Data Article

Data on bioactive peptides derived from chicken hydrolysate with potential alcohol dehydrogenase stabilizing activity and in silico analysis of their potential activity and applicability

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ABSTRACT

Bioactive peptides have attracted extensive attention worldwide as natural alternatives to promote human health and wellness. Previous studies have shown that chicken hydrolysates could enhance alcohol dehydrogenase, and subsequently they facilitate alcohol metabolism and ameliorate alcohol-induced liver injury. The data presented in this article support the accompanying research article “Isolation and identification of alcohol dehydrogenase stabilizing peptides from Alcalase digested chicken breast hydrolysates”. Present article details all 82 peptides identified from the most active fractions of chicken hydrolysates, and 154 peptides from in silico digestion of the 82 identified peptides, together with the prediction of their potential bioactivity and applicability using several in silico assays.

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1. Data

The data in this article include a total 82 peptides from the most active fractions of a chicken hydrolysate after SEC and RP-HPLC separation. Raw data is showed in Table 1 of Supplementary material, including search parameters. Table 1 lists all these peptides together with the potential bioactivity and applicability, indicated by Peptide Ranker score, potential peptide allergenicity, toxicity and physicochemical properties (i.e., hydrophobicity, amphipathicity, steric hindrance, pI, and molecular weight). Also, as potential functional food ingredients, peptides must be digested and absorbed through the gastrointestinal tract to exert activity. Hence, all peptides were further subjected to in silico gastrointestinal digestion and a total of 154 peptides were generated. All the 154 peptides are listed in Table 2, as well as their potential bioactivity and applicability.
2. **Experimental design, materials, and methods**

2.1. **Preparation and separation of chicken peptides**

Peptides were produced and separated according to our previous study with slight modification [1]. In brief, chicken breast was digested in tris-HCl buffer (50 mM, pH 8.0, 1:5 m/v) by Alcalase 2.4L (0.5% w/w, protein basis) for 8 h. The hydrolysates were then centrifuged (10000 rpm, 20 min, 4 °C), and deproteinized (adding 3 volumes of ethanol, stored at 4 °C, 20h before centrifugation). After centrifugation at 10000 rpm at 4 °C for 20 min, the ethanol was removed in a rotatory evaporator, and the peptides were lyophilized and re-dissolved in distilled water for Sephadex G25 separation. The peptides were eluted using 0.01 N HCl at 4 °C with a flow rate of 5 mL/20 min. Fractions were collected, lyophilized and re-dissolved in distilled water for analysis and separation.

The most active fraction obtained from G25 fractionation was further isolated using HPLC with a Symmetry C18 column. The mobile phases consisted of solvent A: 0.1% v/v trifluoroacetic acetic acid (TFA) and solvent B: 0.085% v/v TFA in acetonitrile (ACN). Peptides were diluted using the following gradient: 0% B from 0 to 2 min, linearly increasing to 30% B at 50 min, 60% B at 60 min and 100% B at 65 min under a flow rate of 1 mL/min. Fractions were collected, lyophilized, and re-dissolved for analysis and identification.

2.2. **Identification of peptide sequences**

Peptides were identified using nano-LC tandem nanoelectrospray ionization source-quadrupole-time-of-flight (nanoESI-Q-ToF) MS/MS (AB Sciex Instruments, MA, USA). The sample was concentrated using Zip-Tip C18 (Millipore Corporation, Bedford, MA, USA) before loaded onto an Eksigen trap column (3 μm C18-CL, 350 μm × 0.5 mm). Peptides were eluted using an analytical column (3 μm C18-CL, 75 μm × 123 mm; Nikkyo Technos Co, Ltd. Japan) under a flow rate of 0.3 μL/min at 30 °C. The mobile phases consisted of solvent A: 0.1% v/v formic acid (FA) in water and solvent B: 1% FA in acetonitrile (ACN). Peptides were eluted linearly from 5% to 35% solvent B over the first 20 min, and then from 35% to 65% solvent B for 10 min.

The flow from the LC was ionized applying 2.8 kV. The Q-ToF was operated in positive polarity and information-dependent acquisition mode. MS1 scan was acquired from 350 to 1250 m/z for 250 ms, while MS2 scan was required from 100 to 1500 m/z for 50 ms on 50 of the most intense ions charging from 1 to 5. Up to 25 ions were selected for fragmentation after each survey scan. Dynamic exclusion was set to 15 s.

The database searching of peptides was performed using the Mascot Distiller v2.4.2.0 software (Matrix Science, Inc., Boston, MA; http://www.matrixscience.com), and Mascot search engine with a significance threshold p < 0.05 using Chordata taxonomy, none enzyme digestion, and Uniprot database. The tolerance on the mass measurement was 0.3 Da for MS and 100 ppm for MS/MS.

2.3. **In silico analysis of peptide bioactivity and applicability**

**In silico** gastrointestinal digestion was assessed using the ExPASy PeptideCutter tool (http://web.expasy.org/peptide_cutter/). PeptideCutter predicts the potential cleavage sites by proteases in a given peptide sequence, according to the specific cleavage sites of proteases, and thus generate new peptides [2]. In present study, pepsin (pH 1.3 and pH > 2.0), trypsin, and chymotrypsin were chosen as digesting enzymes [3].

The potential bioactivity was predicted using the Peptide Ranker software (http://distilldeep.ucd.ie/PeptideRanker/) [4]. The prediction of peptide bioactivity was focused on particular amino acid residues as certain classes of bioactive peptides have specific structure features and amino acid sequences [5]. Peptides were scored from 0 to 1 and higher value means higher probability to be bioactive.

