongation factor 1-alpha, partial [Zatania cispai]
6	9855	gi 407021076 gb AFS65398.1	68.36	4	1	1	N	28075	elongation factor 1-alpha, partial [Paratrechina longicornis]
6	9856	gi 460422929 gb AGH12537.1	68.36	4	1	1	N	28137	elongation factor 1-alpha F1, partial [Nylanderia fulva]

total 142 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
6	9857	gi 407021097 gb AFS65409.1	68.36	4	1	1	N	28137	elongation factor 1-alpha, partial [Zatania gl oriosa]
6	9858	gi 407021082 gb AFS65401.1	68.36	4	1	1	N	28137	elongation factor 1-alpha, partial [Prenolepis sp. PHL02]
6	9820	gi 307715730 gb ABK54616.2	68.36	3	1	1	N	39176	elongation factor 1-alpha, partial [Forelius p ruinosus]
6	9821	gi 307715722 gb ABK54576.2	68.36	3	1	1	N	39152	elongation factor 1-alpha, partial [Anonycho myrma gilberti]
6	9822	gi 307715720 gb ABK54574.2	68.36	3	1	1	N	39178	elongation factor 1-alpha, partial [Aneuretus simoni]
6	9823	gi 307715738 gb ABK54632.2	68.36	3	1	1	N	39179	elongation factor 1-alpha, partial [Liometop um apiculatum]
6	23726	gi 289600986 gb ADD13360.1	68.36	3	1	1	N	39162	elongation factor 1-alpha, partial [Dolichode rus decollatus]
6	9824	gi 307715732 gb ABK54628.2	68.36	3	1	1	N	39162	elongation factor 1-alpha, partial [Leptomyr mex sp. AUS01]
6	9825	gi 307715750 gb ABK54674.2	68.36	3	1	1	N	39152	elongation factor 1-alpha, partial [Philidris c ordata]
6	9826	gi 307715744 gb ABK54646.2	68.36	3	1	1	N	39162	elongation factor 1-alpha, partial [Myrmecia pyriformis Smith, 1858]
6	9827	gi 307715748 gb ABK54668.2	68.36	3	1	1	N	39152	elongation factor 1-alpha, partial [Papyrius nitidus]
6	9828	gi 307715746 gb ABK54658.2	68.36	3	1	1	N	39162	elongation factor 1-alpha, partial [Nothomyr mecia macrops]
6	9829	gi 307715762 gb ABK54719.2	68.36	3	1	1	N	39152	elongation factor 1-alpha, partial [Turneria bidentata]
6	9830	gi 307715734 gb ABK54629.2	68.36	3	1	1	N	39162	elongation factor 1-alpha, partial [Leptomyr mex erythrocephalus]
6	9831	gi 307715726 gb ABK54608.2	68.36	3	1	1	N	39150	elongation factor 1-alpha, partial [Dolichode rus scabridus]
6	9832	gi 307715724 gb ABK54585.2	68.36	3	1	1	N	39162	elongation factor 1-alpha, partial [Azteca ov aticeps]
6	9833	gi 307715728 gb ABK54611.2	68.36	3	1	1	N	39162	elongation factor 1-alpha, partial [Dorymyr mex bicolor]
6	9834	gi 307715740 gb ABK54633.2	68.36	3	1	1	N	39179	elongation factor 1-alpha, partial [Liometop um occidentale]
6	9835	gi 307715754 gb ABK54707.2	68.36	3	1	1	N	39189	elongation factor 1-alpha, partial [Tapinoma sessile]
6	9836	gi 307715758 gb ABK54710.2	68.36	3	1	1	N	39179	elongation factor 1-alpha, partial [Technom yrmex sp. MAD05]
6	9837	gi 307715736 gb ABK54631.2	68.36	3	1	1	N	39162	elongation factor 1-alpha, partial [Linepithe ma humile]
6	9838	gi 307715752 gb ABK54697.2	68.36	3	1	1	N	39162	elongation factor 1-alpha, partial [Rhytidopo nera chalybaea]
6	9839	gi 307715756 gb ABK54709.2	68.36	3	1	1	N	39189	elongation factor 1-alpha, partial [Technom yrmex difficilis]
6	9840	gi 307715760 gb ABK54716.2	68.36	3	1	1	N	39148	elongation factor 1-alpha, partial [Tetrapone ra rufonigra]
6	9841	gi 307715742 gb ABK54635.2	68.36	3	1	1	N	39162	elongation factor 1-alpha, partial [Manica br adleyi]
6	23727	gi 815818098 ref XP_012230200.1	68.36	2	1	1	N	50551	PREDICTED: elongation factor 1-alpha [Line pithe ma humile]
10	77	gi 1911819 gb AAB50883.1	53.69	10	1	1	N	11819	Myr p I=allergenic polypeptide {N-terminal} [Myrmecia pilosula=jumper ants, venom, Pe ptide Partial, 112 aa]
10	78	gi 312284 emb CAA49760.1	53.69	10	1	1	N	11849	major allergen [Myrmecia pilosula]
10	76	gi 730091 sp Q07932.1 MYR1_MYRPI	53.69	10	1	1	N	11849	RecName: Full=Pilosulin-1; AltName: Full=A llergen Myr p I; AltName: Full=Major allerge n Myr p 1; AltName: Allergen=Myr p 1; Con tains: RecName: Full=Pilosulin-1; Contains: RecName: Full=Pilosulin-1 65->112; Contai ns: RecNa...
21	23753	gi 769851640 ref XP_011637264.1	47.71	2	1	1	N	48587	PREDICTED: tubulin alpha-2/alpha-4 chain-l ike isoform X2 [Pogonomyrmex barbatus]
21	23754	gi 769851644 ref XP_011637266.1	47.71	2	1	1	N	48587	PREDICTED: tubulin alpha-2/alpha-4 chain-l ike isoform X2 [Pogonomyrmex barbatus]
21	23755	gi 769851642 ref XP_011637265.1	47.71	2	1	1	N	48587	PREDICTED: tubulin alpha-2/alpha-4 chain-l ike isoform X2 [Pogonomyrmex barbatus]
21	23756	gi 769851638 ref XP_011637263.1	47.71	2	1	1	N	50211	PREDICTED: tubulin alpha-2/alpha-4 chain-l ike isoform X1 [Pogonomyrmex barbatus]
21	23782	gi 607363006 gb EZA57250.1	47.71	3	1	1	N	33381	Tubulin alpha-1C chain [Cerapachys biro]
21	5689	gi 307182561 gb EFN69754.1	47.71	2	1	1	N	46140	Tubulin alpha-1 chain [Camponotus floridan us]
21	5690	gi 801383453 ref XP_012054888.1	47.71	2	1	1	N	46271	PREDICTED: tubulin alpha-1 chain-like [Atta cephalotes]
21	5691	gi 780716124 ref XP_011705756.1	47.71	2	1	1	N	46255	PREDICTED: tubulin alpha-1 chain-like [Was mannia auropunctata]

