# BIOPEP-UWM Database of Bioactive Peptides – Current Opportunities

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## Supplement

### Homepage

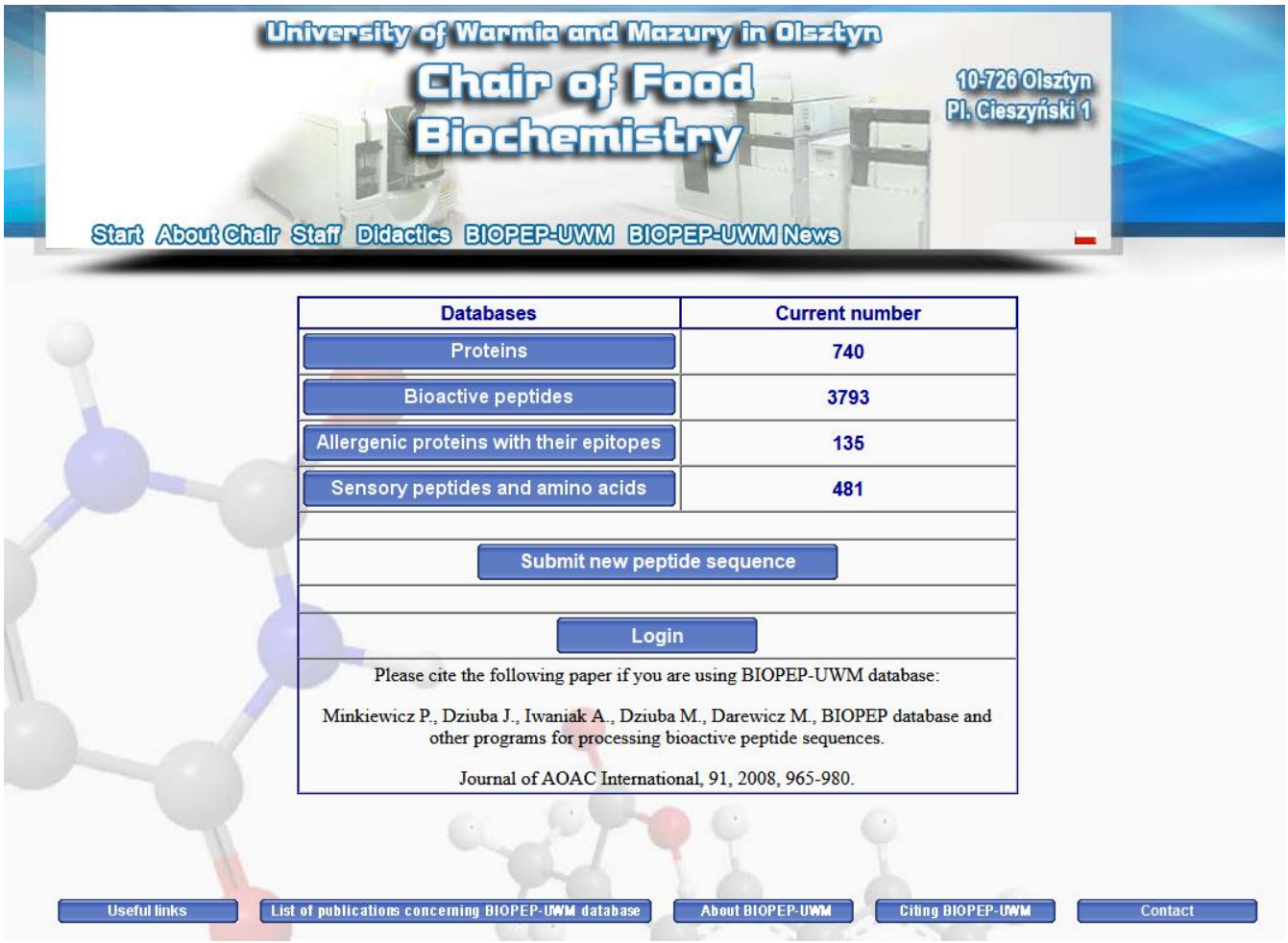



**Figure S1.** BIOPEP-UWM main page screenshot

## “Submit new peptide sequence” tab

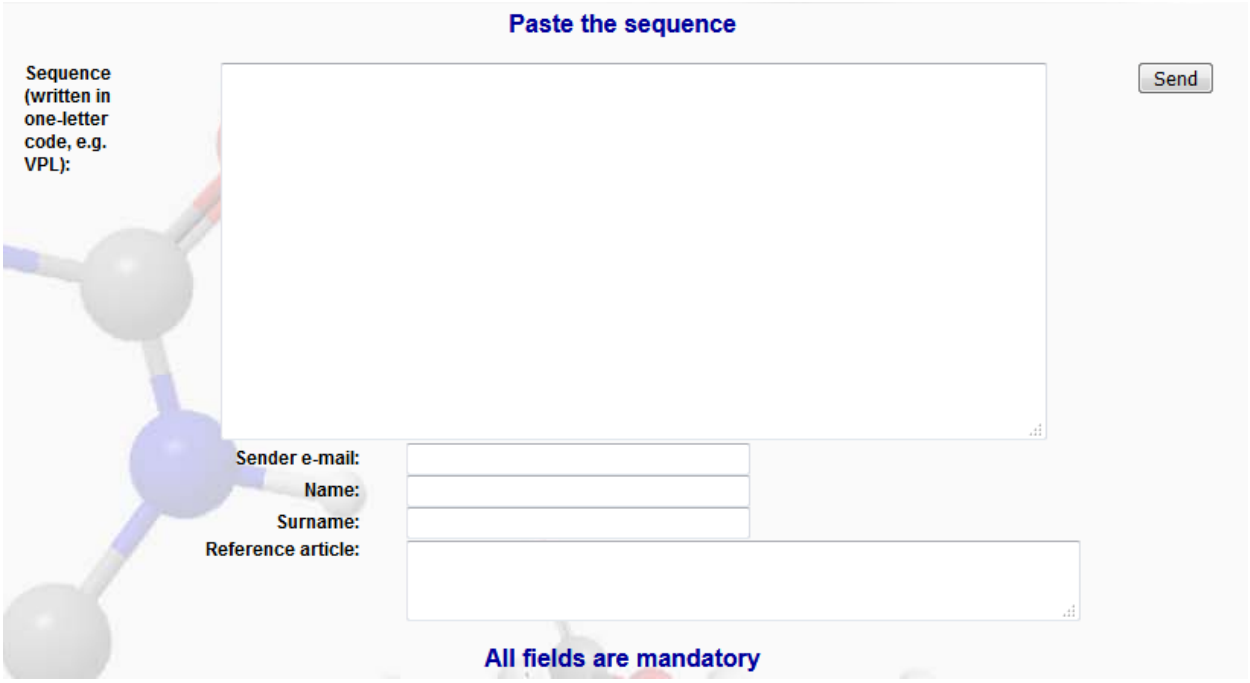
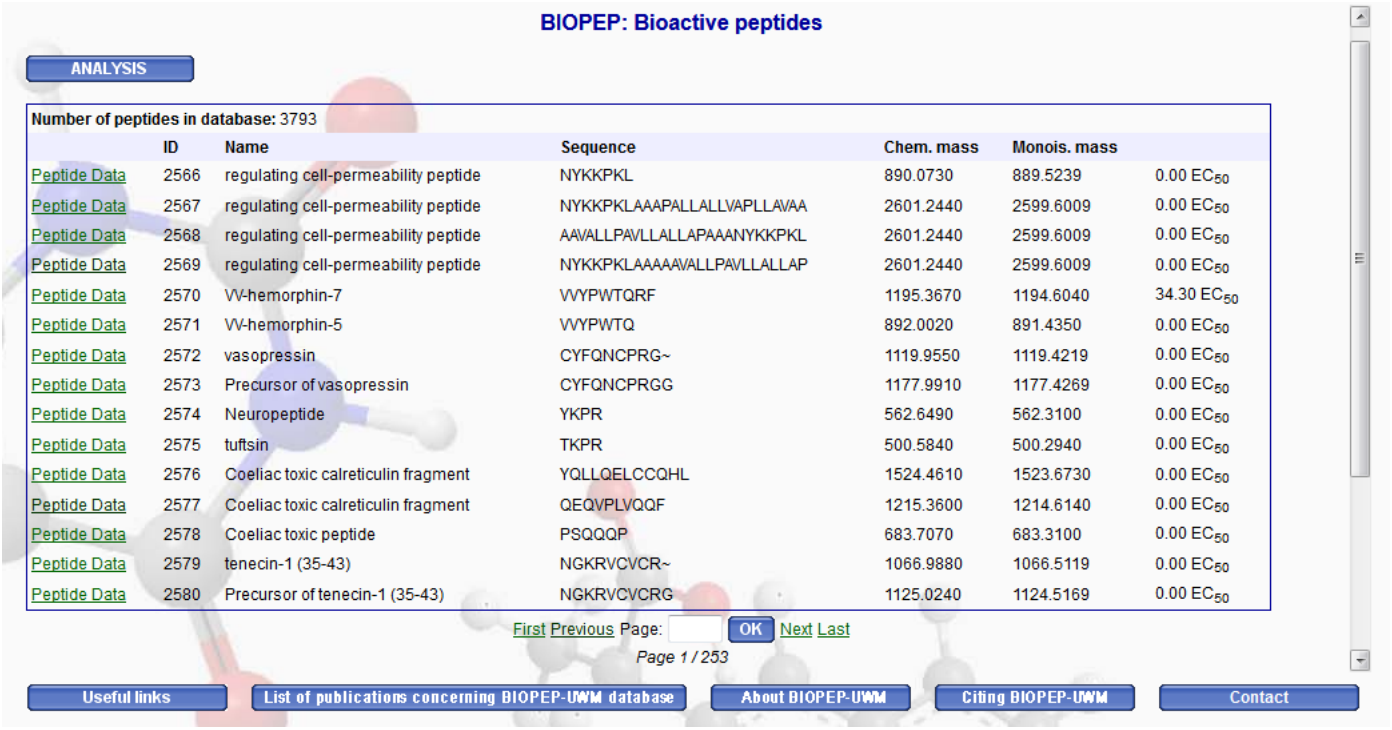