The potential peptide allergenicity was predicted using the AllerTOP v. 2.0 software (http://www.ddg-pharmfac.net/AllerTOP/index.html) [6]. Peptides were classified by k-nearest neighbor algorithm based on training set containing 2427 known allergens from different species and 2427 non-allergens.
| No. | Peptide Sequence | Peptide Ranker Score | Allergenicity Prediction | Nearest Protein | Toxicity Prediction | SVM Score | Steric Hindrance | Amphipathicity | Hydrophobicity | pI | Molecular Weight (Da) |
|-----|------------------|----------------------|--------------------------|----------------|---------------------|----------|-----------------|---------------|---------------|----|---------------------|
| 1   | DPDDFPL          | 0.91                 | non-allergen             | UniProtKB accession number P17676 | Non-Toxin | -0.88       | 0.6            | 0             | -0.17         | 3.43 | 817.35              |
| 2   | NKISVVGVAVGMACAIILMSDLIA | 0.86                | non-allergen             | UniProtKB accession number Q105T8 | Non-Toxin | -1.47       | 0.65           | 0.29          | 0.13          | 8.54 | 2459.33             |
| 3   | DPQYPPGPPAF      | 0.85                 | non-allergen             | UniProtKB accession number Q9S8M0 | Non-Toxin | -0.27       | 0.52           | 0.1           | -0.07         | 3.8  | 1281.60             |
| 4   | ADGPLKGL         | 0.77                 | non-allergen             | UniProtKB accession number Q9NP55 | Non-Toxin | -0.72       | 0.6            | 0.41          | 0.05          | 6.19 | 882.52              |
| 5   | RDQYPPGPPAF      | 0.76                 | non-allergen             | UniProtKB accession number Q9S8M0 | Non-Toxin | -0.35       | 0.53           | 0.28          | -0.2          | 6.19 | 1437.70             |
| 6   | ARDPQYPPGPPAF    | 0.72                 | non-allergen             | UniProtKB accession number Q9S8M0 | Non-Toxin | -0.38       | 0.53           | 0.26          | -0.16         | 6.19 | 1508.74             |
| 7   | LPQPAQYNVINGSHAGNKL  | 0.70                 | non-allergen             | UniProtKB accession number Q9S8M0 | Non-Toxin | -1.14       | 0.59           | 0.27          | 0.03          | 9.11 | 1904.03             |
| 8   | ENPQKYPGTMFGAK  | 0.69                 | non-allergen             | UniProtKB accession number Q9SSX0 | Non-Toxin | -0.89       | 0.64           | 0.89          | -0.13         | 9.84 | 2034.13             |
| 9   | AGFQGDDAPRAVFP   | 0.69                 | non-allergen             | UniProtKB accession number Q8WQYQ3 | Non-Toxin | -1.19       | 0.62           | 0.18          | -0.03         | 4.21 | 1375.65             |
| 10  | GFAGDDAPRAVFP    | 0.67                 | non-allergen             | UniProtKB accession number Q9NP55 | Non-Toxin | -1.16       | 0.61           | 0.19          | -0.04         | 4.21 | 1318.63             |
| 11  | DGPLKGL          | 0.66                 | non-allergen             | UniProtKB accession number Q9NP55 | Non-Toxin | -0.76       | 0.62           | 0.46          | 0.03          | 6.19 | 811.48              |
| 12  | ATGNPNDIVWNLK    | 0.60                 | non-allergen             | UniProtKB accession number P09564 | Non-Toxin | -0.58       | 0.6            | 0.28          | -0.06         | 6.19 | 1423.75             |
| 13  | PPGPQGPGPQPGPGPGHQT | 0.55                 | non-allergen             | UniProtKB accession number Q9S8M0 | Non-Toxin | -0.15       | 0.51           | 0.33          | -0.03         | 9.11 | 2195.19             |
| 14  | FDEKPADLPSL      | 0.53                 | non-allergen             | UniProtKB accession number P23582 | Non-Toxin | -1.19       | 0.58           | 0.45          | -0.15         | 4.03 | 1230.61             |
| 15  | AVNDPFDI         | 0.49                 | non-allergen             | UniProtKB accession number P86071 | Non-Toxin | -1.03       | 0.66           | 0             | 0             | 3.57 | 889.42              |
| 16  | DVPQVPVLDPKPV    | 0.47                 | non-allergen             | UniProtKB accession number QST440 | Non-Toxin | -1.23       | 0.59           | 0.31          | 0.01          | 4.21 | 1247.71             |
| 17  | VIDVPGPRNRL      | 0.45                 | non-allergen             | UniProtKB accession number Q7M2H1 | Non-Toxin | -0.6        | 0.63           | 0.22          | -0.02         | 6.19 | 1177.68             |
| 18  | VNLVDKPGPPAFAF   | 0.42                 | non-allergen             | UniProtKB accession number QST028 | Non-Toxin | -1.16       | 0.59           | 0.28          | 0.02          | 6.19 | 1323.72             |