total 142 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
21	23783	gi 759049960 ref XP_011334048.1	47.71	2	1	1	N	48799	PREDICTED: LOW QUALITY PROTEIN: tubulin alpha-1 chain-like [Ceropachys biroï]
21	5692	gi 795098387 ref XP_011880552.1	47.71	2	1	1	N	49951	PREDICTED: tubulin alpha-1 chain-like [Vollenhovia emeryi]
21	5693	gi 815797181 ref XP_012219276.1	47.71	2	1	1	N	49949	PREDICTED: tubulin alpha-1 chain [Linepithema humile]
21	5694	gi 780688489 ref XP_011699063.1	47.71	2	1	1	N	49937	PREDICTED: tubulin alpha-1 chain-like [Wasmannia auropunctata]
21	5695	gi 751225567 ref XP_011166173.1	47.71	2	1	1	N	49937	PREDICTED: tubulin alpha-1 chain [Solenopsis invicta]
21	5696	gi 749757386 ref XP_011141041.1	47.71	2	1	1	N	49965	PREDICTED: tubulin alpha-1 chain [Harpegnathos saltator]
21	5698	gi 749750076 ref XP_011137280.1	47.71	2	1	1	N	49941	PREDICTED: tubulin alpha-1 chain-like [Harpegnathos saltator]
21	5699	gi 746841278 ref XP_011050824.1	47.71	2	1	1	N	49937	PREDICTED: tubulin alpha-1 chain [Acromyrmex echinator]
21	5700	gi 752873763 ref XP_011254175.1	47.71	2	1	1	N	49965	PREDICTED: tubulin alpha-1 chain-like [Camponotus floridanus]
21	5701	gi 769856071 ref XP_011639616.1	47.71	2	1	1	N	49951	PREDICTED: tubulin alpha-1 chain-like [Pogonomyrmex barbatus]
21	5703	gi 815803306 ref XP_01222352.1	47.71	2	1	1	N	50110	PREDICTED: tubulin alpha-1 chain-like [Linepithema humile]
21	5704	gi 751236429 ref XP_011172049.1	47.71	2	1	1	N	50110	PREDICTED: tubulin alpha-1 chain-like [Solenopsis invicta]
21	5705	gi 795022910 ref XP_011860761.1	47.71	2	1	1	N	50110	PREDICTED: tubulin alpha-1 chain [Vollenhovia emeryi]
21	5706	gi 607355672 gb EZA50232.1	47.71	2	1	1	N	50110	Tubulin alpha-1 chain [Ceropachys biroï]
21	5707	gi 752880372 ref XP_011257750.1	47.71	2	1	1	N	50110	PREDICTED: tubulin alpha-1 chain [Camponotus floridanus]
21	5708	gi 746872703 ref XP_011067628.1	47.71	2	1	1	N	50110	PREDICTED: tubulin alpha-1 chain-like [Acromyrmex echinator]
21	5709	gi 749796492 ref XP_011151658.1	47.71	2	1	1	N	50096	PREDICTED: tubulin alpha-1 chain-like [Harpegnathos saltator]
21	5710	gi 780651001 ref XP_011690375.1	47.71	2	1	1	N	50110	PREDICTED: tubulin alpha-1 chain [Wasmannia auropunctata]
21	5711	gi 769855164 ref XP_011639147.1	47.71	2	1	1	N	50110	PREDICTED: tubulin alpha-1 chain [Pogonomyrmex barbatus]
21	5713	gi 759071477 ref XP_011345341.1	47.71	2	1	1	N	50110	PREDICTED: tubulin alpha-1 chain [Ceropachys biroï]
21	5714	gi 307178877 gb EFN67417.1	47.71	2	1	1	N	50110	Tubulin alpha-1 chain [Camponotus floridanus]
21	5715	gi 801390294 ref XP_012057479.1	47.71	2	1	1	N	52472	PREDICTED: tubulin alpha-1 chain [Atta cephalotes]
total 142 proteins									

Band # 17 Proteins

Summary

1. Notes

2. Result Statistics

Figure 1. False discovery rate (FDR) curve. X axis is the number of peptide-spectrum matches (PSM) being kept. Y axis is the corresponding FDR.

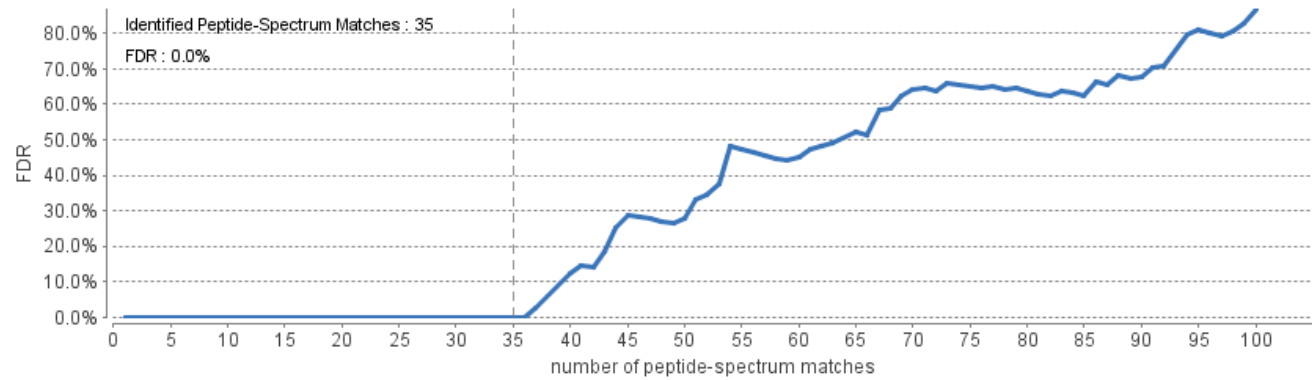


Figure 2. PSM score distribution. (a) Distribution of PEAKS peptide score; (b) Scatterplot of PEAKS peptide score versus precursor mass error.

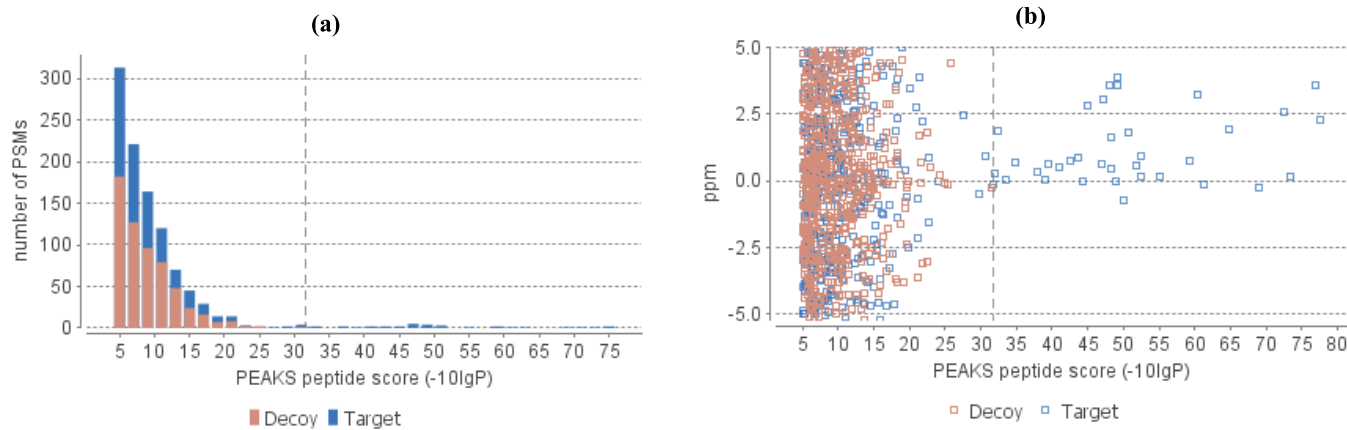


Figure 3. De novo result validation. Distribution of residue local confidence: (a) Residues in de novo sequences validated by confident database peptide assignment; (b) Residues in "de novo only" sequences.