**Figure S2.** Content of the “Submit new peptide sequence” tab (screenshot)

# “Bioactive peptides” tab



BIOPEP: Bioactive peptides

ANALYSIS

Number of peptides in database: 3793

| | ID | Name | Sequence | Chem. mass | Monois. mass | |
|---|---|---|---|---|---|---|
| Peptide Data | 2566 | regulating cell-permeability peptide | NYKKPKL | 890.0730 | 889.5239 | 0.00 $EC_{50}$ |
| Peptide Data | 2567 | regulating cell-permeability peptide | NYKKPKLAAAPALLALLVAPLLAVAA | 2601.2440 | 2599.6009 | 0.00 $EC_{50}$ |
| Peptide Data | 2568 | regulating cell-permeability peptide | AAVALLPAVLLALLAPAAANYKKPKL | 2601.2440 | 2599.6009 | 0.00 $EC_{50}$ |
| Peptide Data | 2569 | regulating cell-permeability peptide | NYKKPKLAAAAAVALLPAVLLALLAP | 2601.2440 | 2599.6009 | 0.00 $EC_{50}$ |
| Peptide Data | 2570 | VV-hemorphin-7 | VVYPWTQRF | 1195.3670 | 1194.6040 | 34.30 $EC_{50}$ |
| Peptide Data | 2571 | VV-hemorphin-5 | VVYPWTQ | 892.0020 | 891.4350 | 0.00 $EC_{50}$ |
| Peptide Data | 2572 | vasopressin | CYFQNCPRG~ | 1119.9550 | 1119.4219 | 0.00 $EC_{50}$ |
| Peptide Data | 2573 | Precursor of vasopressin | CYFQNCPRGG | 1177.9910 | 1177.4269 | 0.00 $EC_{50}$ |
| Peptide Data | 2574 | Neuropeptide | YKPR | 562.6490 | 562.3100 | 0.00 $EC_{50}$ |
| Peptide Data | 2575 | tuftsin | TKPR | 500.5840 | 500.2940 | 0.00 $EC_{50}$ |
| Peptide Data | 2576 | Coeliac toxic calreticulin fragment | YQLLQELCCQHL | 1524.4610 | 1523.6730 | 0.00 $EC_{50}$ |
| Peptide Data | 2577 | Coeliac toxic calreticulin fragment | QEQVPLVQQF | 1215.3600 | 1214.6140 | 0.00 $EC_{50}$ |
| Peptide Data | 2578 | Coeliac toxic peptide | PSQQQP | 683.7070 | 683.3100 | 0.00 $EC_{50}$ |
| Peptide Data | 2579 | tenecin-1 (35-43) | NGKRVCVCR~ | 1066.9880 | 1066.5119 | 0.00 $EC_{50}$ |
| Peptide Data | 2580 | Precursor of tenecin-1 (35-43) | NGKRVCVCRG | 1125.0240 | 1124.5169 | 0.00 $EC_{50}$ |

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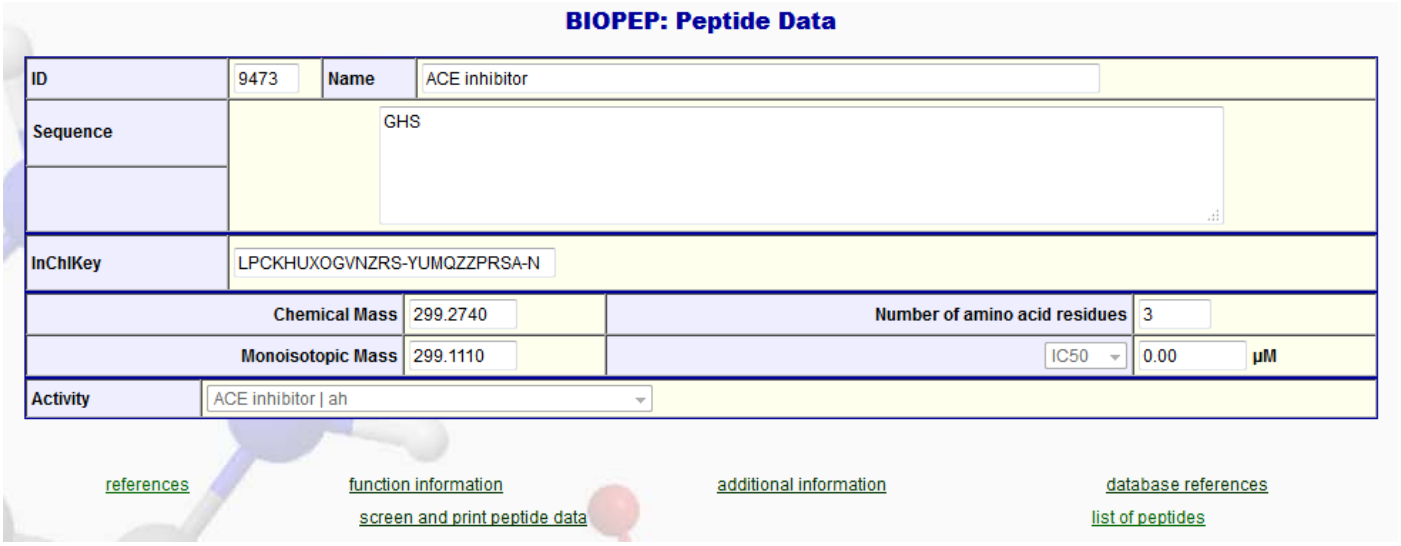
Useful links | List of publications concerning BIOPEP-UWM database | About BIOPEP-UWM | Citing BIOPEP-UWM | Contact

**Figure S3.** List of bioactive peptides – page 1 screenshot



BIOPEP: Peptide Data

| | | | |
|---|---|---|---|
| ID | 9473 | Name | ACE inhibitor |
| Sequence | GHS | | |
| InChIKey | LPCKHUXOGVNZRS-YUMQZZPRSA-N | | |
| Chemical Mass | 299.2740 | Number of amino acid residues | 3 |
| Monoisotopic Mass | 299.1110 | IC50 | 0.00 µM |
| Activity | ACE inhibitor \| ah | | |

references | function information | additional information | database references

screen and print peptide data | list of peptides

**Figure S4.** Page of an individual peptide (“Activity” tab) screenshot

**Table S1**. Content of a page containing representative peptide information (copied from the "Screen and print peptide data" tab)

## BIOPEP: Report

**ID** 9473
**Name** ACE inhibitor
**sequence**
GHS

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**Function:**
Inhibitor of Angiotensin-Converting Enzyme (ACE) (EC 3.4.15.1) (MEROPS ID: M02-001)

**Number of amino acid residues** 3 **Activity code** ah
**Activity :** ACE inhibitor
**Chemical mass** 299.2740 **Monoisotopic mass** 299.1110
**IC50** : 0.00 μM

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**Bibliographic data:**
**Authors**
He R., Malomo S. A., Alashi A., Girgih A. T., Ju X., Aluko R. E.
**Title**
Glycinyl-histidinyl-serine (GHS), a novel rapeseed protein-derived peptide has blood pressure-lowering effect in spontaneously hypertensive rats. J. Agric. Food Chem., 61, 8396-8402, 2013
**Year** **Editor**
2013 Journal

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**Additional information:**
BIOPEP-UWM database of bioactive peptides

SMILES: NCC(=O)N[C@@H](Cc1c[nH]cn1)C(=O)N[C@@]([H])(CO)C(=O)O

InChI=1S/C11H17N5O5/c12-2-9(18)15-7(1-6-3-13-5-14-6)10(19)16-8(4-17)11(20)21/h3,5,7-8,17H,1-2,4,12H2,(H,13,14)(H,15,18)(H,16,19)(H,20,21)/t7-,8-/m0/s1

InChIKey: LPCKHUXOGVNZRS-YUMQZZPRSA-N

Inhibitor of Renin (EC 3.4.23.15) (MEROPS ID: A01.007) according to the BIOPEP-UWM database of bioactive peptides (ID 9472)

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Database reference:
AHTPDB: ID 1053, 2949