| 19  | FDEKPADLPSLVE    | 0.39                 | non-allergen             | UniProtKB accession number P23582 | Non-Toxin | -1.16       | 0.6            | 0.48          | -0.13         | 3.92 | 1458.72             |
|   | Peptide Sequence                  | Allergenicity | UniProtKB Accession Number | Prediction Score | UniProtKB Tip | P-Value | Scores | AUC | Sensitivity | Specificity |Fold Change |
|---|----------------------------------|---------------|----------------------------|------------------|---------------|---------|--------|-----|------------|------------|-------------|
|20| GGFAPNILDNHEALE                 | 0.37          | UniProtKB accession number Q9C0K0 | Non-Toxin -1.23 | 0.59         | 0.27    | -0.03 | 4.14| 1595.76    |             |             |
|21| AEEFFDL                       | 0.33          | UniProtKB accession number Q8BT70 | Non-Toxin -0.63 | 0.61         | 0.48    | -0.16 | 3.51| 948.41     |             |             |
|22| FMVLPVGAA                      | 0.30          | UniProtKB accession number P69448 | Non-Toxin -1.07 | 0.61         | 0       | 0.34  | 5.88| 903.49     |             |             |
|23| PFQSSASSPSPSKNE                 | 0.30          | UniProtKB accession number Q8BWWM7 | Non-Toxin -0.89 | 0.55         | 0.41    | -0.26 | 6.35| 1548.71    |             |             |
|24| DTFTPGPPYAL                    | 0.29          | UniProtKB accession number P54259 | Non-Toxin -0.54  | 0.55         | 0       | 0.01  | 3.8 | 1278.61    |             |             |
|25| IEDPFDQDDWE                    | 0.28          | UniProtKB accession number Q9SLY8 | Non-Toxin -0.69  | 0.67         | 0.34    | -0.29 | 3.26| 1407.55    |             |             |
|26| MVVDGKVLML                     | 0.25          | UniProtKB accession number P48494 | Non-Toxin -1.03  | 0.7          | 0.41    | 0.11  | 6.19| 990.52     |             |             |
|27| NFPYDGKDVRIDL                  | 0.23          | UniProtKB accession number Q9H0F7 | Non-Toxin -1.15  | 0.66         | 0.44    | -0.24 | 4.43| 1651.82    |             |             |
|28| DNHEALELL                      | 0.23          | UniProtKB accession number Q9S8F6 | Non-Toxin -1.14  | 0.55         | 0.44    | -0.13 | 4.14| 1052.51    |             |             |
|29| EAEFLPD                        | 0.21          | UniProtKB accession number A2WLM6 | Non-Toxin -0.72  | 0.61         | 0.48    | -0.16 | 3.51| 948.41     |             |             |
|30| EDLQPVLDDL                     | 0.19          | UniProtKB accession number P02647 | Non-Toxin -1.02  | 0.62         | 0.62    | -0.18 | 4.03| 1168.63    |             |             |
|31| FDPVVEEKI                      | 0.15          | UniProtKB accession number Q9S8N3 | Non-Toxin -1.17  | 0.66         | 0.69    | -0.08 | 4.14| 1074.56    |             |             |
|32| VPEDSQEECAITY                  | 0.15          | UniProtKB accession number Q8T68 | Non-Toxin -0.79  | 0.63         | 0.39    | -0.17 | 3.51| 1482.62    |             |             |
|33| DSNADRLGSEVEQVQ                 | 0.10          | UniProtKB accession number Q97766 | Non-Toxin -1.42  | 0.66         | 0.44    | -0.21 | 3.92| 1905.91    |             |             |
|34| RDKEPSGFLDVIQT                  | 0.10          | UniProtKB accession number Q5SW96 | Non-Toxin -1.42  | 0.63         | 0.51    | -0.27 | 4.23| 1920.94    |             |             |
|35| LTDTOPASPRGSET                  | 0.07          | UniProtKB accession number Q8BWQ3 | Non-Toxin -1.53  | 0.56         | 0.16    | -0.11 | 3.58| 1574.73    |             |             |
|36| SSEEEDNDEAEY                    | 0.05          | UniProtKB accession number Q9BT70 | Non-Toxin -0.85  | 0.67         | 0.74    | -0.43 | 3.32| 1407.52    |             |             |
|37| NVLFLDGLGTFDVSDTIDDGFVEN       | 0.02          | UniProtKB accession number Q9BT70 | Non-Toxin -1.63  | 0.67         | 0.18    | 0     | 3.72| 2896.51    |             |             |
|38| PATIVVIPIDEESRNGTILVDNMLKGTAGPDPIE | 0.02      | UniProtKB accession number Q53JQ4 | Non-Toxin -0.86  | 0.62         | 0.28    | -0.06 | 4.02| 3646.88    |             |             |
|39| RIPVIPLEPDEGIYT                 | 0.15          | UniProtKB accession number Q6UX39 | Non-Toxin -1.7    | 0.63         | 0.36    | -0.06 | 4.14| 1599.85    |             |             |
|40| ELGPMKTPCLCKAA                  | 0.61          | NCBI gi number 6069656 | Non-Toxin -1.41  | 0.57         | 0.61    | -0.04 | 8.54| 1470.79    |             |             |
|41| LEQNQPIIDDMPA                   | 0.32          | UniProtKB accession number Q01412 | Non-Toxin -1.39  | 0.64         | 0.29    | -0.13 | 3.5 | 1482.70    |             |             |