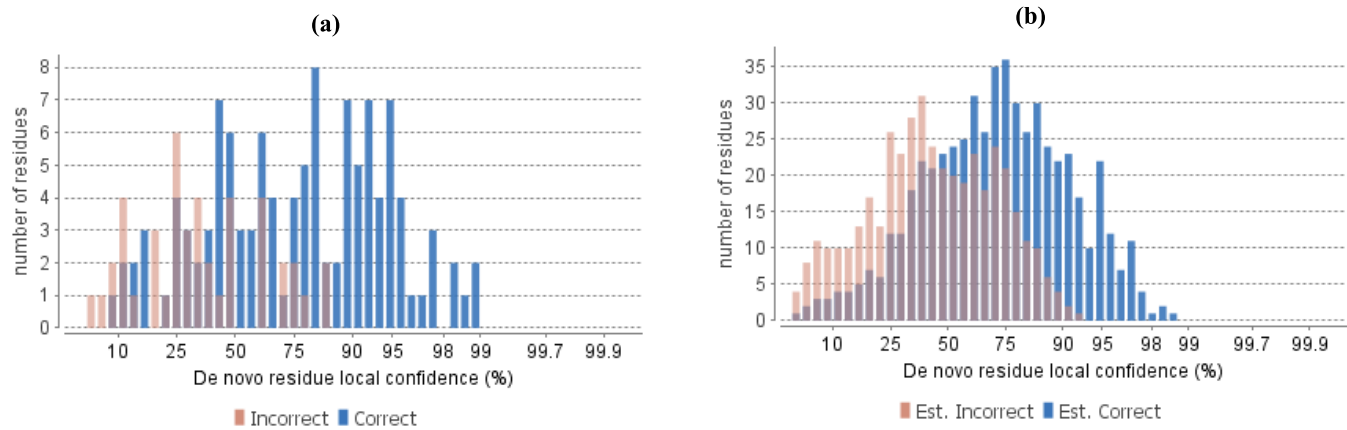


Table 1. Statistics of data.

# of MS Scans	1767
# of MS/MS Scans	2728

Table 4. PTM profile.

Name	Δ Mass	Position	#PSM	-10lgP	Area	AScore
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Table 2. Result filtration parameters.

Peptide -10lgP	≥31.7
Protein -10lgP	≥20
Proteins unique peptides	≥1
De novo ALC Score	≥50%

Table 3. Statistics of filtered result.

Peptide-Spectrum Matches	35
Peptide Sequences	28
Protein Groups	5
Proteins	7
Proteins (#Unique Peptides)	1 (>2); 1 (=2); 5 (=1);
FDR (Peptide-Spectrum Matches)	0.0%
FDR (Peptide Sequences)	0.0%
FDR (Protein)	0.0%
De Novo Only Spectra	89

3. Experiment Control

Figure 4. Precursor mass error of peptide-spectrum matches (PSM) in filtered result. **(a)** Distribution of precursor mass error in ppm; **(b)** Scatterplot of precursor m/z versus precursor mass error in ppm. 

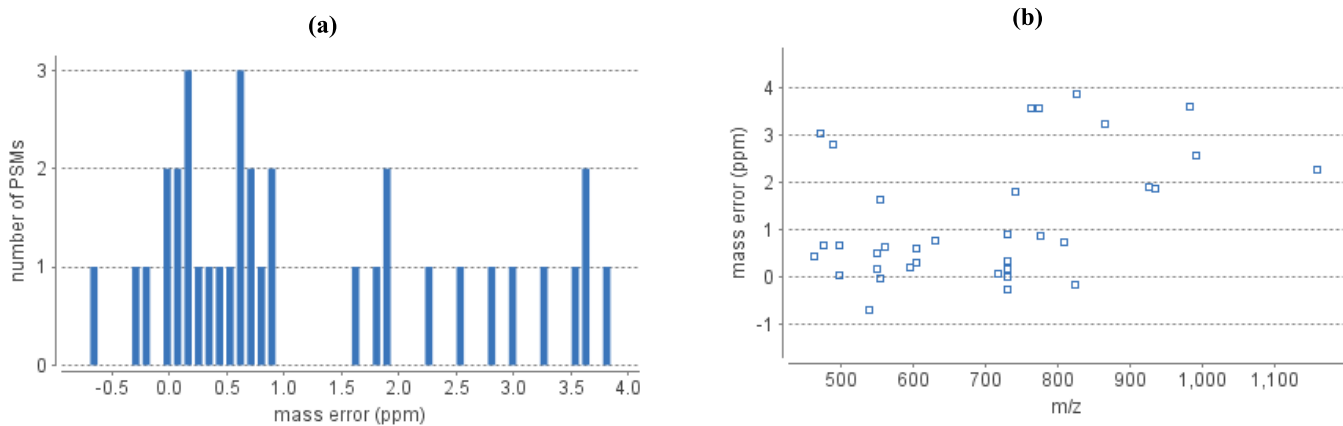


Table 5. Number of identified peptides in each sample by the number of missed cleavages

Missed Cleavages	0	1	2	3	4+
Sample 11	21	6	1	0	0

4. Other Information

Table 6. Search parameters.

Search Engine Name:	PEAKS
Parent Mass Error Tolerance:	5.0 ppm
Fragment Mass Error Tolerance:	0.5 Da
Precursor Mass Search Type:	monoisotopic
Enzyme:	Trypsin
Max Missed Cleavages:	3
Non-specific Cleavage:	one
Variable Modifications:	
Oxidation (M):	15.99
Max variable PTM per peptide:	3
Database:	Ant
Taxon:	All
Searched Entry:	473117
FDR Estimation:	Enabled
Merge Options:	no merge
Precursor Options:	corrected
Charge Options:	no correction

Oxidation	15.99	M	6	72.56	1.03E5	1000.00
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Table 7. Instrument parameters.

Fractions:	TW_17.raw
Ion Source:	ESI(nano-spray)
Fragmentation Mode:	CID, CAD(y and b ions)
MS Scan Mode:	FT-ICR/Orbitrap
MS/MS Scan Mode:	FT-ICR/Orbitrap

Filter Options: no filter
Process: true

Protein List

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
1	25219	gi 815803678 ref XP_012222542.1	221.61	21	17	5	Y	77863	PREDICTED: transferrin [Linepithema humile]
3	14086	gi 1009374605 gb KYM98331.1	187.24	12	8	1	Y	75845	Transferrin [Cyphomyrmex costatus]
4	25220	gi 780662966 ref XP_011693308.1	178.73	12	8	2	Y	77337	PREDICTED: transferrin isoform X2 [Wasmannia auropunctata]
6	14093	gi 861647058 gb KM95759.1	133.85	4	4	1	Y	140001	transferrin [Lasius niger]
7	77	gi 1911819 gb AAB50883.1	52.50	10	1	1	Y	11819	Myr p I=allergenic polypeptide {N-termina l} [Myrmecia pilosula=jumper ants, venom, Peptide Partial, 112 aa]
7	78	gi 312284 emb CAA49760.1	52.50	10	1	1	Y	11849	major allergen [Myrmecia pilosula]
7	76	gi 730091 sp Q07932.1 MYR1_MYRPI	52.50	10	1	1	Y	11849	RecName: Full=Pilosulin-1; AltName: Full=Allergen Myr p I; AltName: Full=Major allergen Myr p 1; AltName: Allergen=Myr p 1; Contains: RecName: Full=Pilosulin-1; Contains: RecName: Full=Pilosulin-1 65->112; Contains: RecNa...
total 7 proteins									

Band # 18 Proteins

Summary

1. Notes

2. Result Statistics

Figure 1. False discovery rate (FDR) curve. X axis is the number of peptide-spectrum matches (PSM) being kept. Y axis is the corresponding FDR.