BioPepDB: ID biopep00354

BIOPEP-UWM database of bioactive peptides: ID 9472

SATPdb: ID satpdb13065

## Search options

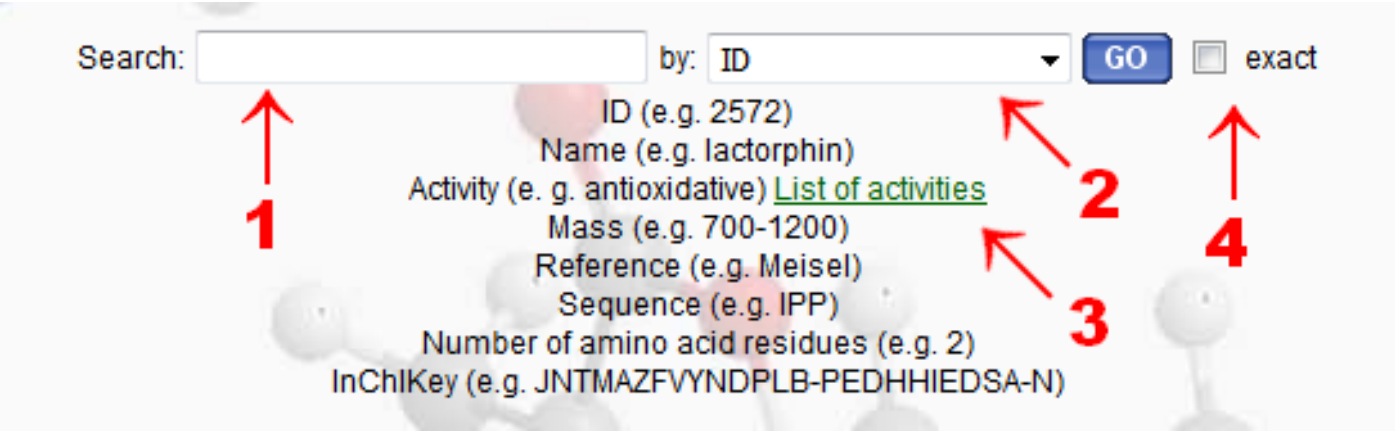



**Figure S5.** Peptide search options available on the page with a list of peptides (screenshot). 1. Window to paste query, 2. Search option choice menu, 3. Link to the list of activities, 4. Icon of “exact search” option

## Analysis

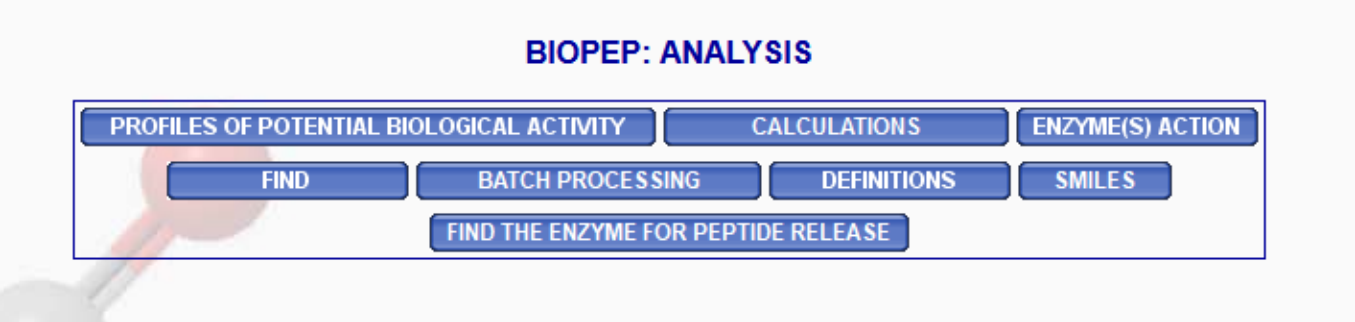



**Figure S6.** Menu of the "Analysis" tab screenshot

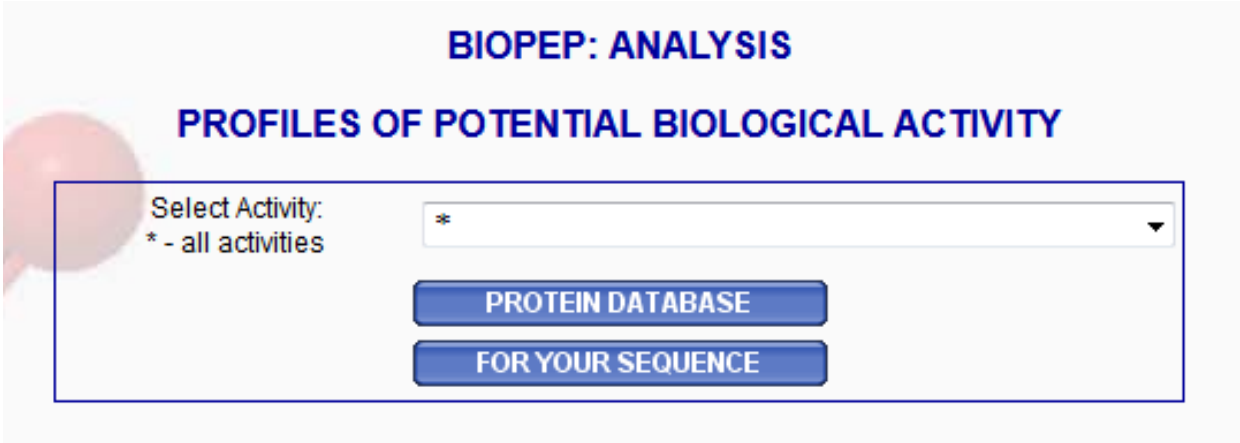



**Figure S7.** Menu of the "Profiles of potential biological activity" tab

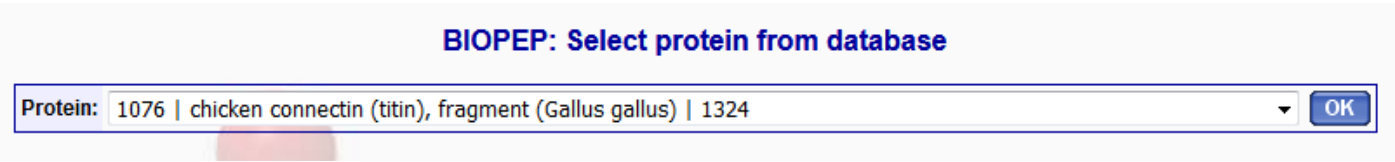



**Figure S8.** Menu for protein selection from the BIOPEP-UWM database of proteins.

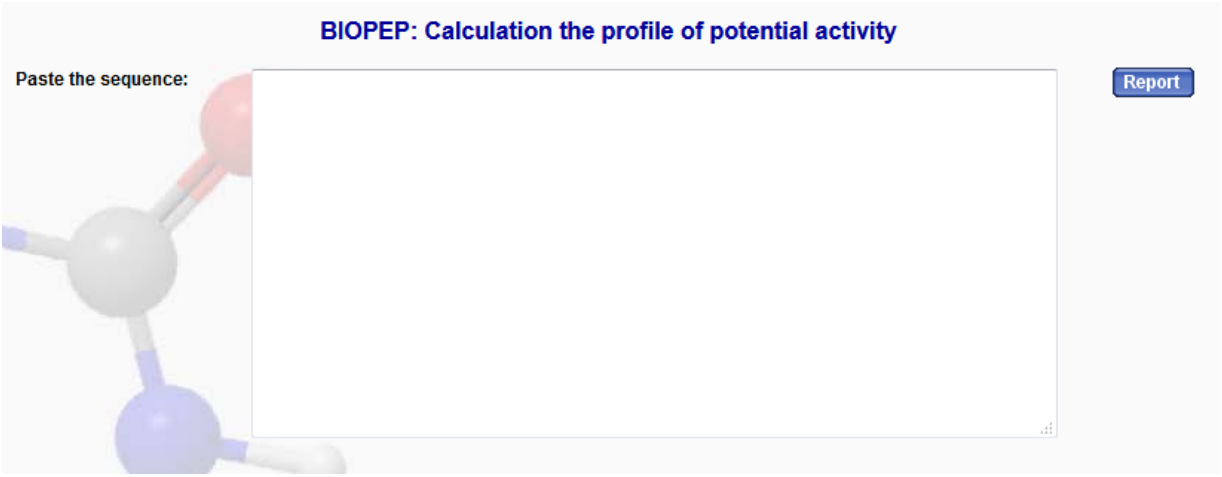



**Figure S9.** Window for user's sequence input for construction of the profile of potential biological activity of protein or peptide fragments. Analysis can be started by clicking "Report" button.