(continued on next page)
| No. | Peptide Sequence       | Peptide Ranker Score | Allergenicity Prediction | Nearest Protein             | Toxicity Prediction | SVM Score | Steric Hindrance | Amphipathicity | Hydrophobicity | pl | Molecular Weight (Da) |
|-----|-----------------------|----------------------|--------------------------|-----------------------------|---------------------|-----------|------------------|----------------|---------------|----|----------------------|
| 42  | AYEPVWAIGKTATPQ       | 0.22                 | allergen                 | UniProtKB accession number P85814 | Non-Toxin | −1.28  | 0.58             | 0.36           | −0.02         | 6.35 | 1788.90              |
| 43  | GEHGDSVPVWSGVNVA      | 0.35                 | allergen                 | UniProtKB accession number O42799 | Non-Toxin | −1.26  | 0.59             | 0.16           | 0             | 4.36 | 1695.79              |
| 44  | DLFDPVQ               | 0.18                 | allergen                 | NCBI gi number 423193       | Non-Toxin | −1.25  | 0.66             | 0.14           | −0.06         | 3.43 | 1060.51              |
| 45  | VPTQHRGPVVL           | 0.18                 | allergen                 | NCBI gi number 741844       | Non-Toxin | −1.23  | 0.54             | 0.47           | −0.08         | 10.11 | 1201.69              |
| 46  | AVGAVFDISNADRL        | 0.39                 | allergen                 | NCBI gi number 1171011      | Non-Toxin | −1.2   | 0.65             | 0.18           | −0.02         | 4.21 | 1446.75              |
| 47  | AVGAVFDIS             | 0.22                 | allergen                 | NCBI gi number 29163773     | Non-Toxin | −1.2   | 0.65             | 0.23           | 3.8           | 877.45 |                   |
| 48  | FPFDVPSEPK            | 0.58                 | allergen                 | NCBI gi number 63052        | Non-Toxin | −1.18  | 0.58             | 0.49           | −0.12         | 4.38  | 1161.57              |
| 49  | LPTGIPNPYE            | 0.19                 | allergen                 | NCBI gi number 50199132     | Non-Toxin | −1.07  | 0.65             | 0.55           | −0.1          | 4.21  | 1073.58              |
| 50  | KDLFDPVQ              | 0.27                 | allergen                 | NCBI gi number 1836010      | Non-Toxin | −1.06  | 0.63             | 0.25           | 0.05          | 3.58  | 1012.51              |
| 51  | GDIGIEIPAE            | 0.18                 | allergen                 | NCBI gi number 542132       | Non-Toxin | −1.04  | 0.64             | 0.78           | −0.22         | 6.42  | 1286.69              |
| 52  | SNKPELIDML            | 0.46                 | allergen                 | NCBI gi number 3004471      | Non-Toxin | −1.03  | 0.6              | 0.13           | 0.18          | 4     | 1100.61              |
| 53  | VPANVINGHSAGNKL       | 0.60                 | allergen                 | UniProtKB accession number BOY665 | Non-Toxin | −1.02  | 0.65             | 0.16           | 0.03          | 3.57  | 945.48               |
| 54  | DLFDPVIQ              | 0.31                 | allergen                 | NCBI gi number 1836010      | Non-Toxin | −0.99  | 0.65             | 0.2            | −0.15         | 3.94  | 1381.65              |
| 55  | DLAGRDLTDYLM          | 0.36                 | allergen                 | UniProtKB accession number Q28049 | Non-Toxin | −0.98  | 0.66             | 0.76           | −0.17         | 4.32  | 1443.78              |
| 56  | TLVDVVEDKLKGE         | 0.06                 | allergen                 | NCBI gi number 14148979     | Non-Toxin | −0.96  | 0.46             | 0.18           | 0.26          | 7.1   | 832.52               |
| 57  | LLILAPGH              | 0.38                 | allergen                 | UniProtKB accession number P01315 | Non-Toxin | −0.94  | 0.65             | 0.26           | −0.06         | 4.03  | 1936.92              |
| 58  | YGKDATNVGDEGGFAPNIL   | 0.32                 | allergen                 | NCBI gi number 160347126    | Non-Toxin | −0.94  | 0.65             | 0.76           | −0.26         | 4.68  | 1471.79              |
| 59  | NDEELNKLGLKVT         | 0.20                 | allergen                 | NCBI gi number 47117355     | Non-Toxin | −0.94  | 0.65             | 0.07           | 0.26          | 7.1   | 965.54               |
| 60  | HLIPKML               | 0.66                 | allergen                 | UniProtKB accession number P35776 | Non-Toxin | −0.92  | 0.54             | 0.64           | −0.03         | 7.09  | 965.54               |
| 61  | IDDHF2DHPVSP          | 0.46                 | allergen                 | NCBI gi number 3914446      | Non-Toxin | −0.92  | 0.58             | 0.39           | −0.08         | 4.42  | 1528.76              |
| 62  | NGDKKSLGLHLTTL        | 0.39                 | allergen                 | NCBI gi number 261865475    | Non-Toxin | −0.92  | 0.59             | 0.72           | −0.17         | 7.1   | 1523.83              |
| 63  | INDHFPDLN             | 0.60                 | allergen                 | NCBI gi number 7228147      | Non-Toxin | −0.9   | 0.67             | 0              | −0.02         | 3.57  | 1059.52              |
| 64  | IDDHF2DHPVSPPL        | 0.71                 | allergen                 | NCBI gi number 3914446      | Non-Toxin | −0.89  | 0.58             | 0.37           | −0.04         | 4.42  | 1641.84              |
| 65  | DDHF2DHPVSPPL         | 0.75                 | allergen                 | NCBI gi number 3914446      | Non-Toxin | −0.87  | 0.57             | 0.39           | −0.1          | 4.42  | 1528.76              |
| 66  | NYILDHLGLSK           | 0.29                 | allergen                 | UniProtKB accession number P00709 | Non-Toxin | −0.87  | 0.58             | 0.47           | −0.06         | 7.09  | 1271.69              |
| 67  | VSHRGETEDTIFADI      | 0.10                 | allergen                 | NCBI gi number 60116876     | Non-Toxin | −0.87  | 0.59             | 0.4            | −0.18         | 4.31  | 1775.83              |
| 68  | DSSNTLSIFIK           | 0.32                 | allergen                 | UniProtKB accession number Q39869 | Non-Toxin | −0.83  | 0.64             | 0.31           | −0.06         | 6.19  | 1280.66              |
| 69  | VHVLLVNPHTGAT         | 0.18                 | allergen                 | NCBI gi number 5689675      | Non-Toxin | −0.82  | 0.5              | 0.22           | 0.09          | 7.26  | 1356.75              |
| 70  | GPPIPILGVT           | 0.83                  | allergen                 | UniProtKB accession number Q9UMD9 | Non-Toxin | −0.81  | 0.57             | 0.1            | 3.8           | 964.52 |                   |
| 71  | DQIDDEIKLI           | 0.25                  | allergen                 | NCBI gi number 28374072     | Non-Toxin | −0.8   | 0.69             | 0.62           | −0.18         | 3.84  | 1200.62              |
|   | Sequence                      | Allergy | NCBI gi number   | UniProtKB accession number | Toxicity | Score  |
|---|------------------------------|---------|------------------|----------------------------|----------|--------|
| 72| DNPVDLI                      | allergen| 105969543        |                            | Non-Toxin| 0.38   |
| 73| AKYGKDATNGDEGGFAPNIL         | allergen| 160347126        |                            | Non-Toxin| 0.28   |
| 74| EVMIDVLK                     | allergen| 19039            |                            | Non-Toxin| 0.14   |
| 75| DQIDDEIKLIGY                 | allergen|                 | UniProtKB accession       | Non-Toxin| 0.30   |
| 76| DDVIQTGVGDNPQHPFIM           | allergen| 7228147          |                            | Non-Toxin| 0.43   |
| 77| SLKPEFVDIINAKH               | allergen|                 | UniProtKB accession       | Non-Toxin| 0.40   |
| 78| LKPEFVDIINAKH                | allergen|                 | UniProtKB accession       | Non-Toxin| 0.28   |
| 79| NVMSGTTMYPGIADRM             | allergen| 62550933         |                            | Non-Toxin| 0.18   |
| 80| GDNPQHPYIM                   | allergen| 14423730         |                            | Non-Toxin| 0.69   |
| 81| PDPLDPTCSLCTCSEGMRCCP        | non-allergen|                | UniProtKB accession      | Toxin    | 0.80   |
| 82| IPGPPTGPIKF                  | non-allergen|            | UniProtKB accession      | Toxin    | 0.88   |