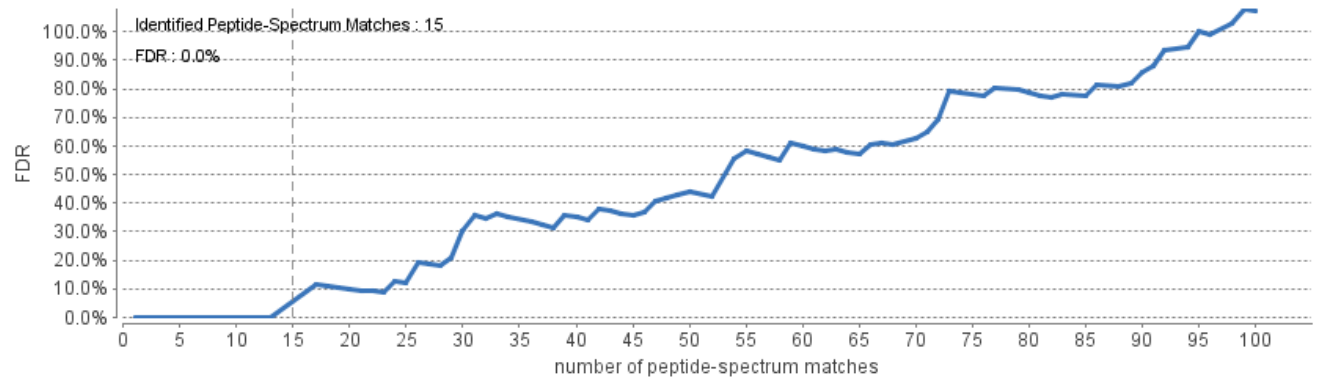


Figure 2. PSM score distribution. (a) Distribution of PEAKS peptide score; (b) Scatterplot of PEAKS peptide score versus precursor mass error.

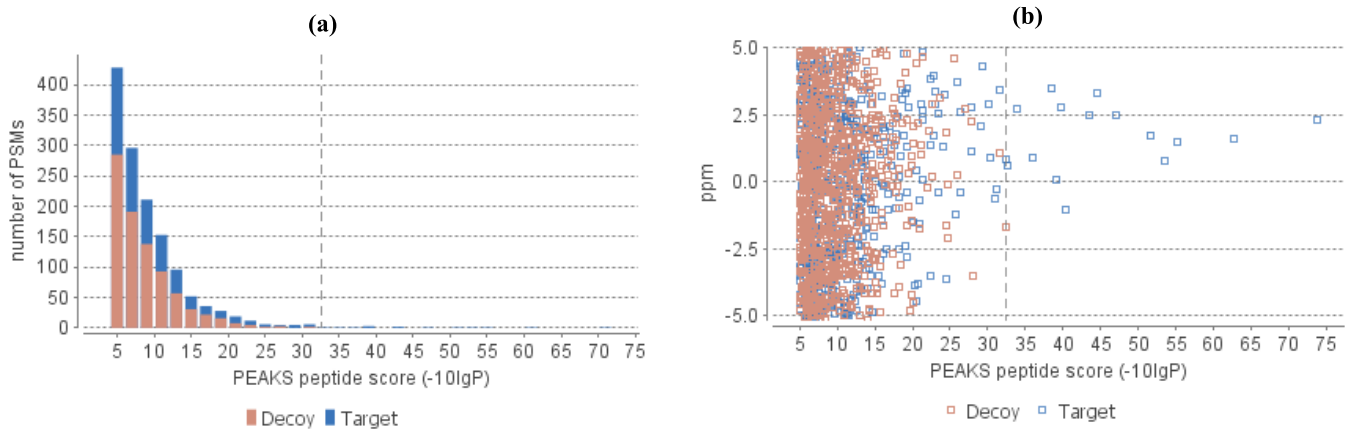


Figure 3. De novo result validation. Distribution of residue local confidence: (a) Residues in de novo sequences validated by confident database peptide assignment; (b) Residues in "de novo only" sequences.

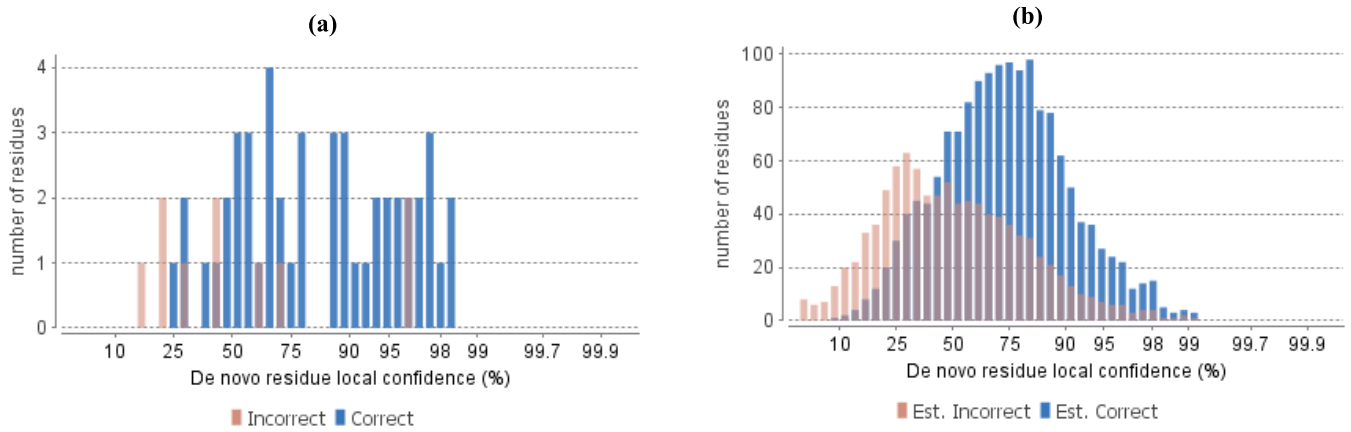


Table 1. Statistics of data.
of MS Scans 1576
of MS/MS Scans 3450

Table 4. PTM profile.
Name ΔMass Position #PSM -10lgP Area AScore

Table 2. Result filtration parameters.

Peptide -10lgP	≥32.5
Protein -10lgP	≥20
Proteins unique peptides	≥1
De novo ALC Score	≥50%

Table 3. Statistics of filtered result.

Peptide-Spectrum Matches	15
Peptide Sequences	13
Protein Groups	7
Proteins	44
Proteins (#Unique Peptides)	0 (>2); 0 (=2); 44 (=1);
FDR (Peptide-Spectrum Matches)	0.0%
FDR (Peptide Sequences)	0.0%
FDR (Protein)	0.0%
De Novo Only Spectra	236

3. Experiment Control

Figure 4. Precursor mass error of peptide-spectrum matches (PSM) in filtered result. **(a)** Distribution of precursor mass error in ppm; **(b)** Scatterplot of precursor m/z versus precursor mass error in ppm. 