**Table S2**. Profile of potential biological activity of an example peptide with the TYHPPPKPPGHP sequence

| ID | Name of peptide | Activity | Number | Sequence | Location |
|---|---|---|---|---|---|
| 3460 | Prolyl endopeptidase inhibitor | antiamnestic | 1 | PG | [9-10] |
| 7601 | ACE inhibitor | ACE inhibitor | 1 | GH | [10-11] |
| 7625 | ACE inhibitor | ACE inhibitor | 1 | PG | [9-10] |
| 7645 | ACE inhibitor from porcine myosin (981-983 | ACE inhibitor | 1 | PPK | [5-7] |
| 7810 | ACE inhibitor from anchovy and bonito | ACE inhibitor | 1 | KP | [7-8] |
| 7836 | ACE inhibitor | ACE inhibitor | 3 | PP | [4-5],[5-6],[8-9] |
| 7842 | ACE inhibitor | ACE inhibitor | 2 | HP | [3-4],[11-12] |
| 9087 | ACE inhibitor | ACE inhibitor | 1 | YH | [2-3] |
| 9172 | ACE inhibitor | ACE inhibitor | 1 | PPP | [4-6] |
| 3285 | Antithrombotic peptide | antithrombotic | 1 | PG | [9-10] |
| 8168 | peptide derived from κ-casein (109-111) | antithrombotic | 1 | PPK | [5-7] |
| 2754 | peptide regulating the stomach mucosal membrane activity | regulating | 1 | PG | [9-10] |
| 8218 | Antioxidative peptide | antioxidative | 1 | KP | [7-8] |
| 8219 | antioxidative peptide | antioxidative | 1 | TY | [1-2] |
| 3761 | dipeptidyl carboxypeptidase inhibitor | inhibitor | 1 | PPPK | [4-7] |
| 3170 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 3 | PP | [4-5],[5-6],[8-9] |
| 8519 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | KP | [7-8] |
| 8520 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 2 | HP | [3-4],[11-12] |
| 8653 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | PPG | [8-10] |
| 8784 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | GH | [10-11] |
| 8855 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | PG | [9-10] |
| 8858 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | PK | [6-7] |
| 8914 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | TY | [1-2] |
| 8937 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | YH | [2-3] |
| 9481 | DPP-III inhibitor | dipeptidyl peptidase III inhibitor | 1 | YH | [2-3] |
| 9496 | DPP-III inhibitor | dipeptidyl peptidase III inhibitor | 2 | HP | [3-4],[11-12] |

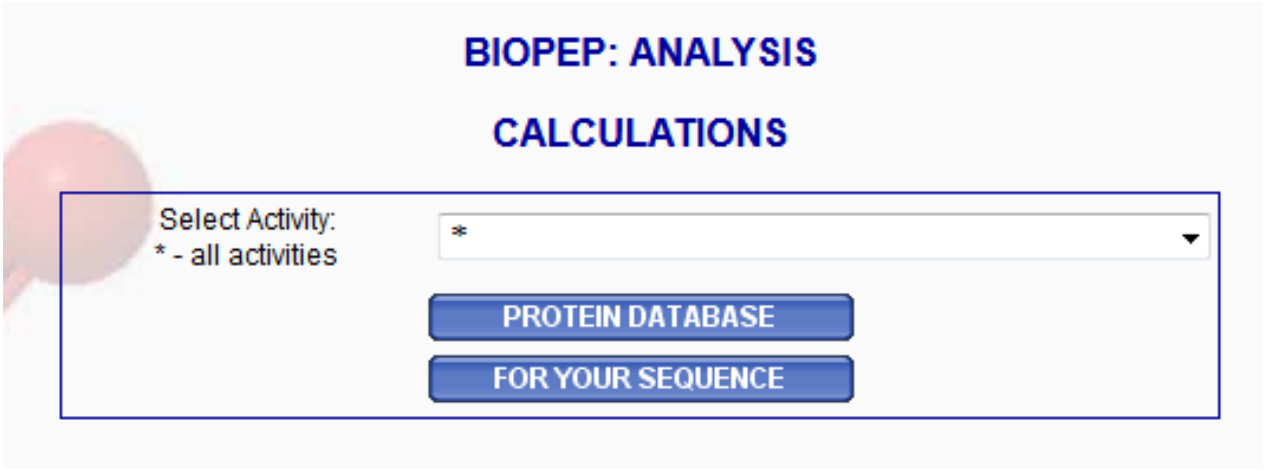



**Figure S10.** "Calculations" menu screenshot. Menus for "Protein database" and "For your sequence" tabs are the same as presented in Figures S8 and S9, respectively.

**Table S3**. Results of A calculation of A and B parameters characterizing the quantitative content of bioactive fragments in the TYHPPPKPPGHP sequence. Definitions of A and B parameters are given in Table 5 in the main text.

| ID | NAME | Activity | A | B |
|---|---|---|---|---|
| --- | ---------- | ACE inhibitor | 0.9167 | 0.021212870691036 |
| --- | ---------- | antiamnestic | 0.0833 | |
| --- | ---------- | antioxidative | 0.1667 | |
| --- | ---------- | antithrombotic | 0.1667 | |
| --- | ---------- | dipeptidyl peptidase III inhibitor | 0.2500 | |
| --- | ---------- | dipeptidyl peptidase IV inhibitor | 1.0000 | 0.00017156514577392 |
| --- | ---------- | inhibitor | 0.0833 | |
| --- | ---------- | regulating | 0.0833 | |