**Toxicity Score Range:**
- Non-Toxin: 0 - 0.06
- Toxin: 0.09 - 0.88

**Score:**
- Score: 105163
Table 2
Peptides obtained from the *in silico* gastrointestinal digestion simulation and prediction of their bioactivity, allergenicity, toxicity, and physicochemical properties.

| No. | Peptide Sequence | Peptide Ranker Score | Allergenicity Prediction | Nearest Protein | Toxicity Prediction | SVM Score | Steric Hindrance | Amphipathicity | Hydrophobicity | pI | Molecular Weight (Da) |
|-----|------------------|----------------------|--------------------------|----------------|---------------------|----------|------------------|----------------|---------------|----|---------------------|
| 1   | IF               | 0.95                 | non-allergen             | UniProtKB accession number Q8WW43 | Non-Toxin | -0.8 | 0.7 | 0 | 0.67 | 5.88 | 278.37 |
| 2   | GPPDPIL          | 0.91                 | non-allergen             | UniProtKB accession number Q9Y2D1 | Non-Toxin | -0.24 | 0.54 | 0 | 0.07 | 3.8 | 707.92 |
| 3   | GG               | 0.89                 | non-allergen             | UniProtKB accession number Q04130 | Non-Toxin | -0.8 | 0.68 | 0 | 0.16 | 5.88 | 132.14 |
| 4   | DPQYPPGPPAF      | 0.88                 | non-allergen             | UniProtKB accession number Q9S8M0 | Non-Toxin | -0.27 | 0.53 | 0.11 | -0.07 | 3.8 | 1185.44 |
| 5   | QKPVL            | 0.82                 | non-allergen             | UniProtKB accession number P49918 | Non-Toxin | -0.88 | 0.59 | 0.98 | -0.16 | 9.11 | 583.8 |
| 6   | KPC              | 0.71                 | non-allergen             | UniProtKB accession number P01075 | Non-Toxin | -0.72 | 0.55 | 1.22 | -0.38 | 8.57 | 346.47 |
| 7   | PEDEGI           | 0.70                 | non-allergen             | UniProtKB accession number Q9S8M0 | Non-Toxin | -0.9 | 0.64 | 0.42 | -0.19 | 3.58 | 658.74 |
| 8   | APGH             | 0.65                 | non-allergen             | UniProtKB accession number Q9S8K1 | Non-Toxin | -0.86 | 0.39 | 0.36 | -0.02 | 7.1 | 380.45 |
| 9   | GIL              | 0.61                 | non-allergen             | UniProtKB accession number O14569 | Non-Toxin | -0.79 | 0.64 | 0 | 0.47 | 5.88 | 301.43 |
| 10  | AVF              | 0.59                 | non-allergen             | UniProtKB accession number P21926 | Non-Toxin | -0.83 | 0.64 | 0 | 0.47 | 5.88 | 335.43 |
| 11  | PDP              | 0.57                 | non-allergen             | UniProtKB accession number Q9T72Q9 | Non-Toxin | -0.82 | 0.49 | 0 | -0.29 | 3.8 | 327.36 |
| 12  | GGDDAPR          | 0.56                 | non-allergen             | UniProtKB accession number Q7M1V9 | Non-Toxin | -1.07 | 0.63 | 0.35 | -0.39 | 4.21 | 686.76 |
| 13  | KPEF             | 0.56                 | non-allergen             | UniProtKB accession number Q6N8M9 | Non-Toxin | -0.89 | 0.6 | 1.23 | -0.3 | 6.35 | 519.64 |
| 14  | ADGP             | 0.56                 | non-allergen             | UniProtKB accession number P83184 | Non-Toxin | -0.71 | 0.58 | 0 | -0.09 | 3.8 | 358.39 |
| 15  | GDSSVPVW         | 0.56                 | non-allergen             | UniProtKB accession number P02747 | Non-Toxin | -0.99 | 0.59 | 0 | 0.04 | 3.8 | 846.01 |
| 16  | AGR              | 0.55                 | non-allergen             | UniProtKB accession number P80806 | Non-Toxin | -0.78 | 0.63 | 0.82 | -0.45 | 10.11 | 302.36 |
| 17  | AG               | 0.55                 | non-allergen             | UniProtKB accession number Q109R6 | Non-Toxin | -0.8 | 0.6 | 0 | 0.21 | 5.88 | 146.16 |
| 18  | PTGIPIV          | 0.54                 | non-allergen             | UniProtKB accession number Q9T2Q0 | Non-Toxin | -0.81 | 0.58 | 0 | 0.26 | 5.88 | 695.96 |
| 19  | AGDDAPR          | 0.54                 | non-allergen             | UniProtKB accession number Q7M1V9 | Non-Toxin | -1.09 | 0.61 | 0.35 | -0.37 | 4.21 | 700.78 |
|   | Sequence                  | Score | Allergy | UniProtKB accession number | Type | IEDB ID | MSA ID | Allergy ID | Score   | Score   | Score   | Score   | Score   | Score   |
|---|--------------------------|-------|---------|----------------------------|------|---------|---------|------------|---------|---------|---------|---------|---------|---------|
| 20| GGGT                     | 0.53  | non-allergen | Q04130                     |      |         |         |             |         |         |         |         |         |         |
| 21| DVPGPVL                  | 0.50  | non-allergen | P83184                      |      |         |         |             |         |         |         |         |         |         |
| 22| VDIINAK                  | 0.40  | non-allergen | Q7M1V6                      |      |         |         |             |         |         |         |         |         |         |
| 23| SGNVNA                   | 0.39  | non-allergen | Q9SSV2                      |      |         |         |             |         |         |         |         |         |         |
| 24| VIDVPGPVR                | 0.34  | non-allergen | P46269                      |      |         |         |             |         |         |         |         |         |         |
| 25| SNK                      | 0.33  | non-allergen | Q7FA6Y6                     |      |         |         |             |         |         |         |         |         |         |
| 26| DPTCS                    | 0.31  | non-allergen | P01076                      |      |         |         |             |         |         |         |         |         |         |
| 27| DR                       | 0.29  | non-allergen | F2YHL2                      |      |         |         |             |         |         |         |         |         |         |
| 28| ACAISI                   | 0.29  | non-allergen | Q7M1U1                      |      |         |         |             |         |         |         |         |         |         |
| 29| ISVVGVAVGM               | 0.29  | non-allergen | Q10ST8                      |      |         |         |             |         |         |         |         |         |         |
| 30| INDP                     | 0.28  | non-allergen | P80819                      |      |         |         |             |         |         |         |         |         |         |
| 31| IPGTGK                   | 0.27  | non-allergen | P00068                      |      |         |         |             |         |         |         |         |         |         |
| 32| GTAAGPDPTIE              | 0.27  | non-allergen | Q9611K1                     |      |         |         |             |         |         |         |         |         |         |
| 33| AGIK                     | 0.25  | non-allergen | Q109R6                      |      |         |         |             |         |         |         |         |         |         |
| 34| PVPAF                    | 0.23  | non-allergen | Q3184                       |      |         |         |             |         |         |         |         |         |         |
| 35| AIGTGBK                  | 0.22  | non-allergen | Q8Y164                      |      |         |         |             |         |         |         |         |         |         |
| 36| VDNM                     | 0.22  | non-allergen | Q8N0T1                      |      |         |         |             |         |         |         |         |         |         |
| 37| CTCEEGSM                 | 0.20  | non-allergen | P30569                      |      |         |         |             |         |         |         |         |         |         |
| 38| AGNPK                    | 0.19  | non-allergen | Q7M1V9                      |      |         |         |             |         |         |         |         |         |         |
| 39| DNPVD                    | 0.19  | non-allergen | P80098                      |      |         |         |             |         |         |         |         |         |         |
| 40| GSK                      | 0.19  | non-allergen | Q13794                      |      |         |         |             |         |         |         |         |         |         |
| 41| DISNADR                  | 0.18  | non-allergen | Q04130                      |      |         |         |             |         |         |         |         |         |         |