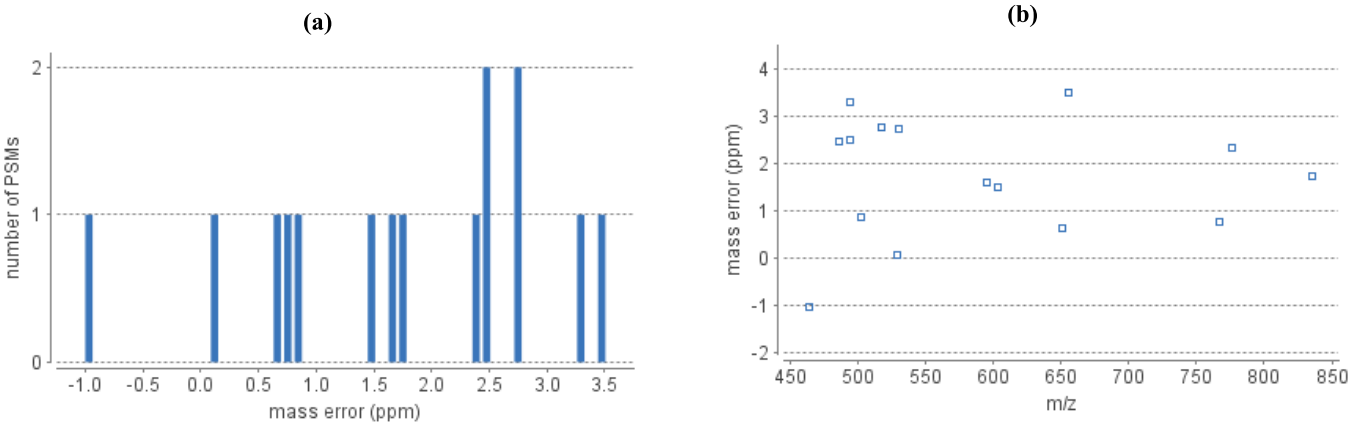


Table 5. Number of identified peptides in each sample by the number of missed cleavages

Missed Cleavages	0	1	2	3	4+
Sample 12	10	3	0	0	0

4. Other Information

Table 6. Search parameters.

Search Engine Name:	PEAKS
Parent Mass Error Tolerance:	5.0 ppm
Fragment Mass Error Tolerance:	0.5 Da
Precursor Mass Search Type:	monoisotopic
Enzyme:	Trypsin
Max Missed Cleavages:	3
Non-specific Cleavage:	one
Variable Modifications:	
Oxidation (M):	15.99
Max variable PTM per peptide:	3
Database:	Ant
Taxon:	All
Searched Entry:	473117
FDR Estimation:	Enabled
Merge Options:	no merge
Precursor Options:	corrected
Charge Options:	no correction

Table 7. Instrument parameters.

Fractions:	TW_18.raw
Ion Source:	ESI(nano-spray)
Fragmentation Mode:	CID, CAD(y and b ions)
MS Scan Mode:	FT-ICR/Orbitrap
MS/MS Scan Mode:	FT-ICR/Orbitrap

Filter Options: no filter

Process: true

Protein List

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
1	26382	gi 769837606 ref XP_011629993.1	125.91	6	4	1	Y	87451	PREDICTED: venom dipeptidyl peptidase 4 [Pogonomyrmex barbatus]
5	26399	gi 749744541 ref XP_011154777.1	75.26	4	2	1	Y	88356	PREDICTED: venom dipeptidyl peptidase 4 [Harpegnathos saltator]
5	26400	gi 307211949 gb EFN87861.1	75.26	4	2	1	Y	92672	Dipeptidyl peptidase 4 [Harpegnathos saltator]
10	77	gi 1911819 gb AAB50883.1	62.65	10	1	1	Y	11819	Myr p I=allergenic polypeptide {N-termina l} [Myrmecia pilosula=jumper ants, venom, Peptide Partial, 112 aa]
10	78	gi 312284 emb CAA49760.1	62.65	10	1	1	Y	11849	major allergen [Myrmecia pilosula]
10	76	gi 730091 sp Q07932.1 MYR1_MYRPI	62.65	10	1	1	Y	11849	RecName: Full=Pilosulin-1; AltName: Full=Allergen Myr p I; AltName: Full=Major allergen Myr p 1; AltName: Allergen=Myr p 1; Contains: RecName: Full=Pilosulin-1; Contains: RecName: Full=Pilosulin-1 65->112; Contains: RecNa...
46	26413	gi 746838195 ref XP_011049616.1	39.04	1	1	1	N	132922	PREDICTED: liprin-alpha-1 isoform X20 [Acromyrmex echinator]
46	4627	gi 749752541 ref XP_011138620.1	39.04	1	1	1	N	135758	PREDICTED: liprin-alpha-1 isoform X11 [Harpegnathos saltator]
46	26414	gi 746838193 ref XP_011049615.1	39.04	1	1	1	N	136490	PREDICTED: liprin-alpha-1 isoform X19 [Acromyrmex echinator]
46	26415	gi 746838191 ref XP_011049614.1	39.04	1	1	1	N	140332	PREDICTED: liprin-alpha-1 isoform X18 [Acromyrmex echinator]
46	26416	gi 746838189 ref XP_011049613.1	39.04	1	1	1	N	140419	PREDICTED: liprin-alpha-1 isoform X17 [Acromyrmex echinator]
46	26417	gi 746838187 ref XP_011049612.1	39.04	1	1	1	N	142003	PREDICTED: liprin-alpha-1 isoform X16 [Acromyrmex echinator]
46	26418	gi 746838185 ref XP_011049611.1	39.04	1	1	1	N	142090	PREDICTED: liprin-alpha-1 isoform X15 [Acromyrmex echinator]
46	26419	gi 746838183 ref XP_011049610.1	39.04	1	1	1	N	141972	PREDICTED: liprin-alpha-1 isoform X14 [Acromyrmex echinator]
46	26420	gi 746838181 ref XP_011049608.1	39.04	1	1	1	N	142384	PREDICTED: liprin-alpha-1 isoform X13 [Acromyrmex echinator]
46	26421	gi 746838179 ref XP_011049607.1	39.04	1	1	1	N	142471	PREDICTED: liprin-alpha-1 isoform X12 [Acromyrmex echinator]
46	26422	gi 746838177 ref XP_011049606.1	39.04	1	1	1	N	142822	PREDICTED: liprin-alpha-1 isoform X11 [Acromyrmex echinator]
46	26423	gi 746838175 ref XP_011049605.1	39.04	1	1	1	N	142910	PREDICTED: liprin-alpha-1 isoform X10 [Acromyrmex echinator]
46	4629	gi 746838173 ref XP_011049604.1	39.04	1	1	1	N	143236	PREDICTED: liprin-alpha-1 isoform X9 [Acromyrmex echinator]
46	26424	gi 746838171 ref XP_011049603.1	39.04	1	1	1	N	143323	PREDICTED: liprin-alpha-1 isoform X8 [Acromyrmex echinator]
46	26425	gi 746838169 ref XP_011049602.1	39.04	1	1	1	N	143930	PREDICTED: liprin-alpha-1 isoform X7 [Acromyrmex echinator]
46	26426	gi 746838163 ref XP_011049599.1	39.04	1	1	1	N	144311	PREDICTED: liprin-alpha-1 isoform X4 [Acromyrmex echinator]
46	26427	gi 746838165 ref XP_011049600.1	39.04	1	1	1	N	144355	PREDICTED: liprin-alpha-1 isoform X5 [Acromyrmex echinator]
46	7502	gi 746838167 ref XP_011049601.1	39.04	1	1	1	N	144211	PREDICTED: liprin-alpha-1 isoform X6 [Acromyrmex echinator]
46	26428	gi 746838161 ref XP_011049597.1	39.04	1	1	1	N	144493	PREDICTED: liprin-alpha-1 isoform X3 [Acromyrmex echinator]
46	26429	gi 746838159 ref XP_011049596.1	39.04	1	1	1	N	144580	PREDICTED: liprin-alpha-1 isoform X2 [Acromyrmex echinator]
46	26430	gi 746838153 ref XP_011049593.1	39.04	1	1	1	N	144962	PREDICTED: liprin-alpha-1 isoform X1 [Acromyrmex echinator]
46	26431	gi 746838157 ref XP_011049595.1	39.04	1	1	1	N	144962	PREDICTED: liprin-alpha-1 isoform X1 [Acromyrmex echinator]
46	26432	gi 746838155 ref XP_011049594.1	39.04	1	1	1	N	144962	PREDICTED: liprin-alpha-1 isoform X1 [Acromyrmex echinator]
46	26433	gi 749752511 ref XP_011138605.1	39.04	1	1	1	N	145269	PREDICTED: liprin-alpha-1 isoform X1 [Harpegnathos saltator]
46	26434	gi 749752517 ref XP_011138608.1	39.04	1	1	1	N	145269	PREDICTED: liprin-alpha-1 isoform X1 [Harpegnathos saltator]
46	26435	gi 749752515 ref XP_011138607.1	39.04	1	1	1	N	145269	PREDICTED: liprin-alpha-1 isoform X1 [Harpegnathos saltator]
46	26436	gi 749752507 ref XP_011138603.1	39.04	1	1	1	N	145269	PREDICTED: liprin-alpha-1 isoform X1 [Harpegnathos saltator]
46	26437	gi 749752513 ref XP_011138606.1	39.04	1	1	1	N	145269	PREDICTED: liprin-alpha-1 isoform X1 [Harpegnathos saltator]