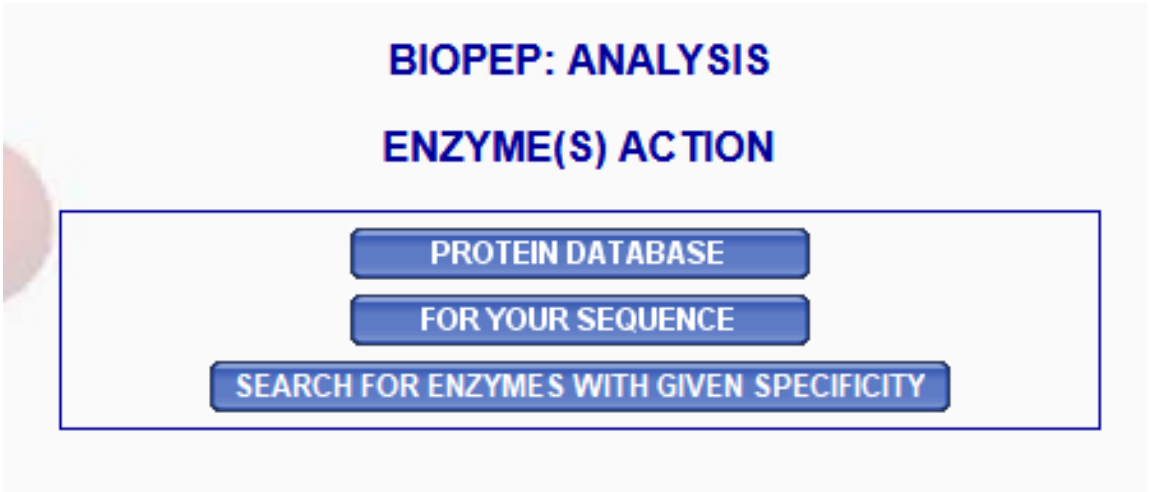



**Figure S11.** Screenshot of "Enzyme(s) action" menu.

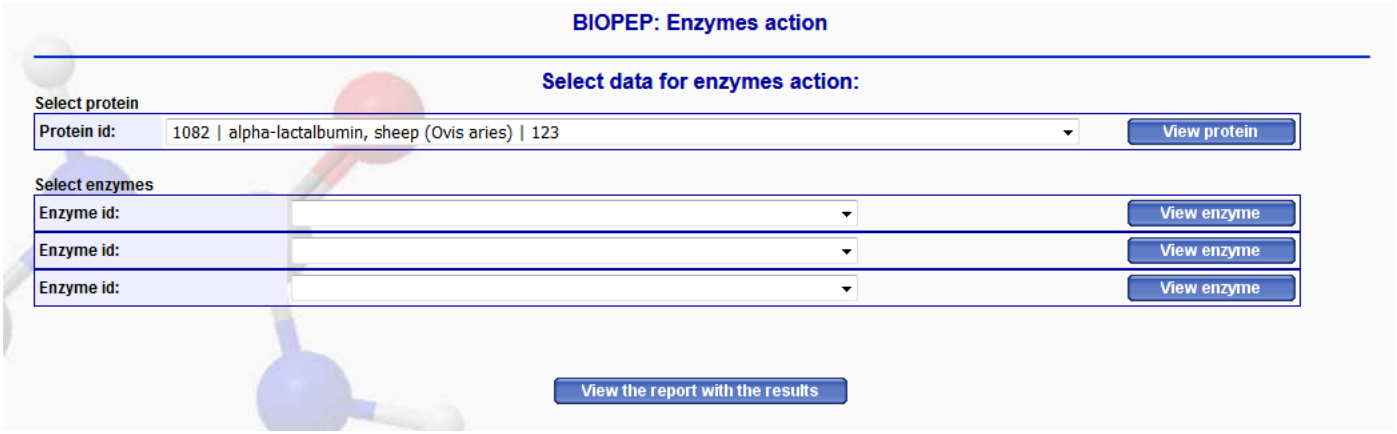



**Figure S12.** Screenshot of the menu for protein and enzyme selection from the BIOPEP-UWM protein database

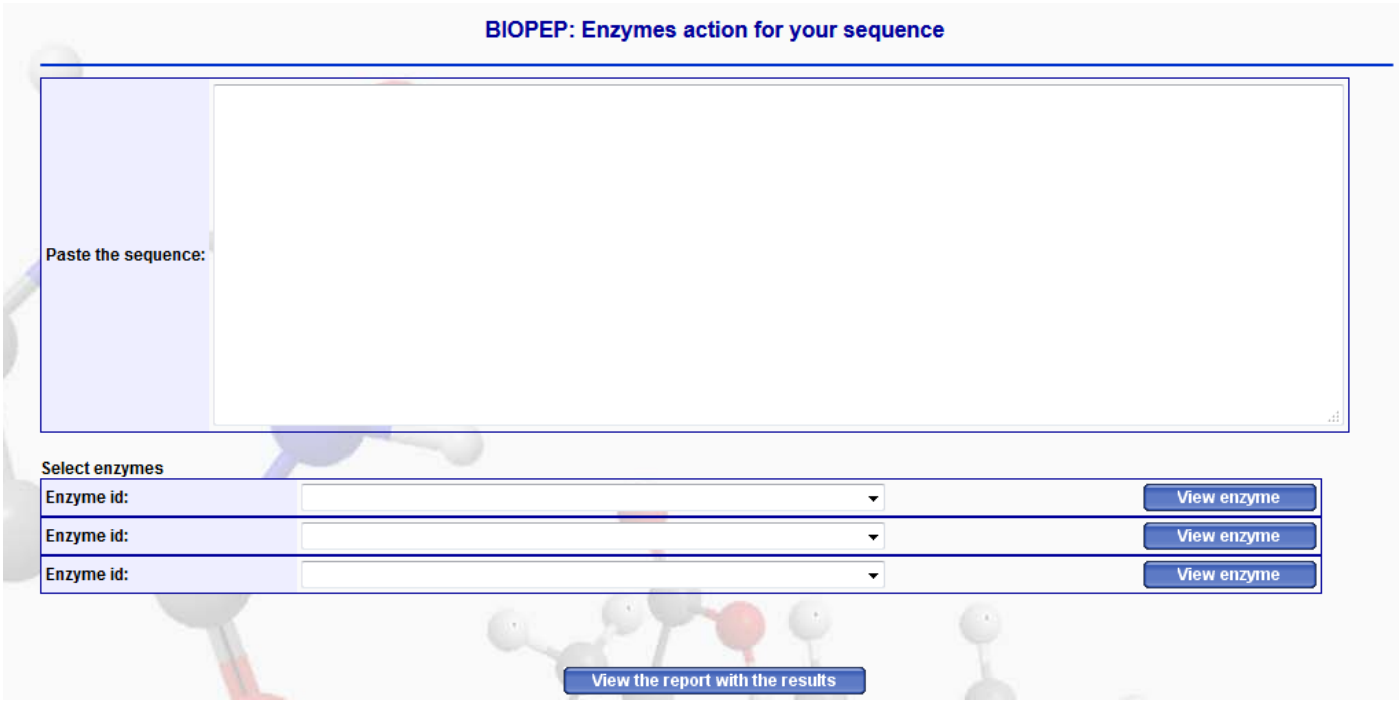
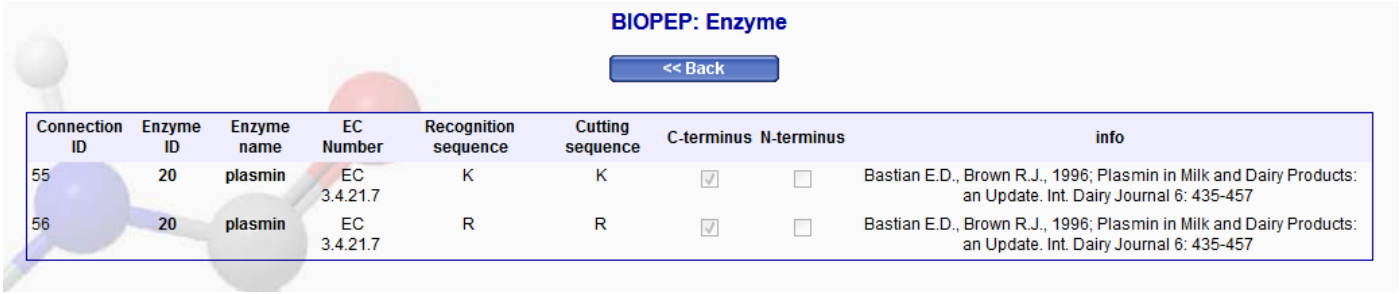



**Figure S13.** Screenshot of the menu for input of user's protein or peptide and enzyme selection.




| Connection ID | Enzyme ID | Enzyme name | EC Number | Recognition sequence | Cutting sequence | C-terminus | N-terminus | info |
|---|---|---|---|---|---|---|---|---|
| 55 | 20 | plasmin | EC 3.4.21.7 | K | K | ☑ | ☐ | Bastian E.D., Brown R.J., 1996; Plasmin in Milk and Dairy Products: an Update. Int. Dairy Journal 6: 435-457 |
| 56 | 20 | plasmin | EC 3.4.21.7 | R | R | ☑ | ☐ | Bastian E.D., Brown R.J., 1996; Plasmin in Milk and Dairy Products: an Update. Int. Dairy Journal 6: 435-457 |

**Figure S14.** Screenshot of an example table containing enzyme data (Plasmin; EC 3.4.21.7; MEROPS ID: S01.233).

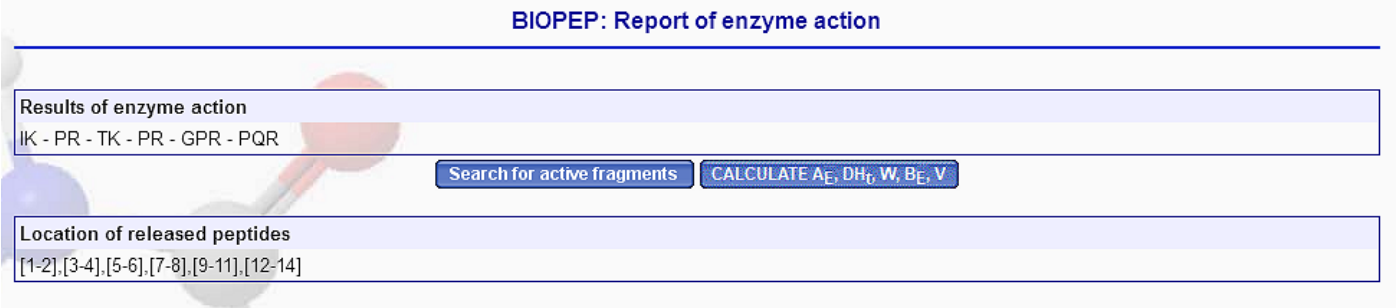



**Figure S15.** Results of preliminary simulation of hydrolysis of peptide IKPRTKPRGPRPQR using plasmin (see Fig. S14). Buttons: "Search for active fragments" and "Calculate $A_E$, $DH_E$, W, $B_E$, V" serve for further analysis of results.

**Table S4**. Results of search for active fragments among products of simulated proteolysis of peptide IKPRTKPRGPRPQR using plasmin

| No | Peptide ID | Sequence | Location | Name | Function | Activity | Monoisotopic mass | Chemical mass |
|---|---|---|---|---|---|---|---|---|
| 1 | 3047 | GPR | [9-11] | Antithrombotic peptide | antithrombotic | antithrombotic | 328.1740 | 328.3570 |
| 2 | 3373 | PQR | [12-14] | ACE inhibitor from beta-CN | Inhibitor of Angiotensin-Converting Enzyme (ACE) (EC 3.4.15.1) (MEROPS ID: M02-001) | ACE inhibitor | 399.2110 | 399.4360 |
| 3 | 3537 | PR | [3-4] | ACE inhibitor | Inhibitor of Angiotensin-Converting Enzyme (ACE) (EC 3.4.15.1) (MEROPS ID: M02-001) | ACE inhibitor | 271.1530 | 271.3050 |
| 4 | 3537 | PR | [7-8] | ACE inhibitor | Inhibitor of Angiotensin-Converting Enzyme (ACE) (EC 3.4.15.1) (MEROPS ID: M02-001) | ACE inhibitor | 271.1530 | 271.3050 |
| 5 | 8904 | TK | [5-6] | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | Inhibitor of Dipeptidyl Peptidase IV (EC 3.4.14.5) (MEROPS ID: S09.003) | dipeptidyl peptidase IV inhibitor | 247.1410 | 247.2790 |
| 6 | 9489 | PR | [3-4] | DPP-III inhibitor | Inhibitor of Dipeptidyl peptidase-III (DPP-III) (EC 3.4.14.4) (MEROPS ID: M49.001) | dipeptidyl peptidase III inhibitor | 271.1530 | 271.3050 |
| 7 | 9489 | PR | [7-8] | DPP-III inhibitor | Inhibitor of Dipeptidyl peptidase-III (DPP-III) (EC 3.4.14.4) (MEROPS ID: M49.001) | dipeptidyl peptidase III inhibitor | 271.1530 | 271.3050 |

**Table S5**. Results of calculation of $A_E$, $DH_E$, W, $B_E$, V parameters characterizing simulated proteolysis of peptide IKPRTKPRGPRPQR using plasmin

| $DH_t$ [%] | | | | | |
|---|---|---|---|---|---|
| 38.4615 | | | | | |
| No | Activity | $A_E$ | W | $B_E$ | V |
| 1 | antithrombotic | 0.0714 | 0.3332 | 0 | |
| 2 | ACE inhibitor | 0.2143 | 0.2728 | 0.035021331688201 | 0.50010828935411 |
| 3 | dipeptidyl peptidase IV inhibitor | 0.0714 | 0.1428 | 0 | 0 |
| 4 | dipeptidyl peptidase III inhibitor | 0.1429 | 0.6668 | 0 | 0 |