(continued on next page)
| No. | Peptide Sequence | Peptide Ranker Score | Allergenicity Prediction | Nearest Protein | Toxicity Prediction | SVM Score | Steric Hindrance | Amphipaticity | Hydrophobicity | pl | Molecular Weight (Da) |
|-----|------------------|----------------------|-------------------------|----------------|---------------------|-----------|-------------------|--------------|----------------|----|----------------------|
| 42  | DVPSEPK          | 0.17                 | non-allergen            | UniProtKB accession number P41208 | Non-Toxin | -1.03 | 0.58              | 0.71         | -0.33          | 4.38 | 770.92               |
| 43  | AVNLP            | 0.16                 | non-allergen            | UniProtKB accession number A0MH06 | Non-Toxin | -0.92 | 0.62              | 0            | -0.13          | 3.8  | 514.59               |
| 44  | IDDHH            | 0.16                 | non-allergen            | UniProtKB accession number P80819 | Non-Toxin | -0.9  | 0.55              | 0.36         | -0.28          | 4.2  | 498.54               |
| 45  | DDSHH            | 0.16                 | non-allergen            | UniProtKB accession number Q9HBK9 | Non-Toxin | -0.82 | 0.51              | 0.48         | -0.61          | 4.2  | 385.36               |
| 46  | DSSNTNG          | 0.16                 | non-allergen            | UniProtKB accession number Q9S8WD | Non-Toxin | -0.59 | 0.63              | 0            | -0.32          | 3.8  | 579.59               |
| 47  | DGAT             | 0.15                 | non-allergen            | UniProtKB accession number Q9T2R4 | Non-Toxin | -0.78 | 0.56              | 0.19         | -0.15          | 3.93 | 1463.73              |
| 48  | DDVIQTGVDNPCHGPF | 0.15                 | non-allergen            | UniProtKB accession number Q968K1 | Non-Toxin | -0.53 | 0.6               | 0.36         | 0.08           | 3.8  | 727.91               |
| 49  | GIEIPAE          | 0.14                 | non-allergen            | UniProtKB accession number Q9691 | Non-Toxin | -0.88 | 0.62              | 0.36         | 0.08           | 3.8  | 727.91               |
| 50  | IEDP             | 0.14                 | non-allergen            | UniProtKB accession number P80819 | Non-Toxin | -0.72 | 0.62              | 0.32         | -0.17          | 3.67 | 472.54               |
| 51  | DNH              | 0.14                 | non-allergen            | UniProtKB accession number Q8WW43 | Non-Toxin | -0.81 | 0.51              | 0.48         | -0.59          | 5.09 | 384.38               |
| 52  | IAD              | 0.14                 | non-allergen            | UniProtKB accession number P86005 | Non-Toxin | -0.81 | 0.66              | 0.09         | 0.32           | 3.8  | 317.37               |
| 53  | IS               | 0.13                 | non-allergen            | UniProtKB accession number P42055 | Non-Toxin | -0.8  | 0.61              | 0.23         | 5.88           |     | 218.27               |
| 54  | TTPGPPY          | 0.13                 | non-allergen            | UniProtKB accession number A0MH06 | Non-Toxin | -0.2  | 0.5               | 0            | -0.06          | 5.88 | 731.89               |
| 55  | DPVIQD           | 0.13                 | non-allergen            | UniProtKB accession number Q9S8N3 | Non-Toxin | -1.12 | 0.66              | 0.21         | -0.15          | 3.57 | 685.81               |
| 56  | VL               | 0.13                 | non-allergen            | UniProtKB accession number P21730 | Non-Toxin | -0.8  | 0.61              | 0.54         | 5.88           |     | 230.33               |
| 57  | VDIINAK          | 0.12                 | non-allergen            | UniProtKB accession number P80818 | Non-Toxin | -0.38 | 0.69              | 0.52         | -0.03          | 6.19 | 772.01               |
| 58  | AVGAV            | 0.12                 | non-allergen            | UniProtKB accession number A9UGV5 | Non-Toxin | -0.8  | 0.62              | 0.35         | 5.88           |     | 415.55               |
| 59  | ETPSG            | 0.11                 | non-allergen            | UniProtKB accession number P26436 | Non-Toxin | -0.99 | 0.56              | 0.25         | -0.19          | 4    | 489.54               |
| 60  | AEEF             | 0.11                 | non-allergen            | UniProtKB accession number P26436 | Non-Toxin | -0.84 | 0.65              | 0.76         | -0.2           | 3.68 | 623.67               |
|   | UniProtKB accession number | Protein Name | Allergen | Non-Toxin | Confirmed-toxin | MRD | Signals | Exp|    |
|---|---------------------------|-------------|----------|-----------|----------------|-----|---------|----|----|
| 61 | Q9S8F6                    | DQDD        | 0.11     | non-allergen | Non-Toxin | 0.85 | 0.74  | 0.31 | -0.71 | 3.43 | 491.45 |
| 62 | P60006                    | DIS         | 0.11     | non-allergen | Non-Toxin | 0.82 | 0.66  | 0    | -0.08 | 3.8  | 333.37 |
| 63 | Q9C0F1                    | VPTQH       | 0.11     | non-allergen | Non-Toxin | 1.04 | 0.45  | 0.54 | -0.16 | 7.1  | 580.71 |
| 64 | P56615                    | ENPK        | 0.11     | non-allergen | Non-Toxin | 0.77 | 0.62  | 1.23 | -0.61 | 6.35 | 486.57 |
| 65 | Q9H246                    | AK          | 0.10     | non-allergen | Non-Toxin | 0.79 | 0.6   | 1.83 | -0.43 | 9.11 | 217.28 |
| 66 | Q9S8F6                    | EAL         | 0.09     | non-allergen | Non-Toxin | 0.84 | 0.58  | 0.42 | 0.05  | 4    | 331.4  |
| 67 | P31110                    | GVT         | 0.09     | non-allergen | Non-Toxin | 0.84 | 0.64  | 0    | 0.17  | 5.88 | 275.34 |
| 68 | Q8NB04                    | EVM         | 0.09     | non-allergen | Non-Toxin | 0.79 | 0.72  | 0.42 | 0.06  | 4    | 377.49 |
| 69 | O00585                    | TAT PQ      | 0.09     | non-allergen | Non-Toxin | 0.91 | 0.52  | 0.25 | -0.17 | 5.88 | 516.61 |
| 70 | Q9NWK09                   | VSH         | 0.07     | non-allergen | Non-Toxin | 0.83 | 0.41  | 0.48 | -0.04 | 7.1  | 341.4  |
| 71 | P86080                    | IDV         | 0.07     | non-allergen | Non-Toxin | 0.8  | 0.72  | 0    | 0.18  | 3.8  | 345.43 |
| 72 | Q08480                    | VID         | 0.06     | non-allergen | Non-Toxin | 0.8  | 0.72  | 0    | 0.18  | 3.8  | 345.43 |
| 73 | P86008                    | VVDGVK      | 0.06     | non-allergen | Non-Toxin | 1.07 | 0.7   | 0.61 | -0.01 | 6.19 | 615.81 |
| 74 | Q9S8N3                    | DPVVEEK     | 0.06     | non-allergen | Non-Toxin | 1.02 | 0.65  | 0.89 | -0.29 | 4.14 | 814.98 |
| 75 | Q75366                    | DT          | 0.05     | non-allergen | Non-Toxin | 0.8  | 0.65  | 0    | -0.45 | 3.8  | 234.22 |
| 76 | Q9BTT0                    | SEVEQVQ     | 0.05     | non-allergen | Non-Toxin | 1.11 | 0.66  | 0.72 | -0.26 | 3.8  | 817.95 |
| 77 | Q99467                    | NVINGGGS    | 0.04     | non-allergen | Non-Toxin | 0.68 | 0.6   | 0.18 | -0.04 | 7.1  | 796.96 |
| 78 | Q99467                    | NDEE        | 0.04     | non-allergen | Non-Toxin | 0.64 | 0.71  | 0.71 | -0.22 | 4.03 | 802.97 |
| 79 | A2XG55                    | NF          | 0.03     | non-allergen | Non-Toxin | 0.76 | 0.72  | 0.64 | -0.65 | 3.58 | 505.48 |
| 80 | P60006                    | SGETEDT     | 0.03     | non-allergen | Non-Toxin | 1.12 | 0.63  | 0.36 | -0.35 | 3.58 | 737.76 |