total 44 proteins

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
46	26438	gi 749752519 ref XP_011138609.1	39.04	1	1	1	N	145269	PREDICTED: liprin-alpha-1 isoform X1 [Harpegnathos saltator]
46	26439	gi 749752509 ref XP_011138604.1	39.04	1	1	1	N	145269	PREDICTED: liprin-alpha-1 isoform X1 [Harpegnathos saltator]
47	143	gi 307184709 gb EFN71038.1	36.05	4	1	1	N	22151	hypothetical protein EAG_09928 [Camponotus floridanus]
47	4127	gi 861653549 gb KMQ99191.1	36.05	1	1	1	N	108034	dynammin-like mitochondrial protein [Lasius niger]
47	195	gi 801397101 ref XP_012058936.1	36.05	1	1	1	N	113731	PREDICTED: dynammin-like 120 kDa protein, mitochondrial isoform X3 [Atta cephalotes]
47	4128	gi 801397099 ref XP_012058935.1	36.05	1	1	1	N	113933	PREDICTED: dynammin-like 120 kDa protein, mitochondrial isoform X2 [Atta cephalotes]
47	4129	gi 801397097 ref XP_012058934.1	36.05	1	1	1	N	114004	PREDICTED: dynammin-like 120 kDa protein, mitochondrial isoform X1 [Atta cephalotes]
27	192	gi 1009422031 gb KYN40424.1	33.85	1	1	1	N	84216	hypothetical protein ALC56_05369 [Trachymyrmex septentrionalis]
11	180	gi 951525616 ref XP_014489536.1	32.61	1	1	1	N	111966	PREDICTED: protein stum-like [Dinoponera quadricaps]
11	181	gi 951525618 ref XP_014489537.1	32.61	1	1	1	N	111966	PREDICTED: protein stum-like [Dinoponera quadricaps]
total 44 proteins									

Prepared with PEAKS™ (bioinform.com)

Band # 19 Proteins

Summary

1. Notes

2. Result Statistics

Figure 1. False discovery rate (FDR) curve. X axis is the number of peptide-spectrum matches (PSM) being kept. Y axis is the corresponding FDR.

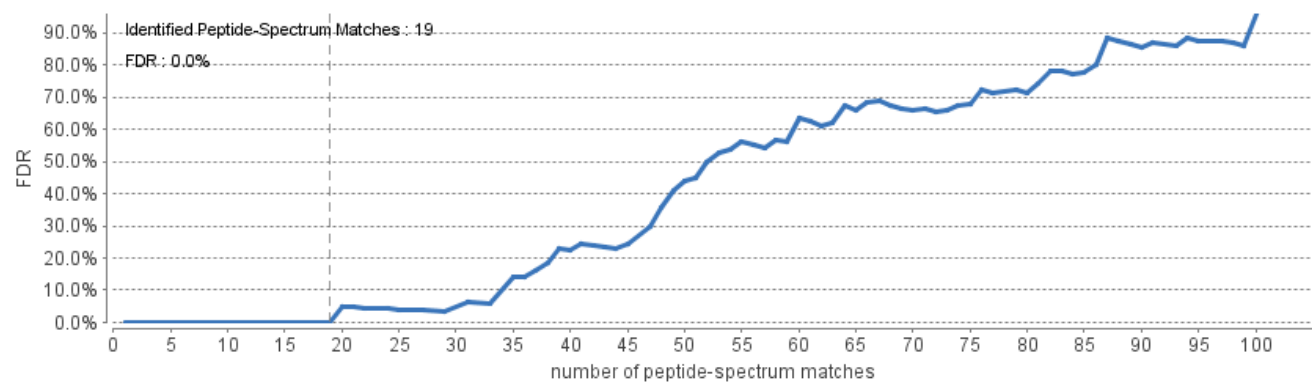


Figure 2. PSM score distribution. (a) Distribution of PEAKS peptide score; (b) Scatterplot of PEAKS peptide score versus precursor mass error.

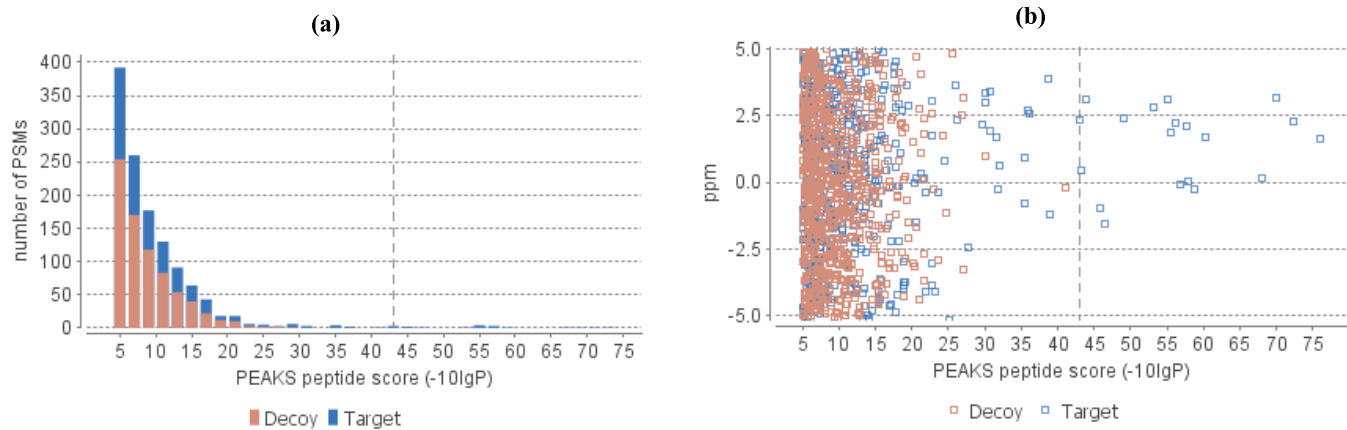


Figure 3. De novo result validation. Distribution of residue local confidence: (a) Residues in de novo sequences validated by confident database peptide assignment; (b) Residues in "de novo only" sequences.