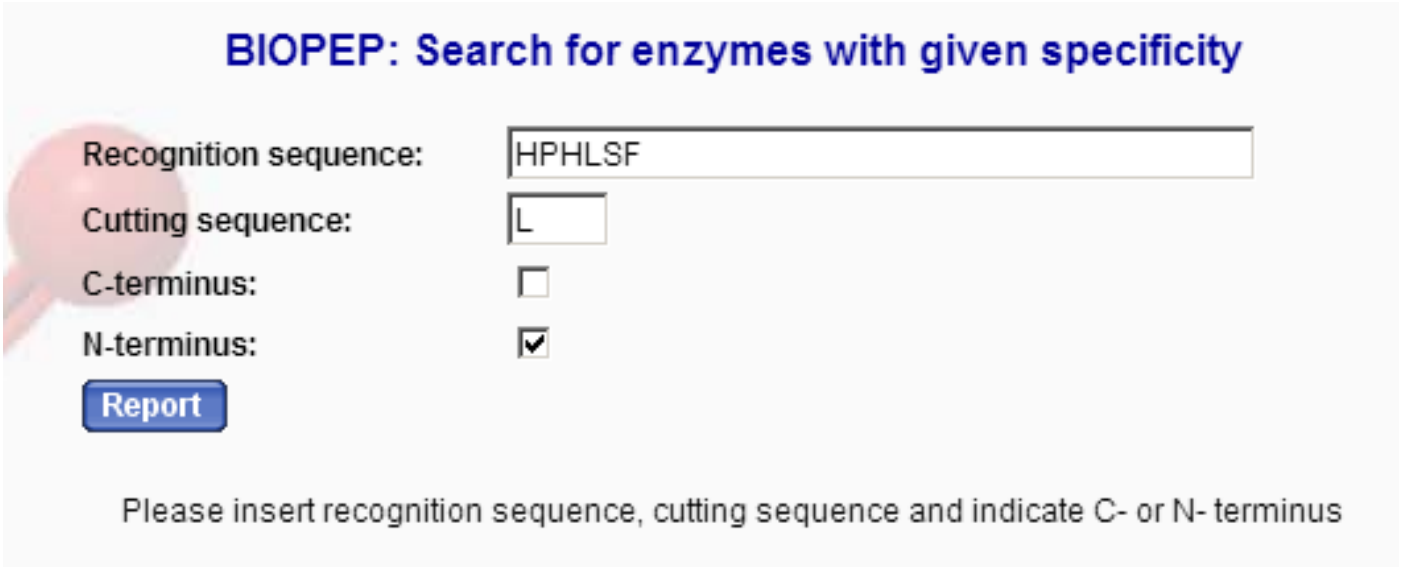



**Figure S15.** Screenshot of the menu for the "Search for enzymes with given specificity" option

**Table S6**. Results of search for enzyme with specificity defined as shown in Figure S15.

| No | Enzyme name | EC Number | Enzyme ID | Connection ID |
|---|---|---|---|---|
| 1 | ginger protease (zingipain) | EC 3.4.22.67 | 43 | 140 |

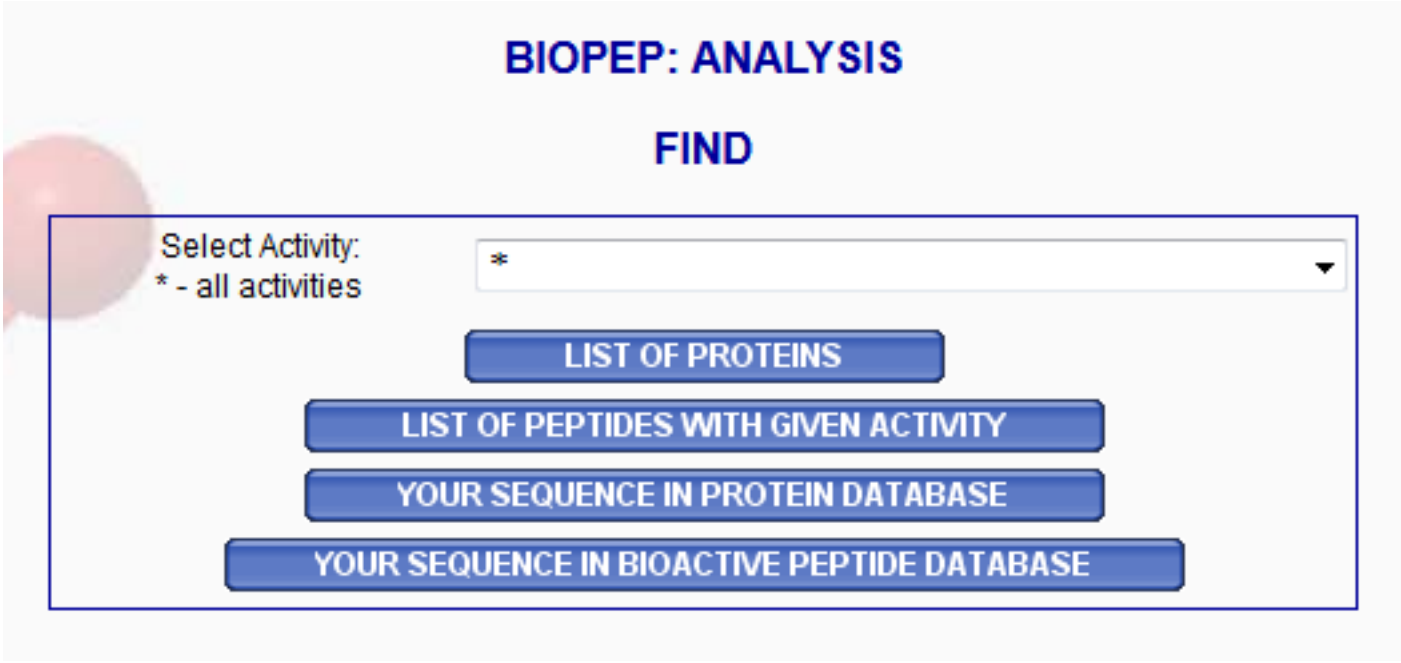



**Figure S17.** Screenshot of the menu of the "Find" tab.

**Table S7**. Results from the "Find your sequence in bioactive peptide database" tab. The VPP sequence has been used as a query.

| | ID | Name | Sequence |
|---|---|---|---|
| Peptide data | 2682 | Erythropoietin receptor agonist | DLEGCRLGWVGHCNVWGGDEYTKRTS HSVPPSHKSKLL |
| Peptide data | 3153 | Erythropoietin receptor agonist peptide | DVEACGGGWVGHCNYWLRDEYASKPI KQVPPGNHNQPS |
| Peptide data | 3503 | ACE inhibitor (bCN fr.80-90) | TPVVVPPFLQP |
| Peptide data | 3524 | ACE inhibitor (from bovine beta-CN) | VPP |
| Peptide data | 7664 | ACE inhibitor | VVPPA |
| Peptide data | 8308 | ACE inhibitor | VVPP |
| Peptide data | 8456 | Antioxidant peptide from marine bivalve (Mactra veneriformis) | VAMVPPFET |
| Peptide data | 8661 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | VPPFIQPE |
| Peptide data | 9237 | ACE inhibitor | LTQTPVVVPPF |
| Peptide data | 9251 | ACE inhibitor | VVVPPF |
| Peptide data | 9399 | Antioxidative peptide | GQVPP |
| Peptide data | 9409 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | VPPFIQPE |
| Peptide data | 9453 | Antifungal peptide | FPSHTGMSVPPP |

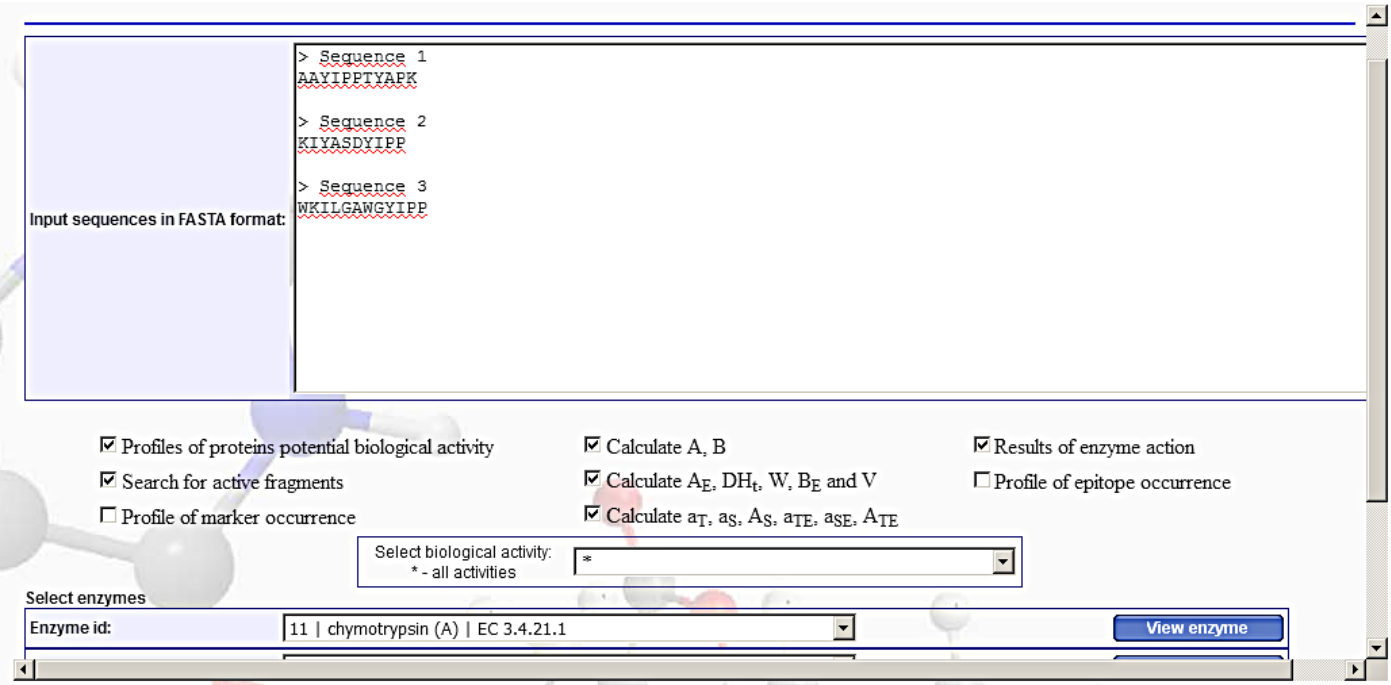



**Figure S18.** Screenshot of the menu of the "Batch processing" tab. Results for the query sequences displayed in the Figure are presented in Tables S8 and S9.