(continued on next page)
| No. | Peptide Sequence | Peptide Ranker Score | Allergenicity Prediction | Nearest Protein | Toxicity Prediction | SVM Score | Steric Hindrance | Amphipathicity | Hydrophobicity | pI | Molecular Weight (Da) |
|-----|-----------------|----------------------|--------------------------|-----------------|-------------------|------------|-----------------|----------------|--------------|----|----------------------|
| 82  | EAAE            | 0.03                 | non-allergen             | UniProtKB accession number Q9T2R4 | Non-Toxin | -0.9         | 0.64            | 0.95           | -0.4         | 3.68 | 476.48               |
| 83  | EQNQPIDDMM      | 0.27                 | allergen                 | UniProtKB accession number Q9BT70 | Non-Toxin | -1.34        | 0.68            | 0.42           | -0.35        | 3.5  | 1089.27              |
| 84  | ASPGSGGET       | 0.14                 | allergen                 | NCBI gi number 285005079 | Non-Toxin | -1.27        | 0.58            | 0.28           | -0.16        | 3.8  | 833.92               |
| 85  | PVGAA           | 0.31                 | allergen                 | NCBI gi number 1588669 | Non-Toxin | -1.14        | 0.56            | 0.23           | 5.88         | 413.53 |
| 86  | IPVVL           | 0.24                 | allergen                 | UniProtKB accession number P01504 | Non-Toxin | -1.06        | 0.6             | 0.45           | 5.88         | 539.79 |
| 87  | TDITPL          | 0.04                 | allergen                 | UniProtKB accession number Q60748 | Non-Toxin | -0.97        | 0.54            | 0              | -0.13        | 3.8  | 646.77               |
| 88  | EPVW            | 0.49                 | allergen                 | UniProtKB accession number P09944 | Non-Toxin | -0.94        | 0.56            | 0.32           | .            | 4    | 529.64               |
| 89  | PGADR           | 0.13                 | allergen                 | UniProtKB accession number Q7M278 | Non-Toxin | -0.93        | 0.62            | 0.41           | -0.24        | 6.19  | 627.77               |
| 90  | KPEL            | 0.19                 | allergen                 | NCBI gi number 3004471 | Non-Toxin | -0.92        | 0.56            | 1.23           | -0.32        | 6.35  | 485.63               |
| 91  | DPVQ            | 0.17                 | allergen                 | NCBI gi number 7228147 | Non-Toxin | -0.91        | 0.64            | 0.25           | -0.04        | 3.8   | 570.71               |
| 92  | DDVQQT          | 0.09                 | allergen                 | NCBI gi number 7435005 | Non-Toxin | -0.99        | 0.69            | 0.21           | -0.17        | 3.57  | 689.8                |
| 93  | DEKPADL         | 0.19                 | allergen                 | NCBI gi number 1480457 | Non-Toxin | -0.89        | 0.61            | 0.71           | -0.35        | 4.03  | 786.92               |
| 94  | VPAF            | 0.77                 | allergen                 | UniProtKB accession number O96522 | Non-Toxin | -0.88        | 0.57            | 0              | 0.33         | 5.88  | 432.56               |
| 95  | VPEDSQEECAIT    | 0.14                 | allergen                 | UniProtKB accession number P092636 | Non-Toxin | -0.88        | 0.62            | 0.42           | -0.19        | 3.51  | 1320.55              |
| 96  | DVSIF           | 0.07                 | allergen                 | UniProtKB accession number Q94907 | Non-Toxin | -0.88        | 0.67            | 0              | 0.07         | 3.8   | 432.52               |
| 97  | VNHPI           | 0.20                 | allergen                 | NCBI gi number 41017429 | Non-Toxin | -0.87        | 0.45            | 0.36           | -0.14        | 7.1   | 465.56               |
| 98  | GPVQ            | 0.21                 | allergen                 | NCBI gi number 1315111 | Non-Toxin | -0.86        | 0.61            | 0              | 0.29         | 5.88  | 337.5                |
| 99  | DPQDFF          | 0.81                 | allergen                 | NCBI gi number 110346534 | Non-Toxin | -0.85        | 0.67            | 0              | -0.32        | 3.43  | 607.62               |
| 100 | SEEDNEEEAEV     | 0.13                 | allergen                 | UniProtKB accession number P08334 | Non-Toxin | -0.85        | 0.67            | 0.74           | -0.43        | 3.32  | 1408.46              |
| 101 | APNI            | 0.38                 | allergen                 | NCBI gi number 1174276 | Non-Toxin | -0.84        | 0.58            | 0              | 0.07         | 5.88  | 413.52               |
| 102 | QTL             | 0.35                 | allergen                 | UniProtKB accession number Q15517 | Non-Toxin | -0.83        | 0.58            | 0.42           | -0.11        | 5.88  | 360.45               |
| 103 | PDL             | 0.41                 | allergen                 | UniProtKB accession number P09945 | Non-Toxin | -0.82        | 0.55            | 0              | -0.09        | 3.8   | 343.41               |
| 104 | PTY             | 0.27                 | allergen                 | NCBI gi number 50199132 | Non-Toxin | -0.82        | 0.53            | 0              | -0.08        | 5.88  | 379.44               |
| 105 | RPF             | 0.14                 | allergen                 | NCBI gi number 112559 | Non-Toxin | -0.82        | 0.58            | 1.22           | -0.21        | 9.11  | 342.47               |
| 106 | TKP             | 0.13                 | allergen                 | NCBI gi number 112559 | Non-Toxin | -0.82        | 0.52            | 1.22           | -0.45        | 9.11  | 344.44               |
|   | Accession | Allergen | UniProtKB accession number |    |      |      |      |      |      |      |      |      |      |
|---|-----------|----------|-----------------------------|---|----|----|----|----|----|----|----|----|----|
| 107 | DKPVSP    | 0.19     | Non-Toxin                   | −0.81 | 0.57 | 0.61 | −0.28 | 6.19 | 641.79 |
| 108 | VNV       | 0.03     | NCBI gi number 84698        | −0.81 | 0.72 | 0    | 0.15  | 5.88 | 330.42 |
| 109 | EVK       | 0.02     | UniProtKB accession number  | −0.81 | 0.69 | 1.65 | −0.39 | 6.35 | 374.47 |
| 110 | GF        | 0.99     | Non-Toxin                   | −0.8  | 0.69 | 0    | 0.39  | 5.88 | 222.26 |
| 111 | PSL       | 0.94     | NCBI gi number 33323477     | −0.8  | 0.47 | 0    | 0.07  | 5.88 | 315.4  |
| 112 | IM        | 0.70     | NCBI gi number 256636       | −0.8  | 0.74 | 0    | 0.49  | 5.88 | 262.39 |
| 113 | IG        | 0.50     | NCBI gi number 208605348    | −0.8  | 0.69 | 0    | 0.45  | 5.88 | 188.25 |
| 114 | IPA       | 0.43     | NCBI gi number 23616947     | −0.8  | 0.53 | 0    | 0.3   | 5.88 | 299.4  |
| 115 | AR        | 0.39     | Non-Toxin                   | −0.8  | 0.6  | 1.23 | −0.76 | 10.11 | 245.29 |
| 116 | GD        | 0.39     | UniProtKB accession number  | −0.8  | 0.72 | 0    | −0.28 | 3.8  | 190.17  |
| 117 | PATIVPIDEESR | 0.22 | allergen                   | −0.8  | 0.6  | 0.42 | −0.17 | 4.14 | 1326.63 |
| 118 | IH        | 0.21     | NCBI gi number 729979       | −0.8  | 0.35 | 0.72 | 0.16  | 7.1  | 268.34  |
| 119 | AA        | 0.19     | UniProtKB accession number  | −0.8  | 0.52 | 0    | 0.25  | 5.88 | 160.18 |
| 120 | NK        | 0.16     | NCBI gi number 218059728    | −0.8  | 0.72 | 1.83 | −0.87 | 9.11 | 260.31  |
| 121 | DH        | 0.15     | UniProtKB accession number  | −0.8  | 0.38 | 0.72 | −0.56 | 5.09 | 270.26 |
| 122 | GEH       | 0.13     | NCBI gi number 102834       | −0.8  | 0.45 | 0.91 | −0.29 | 5.25 | 341.36 |
| 123 | ID        | 0.13     | UniProtKB accession number  | −0.8  | 0.73 | 0    | 0.01  | 3.8  | 246.28 |
| 124 | GE        | 0.11     | UniProtKB accession number  | −0.8  | 0.68 | 0.64 | −0.23 | 4    | 204.2 |
| 125 | SL        | 0.11     | NCBI gi number 267048       | −0.8  | 0.53 | 0    | 0.14  | 5.88 | 218.27  |
| 126 | IK        | 0.10     | NCBI gi number 157829757    | −0.8  | 0.69 | 1.83 | −0.19 | 9.11 | 259.37 |
| 127 | TD        | 0.09     | NCBI gi number 50199132     | −0.8  | 0.65 | 0    | −0.45 | 3.8  | 234.22 |
| 128 | PD        | 0.09     | NCBI gi number 4138171      | −0.8  | 0.56 | 0    | −0.4  | 3.8  | 230.23 |
| 129 | TIDDGI    | 0.09     | UniProtKB accession number  | −0.8  | 0.69 | 0    | 0   | 3.57 | 632.75  |
| 130 | VH        | 0.07     | UniProtKB accession number  | −0.8  | 0.35 | 0.72 | 0.07  | 7.1  | 254.31  |
| 131 | NV        | 0.06     | NCBI gi number 14423664     | −0.8  | 0.73 | 0    | −0.05 | 5.88 | 231.27 |
| 132 | DK        | 0.06     | UniProtKB accession number  | −0.8  | 0.72 | 1.83 | −0.91 | 6.19 | 261.29 |
| 133 | ED        | 0.03     | UniProtKB accession number  | −0.8  | 0.72 | 0.64 | −0.67 | 3.67 | 262.23 |
| 134 | VT        | 0.03     | allergen                   | −0.8  | 0.61 | 0    | 0.18  | 5.88 | 218.27 |