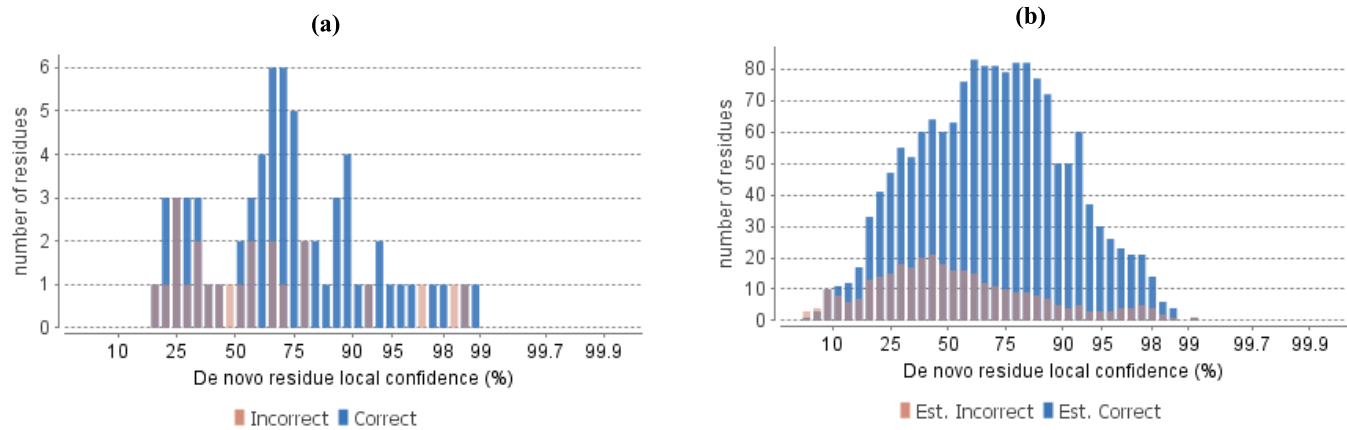


Table 1. Statistics of data.

# of MS Scans	1651
# of MS/MS Scans	3148

Table 4. PTM profile.

Name	Δ Mass	Position	#PSM	-10lgP	Area	AScore
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Table 2. Result filtration parameters.

Peptide -10lgP	≥43
Protein -10lgP	≥20
Proteins unique peptides	≥1
De novo ALC Score	≥50%

Table 3. Statistics of filtered result.

Peptide-Spectrum Matches	19
Peptide Sequences	14
Protein Groups	4
Proteins	45
Proteins (#Unique Peptides)	12 (>2); 0 (=2); 33 (=1);
FDR (Peptide-Spectrum Matches)	0.0%
FDR (Peptide Sequences)	0.0%
FDR (Protein)	0.0%
De Novo Only Spectra	183

3. Experiment Control

Figure 4. Precursor mass error of peptide-spectrum matches (PSM) in filtered result. **(a)** Distribution of precursor mass error in ppm; **(b)** Scatterplot of precursor m/z versus precursor mass error in ppm.

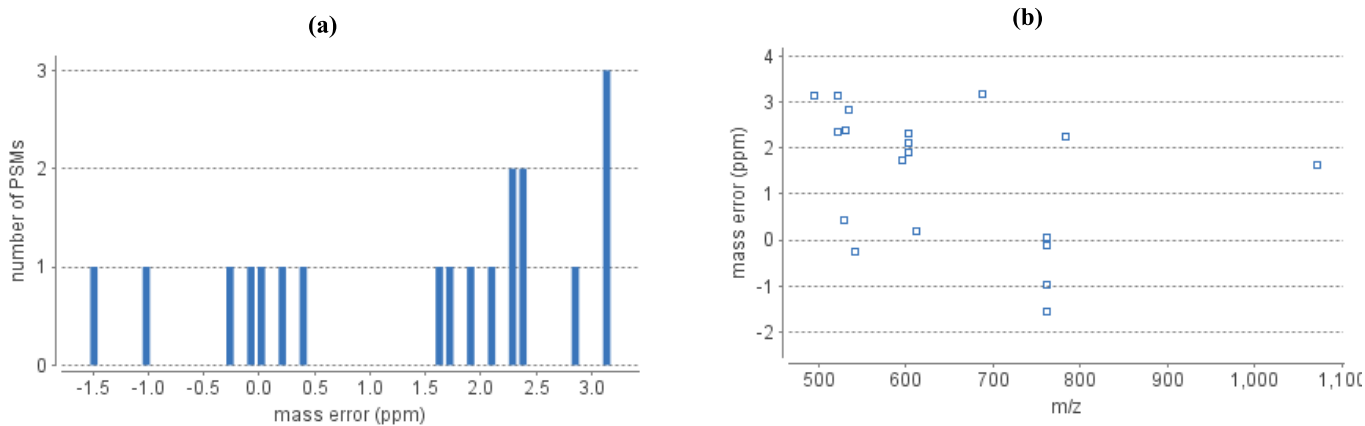


Table 5. Number of identified peptides in each sample by the number of missed cleavages

Missed Cleavages	0	1	2	3	4+
Sample 18	8	6	0	0	0

4. Other Information

Table 6. Search parameters.

Search Engine Name:	PEAKS
Parent Mass Error Tolerance:	5.0 ppm
Fragment Mass Error Tolerance:	0.5 Da
Precursor Mass Search Type:	monoisotopic
Enzyme:	Trypsin
Max Missed Cleavages:	3
Non-specific Cleavage:	one
Variable Modifications:	
Oxidation (M):	15.99
Max variable PTM per peptide:	3
Database:	Ant
Taxon:	All
Searched Entry:	473117
FDR Estimation:	Enabled
Merge Options:	no merge
Precursor Options:	corrected
Charge Options:	no correction