**Table S8**. Results of batch processing – step 1. The set of processed sequences was as follows: sequence 1: AAYIPPTYAPK; sequence 2: KIYASDYIPP; sequence 3: WKILGAWGYIPP. The enzyme chymotrypsin A (EC 3.4.21.1; MEROPS ID: S01.001; BIOPEP-UWM ID: 11) was used for proteolysis simulation. Results of calculation of the parameters $a_T$, $a_S$, $A_S$, $a_{TE}$, $a_{SE}$, $A_{TE}$ for selected peptides may be displayed by pressing the "View the report with the results" button below the table. Peptides may be selected by clicking icons in the left column in the table showing profile of potential biological activity of fragments or by clicking the "Check all" button to select all peptides.

| Protein name: Sequence 1 | | | | | | |
|---|---|---|---|---|---|---|
| Protein sequence: AAYIPPTYAPK | | | | | | |
| Profiles of proteins potential biological activity | | | | | | |
| As | ID | Name of peptide | Activity | Number | Sequence | Location |
| ☐ | 3522 | ACE inhibitor (from bovine b-CN) | ACE inhibitor | 1 | IPP | [4-6] |
| ☐ | 3563 | ACE inhibitor | ACE inhibitor | 1 | AY | [2-3] |
| ☐ | 7581 | ACE inhibitor | ACE inhibitor | 1 | IP | [4-5] |
| ☐ | 7584 | ACE inhibitor | ACE inhibitor | 1 | AP | [9-10] |
| ☐ | 7589 | ACE inhibitor | ACE inhibitor | 1 | YA | [8-9] |
| ☐ | 7590 | ACE inhibitor | ACE inhibitor | 1 | AA | [1-2] |
| ☐ | 7833 | ACE inhibitor | ACE inhibitor | 1 | PT | [6-7] |
| ☐ | 7836 | ACE inhibitor | ACE inhibitor | 1 | PP | [5-6] |
| ☐ | 7866 | peptide from Okara protein | antioxidative | 1 | AY | [2-3] |
| ☐ | 8219 | antioxidative peptide | antioxidative | 1 | TY | [7-8] |
| ☐ | 2886 | Opioid peptide | opioid antagonist | 1 | YIPP | [3-6] |
| ☐ | 3170 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | PP | [5-6] |

| | | | | | | |
|---|---|---|---|---|---|---|
| ☐ | 3177 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | AP | [9-10] |
| ☐ | 8501 | Dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | IP | [4-5] |
| ☐ | 8637 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | AA | [1-2] |
| ☐ | 8765 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | AY | [2-3] |
| ☐ | 8858 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | PK | [10-11] |
| ☐ | 8863 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | PT | [6-7] |
| ☐ | 8914 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | TY | [7-8] |
| ☐ | 8932 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | YA | [8-9] |
| ☐ | 8938 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | YI | [3-4] |
| ☐ | 9510 | DPP-III inhibitor | dipeptidyl peptidase III inhibitor | 1 | YI | [3-4] |
| ☐ | 9433 | Renin inhibitor | renin inhibitor | 1 | YA | [8-9] |

Calculations

| ID | NAME | Activity | A | B |
|---|---|---|---|---|
| --- | ---------- | ACE inhibitor | 0.7273 | 0.024405320817811 |
| --- | ---------- | antioxidative | 0.1818 | |
| --- | ---------- | dipeptidyl peptidase III inhibitor | 0.0909 | |
| --- | ---------- | dipeptidyl peptidase IV inhibitor | 0.9091 | 0.00025834927242301 |
| --- | ---------- | opioid antagonist | 0.0909 | |
| --- | ---------- | renin inhibitor | 0.0909 | |

Results of enzyme action

AAY - IPPTY - APK

Location of released peptides

[1-3],[4-8],[9-11]

Search for active fragments

| No | Peptide ID | Sequence | Location | Name | Function | Activity | Monoisotopic mass | Chemical mass |
|---|---|---|---|---|---|---|---|---|

$DH_t$ [%]

20.0000

CALCULATE $A_E$, W, $B_E$ and V

| No | Activity | $A_E$ | W | $B_E$ | V |
|---|---|---|---|---|---|

Protein name: Sequence 2

Protein sequence: KIYASDYIPP

Profiles of proteins potential biological activity

| As | ID | Name of peptide | Activity | Number | Sequence | Location |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| ☐ | 3383 | ACE inhibitor | ACE inhibitor | 1 | IY | [2-3] |
| ☐ | 3522 | ACE inhibitor (from bovine b-CN) | ACE inhibitor | 1 | IPP | [8-10] |
| ☐ | 7581 | ACE inhibitor | ACE inhibitor | 1 | IP | [8-9] |
| ☐ | 7589 | ACE inhibitor | ACE inhibitor | 1 | YA | [3-4] |
| ☐ | 7836 | ACE inhibitor | ACE inhibitor | 1 | PP | [9-10] |
| ☐ | 9072 | ACE inhibitor | ACE inhibitor | 1 | DY | [6-7] |
| ☐ | 2749 | peptide regulating ion flow | regulating | 1 | DY | [6-7] |
| ☐ | 7873 | peptide from soybean protein isolates: beta-conglycinin and glycinin | antioxidative | 1 | IY | [2-3] |
| ☐ | 2886 | Opioid peptide | opioid antagonist | 1 | YIPP | [7-10] |
| ☐ | 3170 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | PP | [9-10] |
| ☐ | 8501 | Dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | IP | [8-9] |
| ☐ | 8762 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | AS | [4-5] |
| ☐ | 8812 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | KI | [1-2] |
| ☐ | 8932 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | YA | [3-4] |
| ☐ | 8938 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | YI | [7-8] |
| ☐ | 9510 | DPP-III inhibitor | dipeptidyl peptidase III inhibitor | 1 | YI | [7-8] |
| ☐ | 9433 | Renin inhibitor | renin inhibitor | 1 | YA | [3-4] |

Calculations

| ID | NAME | Activity | A | B |
|---|---|---|---|---|
| --- | ---------- | ACE inhibitor | 0.6000 | 0.069605669692626 |
| --- | ---------- | antioxidative | 0.1000 | |
| --- | ---------- | dipeptidyl peptidase III inhibitor | 0.1000 | |
| --- | ---------- | dipeptidyl peptidase IV inhibitor | 0.6000 | 0.00026096728544077 |
| --- | ---------- | opioid antagonist | 0.1000 | |
| --- | ---------- | regulating | 0.1000 | |
| --- | ---------- | renin inhibitor | 0.1000 | |

Results of enzyme action

KIY - ASDY - IPP

Location of released peptides

[1-3],[4-7],[8-10]

Search for active fragments

| No | Peptide ID | Sequence | Location | Name | Function | Activity | Monoisotopic mass | Chemical mass |
|---|---|---|---|---|---|---|---|---|

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 1 | 3522 | IPP | [8-10] | ACE inhibitor (from bovine b-CN) | | ACE inhibitor | 325.1880 | 325.3940 |

| $DH_t$ [%] |
|---|
| 22.2222 |
| CALCULATE $A_E$, W, $B_E$ and V |

| No | Activity | $A_E$ | W | $B_E$ | V |
|---|---|---|---|---|---|
| 1 | ACE inhibitor | 0.1000 | 0.1667 | 0.02 | 0.28733291538345 |

| Protein name: Sequence 3 |
|---|
| Protein sequence: WKILGAWGYIPP |
| Profiles of proteins potential biological activity |