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| No. | Peptide Sequence | Peptide Ranker Score | Allergenicity Prediction | Nearest Protein | Toxicity Prediction | SVM Score | Steric Hindrance | Amphiphaticity | Hydrophobicity | pl | Molecular Weight (Da) |
|-----|-----------------|----------------------|--------------------------|----------------|---------------------|----------|-----------------|----------------|---------------|----|---------------------|
| 135 | VE              | 0.02                 | allergen                 | NCBI gi number 76097511 | Non-Toxin          | -0.8     | 0.69            | 0.64           | -0.04         | 4  | 246.28              |
| 136 | IDM             | 0.48                 | allergen                 | UniProtKB accession number Q94507 | Non-Toxin          | -0.79    | 0.75            | 0              | 0.09          | 3.8 | 377.49              |
| 137 | GK              | 0.30                 | allergen                 | UniProtKB accession number P09944 | Non-Toxin          | -0.79    | 0.68            | 1.83           | -0.47         | 9.11| 203.26              |
| 138 | DIPK            | 0.28                 | allergen                 | NCBI gi number 208605348 | Non-Toxin          | -0.79    | 0.62            | 0.92           | -0.29         | 6.19| 471.6               |
| 139 | DATNVGDEGG      | 0.10                 | allergen                 | NCBI gi number 160347120 | Non-Toxin          | -0.79    | 0.68            | 0.13           | -0.16         | 3.5 | 934.02              |
| 140 | NVM             | 0.13                 | allergen                 | UniProtKB accession number P00777 | Non-Toxin          | -0.78    | 0.75            | 0              | 0.05          | 5.88| 362.48              |
| 141 | CQK             | 0.28                 | allergen                 | NCBI gi number 3318885 | Non-Toxin          | -0.77    | 0.66            | 1.64           | -0.58         | 8.57| 377.49              |
| 142 | QSSASSPSPSK     | 0.27                 | allergen                 | NCBI gi number 868967 | Non-Toxin          | -0.76    | 0.53            | 0.45           | -0.29         | 9.11| 1062.23             |
| 143 | DGK             | 0.21                 | allergen                 | UniProtKB accession number O60023 | Non-Toxin          | -0.76    | 0.71            | 1.22           | -0.55         | 6.19| 318.36              |
| 144 | DGP             | 0.66                 | allergen                 | NCBI gi number 122064581 | Non-Toxin          | -0.74    | 0.6             | 0              | -0.21         | 3.8 | 287.3               |
| 145 | GPM             | 0.96                 | allergen                 | UniProtKB accession number P00974 | Non-Toxin          | -0.71    | 0.61            | 0              | 0.12          | 5.88| 303.41              |
| 146 | NGTI            | 0.15                 | allergen                 | NCBI gi number 18568322 | Non-Toxin          | -0.71    | 0.67            | 0              | 0.02          | 5.88| 403.49              |
| 147 | NGDK            | 0.94                 | allergen                 | UniProtKB accession number Q2YFF0 | Non-Toxin          | -0.69    | 0.72            | 0.92           | -0.57         | 6.19| 432.48              |
| 148 | DQIDDEIK        | 0.13                 | allergen                 | NCBI gi number 47117350 | Non-Toxin          | -0.61    | 0.71            | 0.77           | -0.39         | 3.84| 975.13              |
| 149 | DKPQPPAA        | 0.50                 | allergen                 | NCBI gi number 27806257 | Non-Toxin          | -0.55    | 0.53            | 0.46           | -0.17         | 6.19| 751.93              |
| 150 | GVDNPGHP        | 0.42                 | allergen                 | NCBI gi number 285005081 | Non-Toxin          | -0.53    | 0.54            | 0.18           | -0.13         | 5.09| 791.93              |
| 151 | ATGNNPNDIV      | 0.23                 | allergen                 | NCBI gi number 7489357 | Non-Toxin          | -0.42    | 0.61            | 0              | 0.06          | 3.8 | 997.21              |
| 152 | SGTTMY          | 0.05                 | allergen                 | NCBI gi number 56417504 | Non-Toxin          | -0.38    | 0.63            | 0              | 0            | 5.88| 715.87              |
| 153 | PPGKPPPPPGPQGQH | 0.38                 | allergen                 | NCBI gi number 1168171 | Non-Toxin          | -0.09    | 0.5             | 0.32           | -0.02         | 9.11| 1854.45             |
| 154 | IPCGPTGPIK      | 0.72                 | non-allergen             | UniProtKB accession number Q9S8M0 | Toxin             | 0.07     | 0.54            | 0.37           | 0.02          | 9.11| 976.33              |
Peptide toxicity and physicochemical properties (i.e., hydrophobicity, amphipathicity, steric hindrance, pI, and molecular weight) were studied using the ToxinPred software (http://crdd.osdd.net/raghava/toxinpred/) [7]. Peptide toxicity was predicted mainly according to the amino acid composition and position of peptides. The models were developed based on machine learning technique and quantitative matrix using more than 1805 toxic peptides.

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Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.dib.2020.105163.

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