Filter Options: no filter

Process: true

Protein List

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
1	77	gi 1911819 gb AAB50883.1	149.12	20	4	4	Y	11819	Myr p I=allergenic polypeptide {N-terminal} [Myrmecia pilosula=jumper ants, venom, Peptide Partial, 112 aa]
1	78	gi 312284 emb CAA49760.1	149.12	20	4	4	Y	11849	major allergen [Myrmecia pilosula]
1	76	gi 730091 sp Q07932.1 MYR1_MYRPI	149.12	20	4	4	Y	11849	RecName: Full=Pilosulin-1; AltName: Full=Allergen Myr p I; AltName: Full=Major allergen Myr p 1; AltName: Allergen=Myr p 1; Contains: RecName: Full=Pilosulin-1; Contains: RecName: Full=Pilosulin-1 65->112; Contains: RecNa...
4	34801	gi 161788856 dbj BAF95069.1	109.17	22	3	3	N	9816	pilosulin 5 [Myrmecia banksi]
4	34802	gi 347602359 sp A9CM07.1 MYRB5_MYRBA	109.17	22	3	3	N	9816	RecName: Full=Pilosulin-5; Flags: Precursor
2	34794	gi 746831859 ref XP_011055222.1	105.28	24	3	3	N	14703	PREDICTED: ubiquitin-60S ribosomal protein L40 [Acromyrmex echinatio]
2	34795	gi 607368776 gb EZA62882.1	105.28	24	3	3	N	14703	Ubiquitin-60S ribosomal protein L40 [Ceraapachys biroi]
2	34796	gi 607366383 gb EZA60553.1	105.28	20	3	3	N	17940	Ubiquitin-40S ribosomal protein S27a [Ceraapachys biroi]
2	34797	gi 607352215 gb EZA47229.1	105.28	7	3	3	N	51356	Polyubiquitin-A [Ceraapachys biroi]
2	34798	gi 746860486 ref XP_011061085.1	105.28	7	3	3	N	51500	PREDICTED: polyubiquitin [Acromyrmex echinatio]
2	34799	gi 746853516 ref XP_011057361.1	105.28	6	3	3	N	59878	PREDICTED: polyubiquitin-like [Acromyrmex echinatio]
2	34800	gi 607364060 gb EZA58281.1	105.28	4	3	3	N	94034	Polyubiquitin-A [Ceraapachys biroi]
44	34804	gi 752870746 ref XP_011252539.1	43.22	1	1	1	N	118026	PREDICTED: liprin-alpha-1 isoform X14 [Camponotus floridanus]
44	34805	gi 780646574 ref XP_011689328.1	43.22	1	1	1	N	120409	PREDICTED: liprin-alpha-1 isoform X13 [Wasmannia auropunctata]
44	26413	gi 746838195 ref XP_011049616.1	43.22	1	1	1	N	132922	PREDICTED: liprin-alpha-1 isoform X20 [Acromyrmex echinatio]
44	26414	gi 746838193 ref XP_011049615.1	43.22	1	1	1	N	136490	PREDICTED: liprin-alpha-1 isoform X19 [Acromyrmex echinatio]
44	26415	gi 746838191 ref XP_011049614.1	43.22	1	1	1	N	140332	PREDICTED: liprin-alpha-1 isoform X18 [Acromyrmex echinatio]
44	26416	gi 746838189 ref XP_011049613.1	43.22	1	1	1	N	140419	PREDICTED: liprin-alpha-1 isoform X17 [Acromyrmex echinatio]
44	26417	gi 746838187 ref XP_011049612.1	43.22	1	1	1	N	142003	PREDICTED: liprin-alpha-1 isoform X16 [Acromyrmex echinatio]
44	26418	gi 746838185 ref XP_011049611.1	43.22	1	1	1	N	142090	PREDICTED: liprin-alpha-1 isoform X15 [Acromyrmex echinatio]
44	26419	gi 746838183 ref XP_011049610.1	43.22	1	1	1	N	141972	PREDICTED: liprin-alpha-1 isoform X14 [Acromyrmex echinatio]
44	26420	gi 746838181 ref XP_011049608.1	43.22	1	1	1	N	142384	PREDICTED: liprin-alpha-1 isoform X13 [Acromyrmex echinatio]
44	26421	gi 746838179 ref XP_011049607.1	43.22	1	1	1	N	142471	PREDICTED: liprin-alpha-1 isoform X12 [Acromyrmex echinatio]
44	34806	gi 752870728 ref XP_011252530.1	43.22	1	1	1	N	142428	PREDICTED: liprin-alpha-1 isoform X5 [Camponotus floridanus]
44	26422	gi 746838177 ref XP_011049606.1	43.22	1	1	1	N	142822	PREDICTED: liprin-alpha-1 isoform X11 [Acromyrmex echinatio]
44	26423	gi 746838175 ref XP_011049605.1	43.22	1	1	1	N	142910	PREDICTED: liprin-alpha-1 isoform X10 [Acromyrmex echinatio]
44	4629	gi 746838173 ref XP_011049604.1	43.22	1	1	1	N	143236	PREDICTED: liprin-alpha-1 isoform X9 [Acromyrmex echinatio]
44	26424	gi 746838171 ref XP_011049603.1	43.22	1	1	1	N	143323	PREDICTED: liprin-alpha-1 isoform X8 [Acromyrmex echinatio]
44	34807	gi 752870716 ref XP_011252523.1	43.22	1	1	1	N	143179	PREDICTED: liprin-alpha-1 isoform X1 [Camponotus floridanus]
44	26425	gi 746838169 ref XP_011049602.1	43.22	1	1	1	N	143930	PREDICTED: liprin-alpha-1 isoform X7 [Acromyrmex echinatio]
44	26426	gi 746838163 ref XP_011049599.1	43.22	1	1	1	N	144311	PREDICTED: liprin-alpha-1 isoform X4 [Acromyrmex echinatio]
44	26427	gi 746838165 ref XP_011049600.1	43.22	1	1	1	N	144355	PREDICTED: liprin-alpha-1 isoform X5 [Acromyrmex echinatio]
44	7502	gi 746838167 ref XP_011049601.1	43.22	1	1	1	N	144211	PREDICTED: liprin-alpha-1 isoform X6 [Acromyrmex echinatio]
44	26428	gi 746838161 ref XP_011049597.1	43.22	1	1	1	N	144493	PREDICTED: liprin-alpha-1 isoform X3 [Acromyrmex echinatio]
44	26429	gi 746838159 ref XP_011049596.1	43.22	1	1	1	N	144580	PREDICTED: liprin-alpha-1 isoform X2 [Acromyrmex echinatio]
total 45 proteins									

Protein Group	Protein ID	Accession	-10lgP	Coverage (%)	#Peptides	#Unique	PTM	Avg. Mass	Description
44	26430	gi 746838153 ref XP_011049593.1	43.22	1	1	1	N	144962	PREDICTED: liprin-alpha-1 isoform X 1 [Acromyrmex echinator]
44	26431	gi 746838157 ref XP_011049595.1	43.22	1	1	1	N	144962	PREDICTED: liprin-alpha-1 isoform X 1 [Acromyrmex echinator]
44	26432	gi 746838155 ref XP_011049594.1	43.22	1	1	1	N	144962	PREDICTED: liprin-alpha-1 isoform X 1 [Acromyrmex echinator]
44	26433	gi 749752511 ref XP_011138605.1	43.22	1	1	1	N	145269	PREDICTED: liprin-alpha-1 isoform X 1 [Harpegnathos saltator]
44	26434	gi 749752517 ref XP_011138608.1	43.22	1	1	1	N	145269	PREDICTED: liprin-alpha-1 isoform X 1 [Harpegnathos saltator]
44	26435	gi 749752515 ref XP_011138607.1	43.22	1	1	1	N	145269	PREDICTED: liprin-alpha-1 isoform X 1 [Harpegnathos saltator]
44	26436	gi 749752507 ref XP_011138603.1	43.22	1	1	1	N	145269	PREDICTED: liprin-alpha-1 isoform X 1 [Harpegnathos saltator]
44	26437	gi 749752513 ref XP_011138606.1	43.22	1	1	1	N	145269	PREDICTED: liprin-alpha-1 isoform X 1 [Harpegnathos saltator]
44	26438	gi 749752519 ref XP_011138609.1	43.22	1	1	1	N	145269	PREDICTED: liprin-alpha-1 isoform X 1 [Harpegnathos saltator]
44	26439	gi 749752509 ref XP_011138604.1	43.22	1	1	1	N	145269	PREDICTED: liprin-alpha-1 isoform X 1 [Harpegnathos saltator]
total 45 proteins									

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