| As | ID | Name of peptide | Activity | Number | Sequence | Location |
|---|---|---|---|---|---|---|
| ☐ | 3522 | ACE inhibitor (from bovine b-CN) | ACE inhibitor | 1 | IPP | [10-12] |
| ☐ | 3532 | ACE inhibitor | ACE inhibitor | 1 | GY | [8-9] |
| ☐ | 7543 | ACE inhibitor | ACE inhibitor | 1 | AW | [6-7] |
| ☐ | 7581 | ACE inhibitor | ACE inhibitor | 1 | IP | [10-11] |
| ☐ | 7598 | ACE inhibitor | ACE inhibitor | 1 | GA | [5-6] |
| ☐ | 7613 | ACE inhibitor | ACE inhibitor | 1 | WG | [7-8] |
| ☐ | 7619 | ACE inhibitor | ACE inhibitor | 1 | LG | [4-5] |
| ☐ | 7836 | ACE inhibitor | ACE inhibitor | 1 | PP | [11-12] |
| ☐ | 9079 | ACE inhibitor | ACE inhibitor | 1 | IL | [3-4] |
| ☐ | 8323 | Glucose uptake stimulating peptide | stimulating | 1 | IL | [3-4] |
| ☐ | 8460 | Antioxidant peptide from marine bivalve (Mactra veneriformis) | antioxidative | 1 | AW | [6-7] |
| ☐ | 9082 | Antioxidative peptide | antioxidative | 1 | WG | [7-8] |
| ☐ | 3201 | chymotrypsin inhibitor | inhibitor | 1 | GAW | [5-7] |
| ☐ | 2886 | Opioid peptide | opioid antagonist | 1 | YIPP | [9-12] |
| ☐ | 3170 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | PP | [11-12] |
| ☐ | 8501 | Dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | IP | [10-11] |
| ☐ | 8524 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | GA | [5-6] |
| ☐ | 8676 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | WK | [1-2] |
| ☐ | 8695 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | AW | [6-7] |
| ☐ | 8697 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | WG | [7-8] |
| ☐ | 8788 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | GY | [8-9] |
| ☐ | 8802 | dipeptidyl peptidase IV inhibitor | dipeptidyl peptidase IV | 1 | IL | [3-4] |

| | | | | | | |
|---|---|---|---|---|---|---|
| | | (DPP IV inhibitor) | inhibitor | | | |
| ☐ | 8812 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | KI | [2-3] |
| ☐ | 8938 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | YI | [9-10] |
| ☐ | 9510 | DPP-III inhibitor | dipeptidyl peptidase III inhibitor | 1 | YI | [9-10] |

Calculations

| ID | NAME | Activity | A | B |
|---|---|---|---|---|
| --- | ---------- | ACE inhibitor | 0.7500 | 0.027619641874223 |
| --- | ---------- | antioxidative | 0.1667 | |
| --- | ---------- | dipeptidyl peptidase III inhibitor | 0.0833 | |
| --- | ---------- | dipeptidyl peptidase IV inhibitor | 0.8333 | 0.0022700178938607 |
| --- | ---------- | inhibitor | 0.0833 | |
| --- | ---------- | opioid antagonist | 0.0833 | |
| --- | ---------- | stimulating | 0.0833 | |

Results of enzyme action

W - KIL - GAW - GY - IPP

Location of released peptides

[1-1],[2-4],[5-7],[8-9],[10-12]

Search for active fragments

| No | Peptide ID | Sequence | Location | Name | Function | Activity | Monoisotopic mass | Chemical mass |
|---|---|---|---|---|---|---|---|---|
| 1 | 3201 | GAW | [5-7] | chymotrypsin inhibitor | | inhibitor | 332.1370 | 332.3440 |
| 2 | 3522 | IPP | [10-12] | ACE inhibitor (from bovine b-CN) | | ACE inhibitor | 325.1880 | 325.3940 |
| 3 | 3532 | GY | [8-9] | ACE inhibitor | Inhibitor of Angiotensin-Converting Enzyme (ACE) (EC 3.4.15.1) (MEROPS ID: XM02-001) | ACE inhibitor | 238.0840 | 238.2220 |
| 4 | 8788 | GY | [8-9] | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | Inhibitor of Dipeptidyl Peptidase IV (EC 3.4.14.5) (MEROPS ID: S09.003) | dipeptidyl peptidase IV inhibitor | 238.0840 | 238.2220 |

$DH_t$ [%]

36.3636

CALCULATE $A_E$, W, $B_E$ and V

| No | Activity | $A_E$ | W | $B_E$ | V |
|---|---|---|---|---|---|
| 1 | inhibitor | 0.0833 | 1.0000 | 0 | |
| 2 | ACE inhibitor | 0.1667 | 0.2223 | 0.033730158730159 | 1.2212380914916 |
| 3 | dipeptidyl peptidase IV inhibitor | 0.0833 | 0.1000 | 0 | 0 |

View the report with the results

**Table S9**. Final results of batch processing. The set of processed sequences was as follows: sequence 1: AAYIPPTYAPK; sequence 2: KIYASDYIPP; sequence 3: WKILGAWGYIPP. The enzyme chymotrypsin A (EC 3.4.21.1; MEROPS ID: S01.001; BIOPEP-UWM ID: 11) was used for proteolysis simulation. Results of calculation of the parameters $a_T$, $a_S$, $A_S$, $a_{TE}$, $a_{SE}$, $A_{TE}$ for selected peptides may be displayed by pressing the "View the report with the results" button below the table with results of step 1 (Table S8).

| Protein name: Sequence 1 | | | | | |
|---|---|---|---|---|---|
| Protein sequence: AAYIPPTYAPK | | | | | |
| Profiles of proteins potential biological activity | | | | | |
| ID | Name of peptide | Activity | Number | Sequence | Location |
| 3522 | ACE inhibitor (from bovine b-CN) | ACE inhibitor | 1 | IPP | [4-6] |
| 3563 | ACE inhibitor | ACE inhibitor | 1 | AY | [2-3] |
| 7581 | ACE inhibitor | ACE inhibitor | 1 | IP | [4-5] |
| 7584 | ACE inhibitor | ACE inhibitor | 1 | AP | [9-10] |
| 7589 | ACE inhibitor | ACE inhibitor | 1 | YA | [8-9] |
| 7590 | ACE inhibitor | ACE inhibitor | 1 | AA | [1-2] |
| 7833 | ACE inhibitor | ACE inhibitor | 1 | PT | [6-7] |
| 7836 | ACE inhibitor | ACE inhibitor | 1 | PP | [5-6] |
| 7866 | peptide from Okara protein | antioxidative | 1 | AY | [2-3] |
| 8219 | antioxidative peptide | antioxidative | 1 | TY | [7-8] |
| 2886 | Opioid peptide | opioid antagonist | 1 | YIPP | [3-6] |
| 3170 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | PP | [5-6] |
| 3177 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | AP | [9-10] |
| 8501 | Dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | IP | [4-5] |
| 8637 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | AA | [1-2] |
| 8765 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | AY | [2-3] |
| 8858 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | PK | [10-11] |
| 8863 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | PT | [6-7] |
| 8914 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | TY | [7-8] |
| 8932 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | YA | [8-9] |
| 8938 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | YI | [3-4] |
| 9510 | DPP-III inhibitor | dipeptidyl peptidase III inhibitor | 1 | YI | [3-4] |
| 9433 | Renin inhibitor | renin inhibitor | 1 | YA | [8-9] |
| Calculations | | | | | |

| ID | NAME | Activity | A | B |
|---|---|---|---|---|
| --- | ---------- | ACE inhibitor | 0.7273 | 0.024405320817811 |
| --- | ---------- | antioxidative | 0.1818 | |
| --- | ---------- | dipeptidyl peptidase III inhibitor | 0.0909 | |
| --- | ---------- | dipeptidyl peptidase IV inhibitor | 0.9091 | 0.00025834927242301 |
| --- | ---------- | opioid antagonist | 0.0909 | |
| --- | ---------- | renin inhibitor | 0.0909 | |

Results of enzyme action

AAY - IPPTY - APK

Location of released peptides

[1-3],[4-8],[9-11]

Search for active fragments

| No | Peptide ID | Sequence | Location | Name | Function | Activity | Monoisotopic mass | Chemical mass |
|---|---|---|---|---|---|---|---|---|

$DH_t$ [%]

20.0000

CALCULATE $A_E$, W, $B_E$ and V

| No | Activity | $A_E$ | W | $B_E$ | V |
|---|---|---|---|---|---|

Protein name: Sequence 2

Protein sequence: KIYASDYIPP

Profiles of proteins potential biological activity

| ID | Name of peptide | Activity | Number | Sequence | Location |
|---|---|---|---|---|---|
| 3383 | ACE inhibitor | ACE inhibitor | 1 | IY | [2-3] |
| 3522 | ACE inhibitor (from bovine b-CN) | ACE inhibitor | 1 | IPP | [8-10] |
| 7581 | ACE inhibitor | ACE inhibitor | 1 | IP | [8-9] |
| 7589 | ACE inhibitor | ACE inhibitor | 1 | YA | [3-4] |
| 7836 | ACE inhibitor | ACE inhibitor | 1 | PP | [9-10] |
| 9072 | ACE inhibitor | ACE inhibitor | 1 | DY | [6-7] |
| 2749 | peptide regulating ion flow | regulating | 1 | DY | [6-7] |
| 7873 | peptide from soybean protein isolates: beta-conglycinin and glycinin | antioxidative | 1 | IY | [2-3] |
| 2886 | Opioid peptide | opioid antagonist | 1 | YIPP | [7-10] |
| 3170 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | PP | [9-10] |
| 8501 | Dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | IP | [8-9] |
| 8762 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | AS | [4-5] |
| 8812 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | KI | [1-2] |
| 8932 | dipeptidyl peptidase IV inhibitor | dipeptidyl peptidase IV | 1 | YA | [3-4] |

| | | | | | |
|---|---|---|---|---|---|
| | (DPP IV inhibitor) | inhibitor | | | |
| 8938 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | YI | [7-8] |
| 9510 | DPP-III inhibitor | dipeptidyl peptidase III inhibitor | 1 | YI | [7-8] |
| 9433 | Renin inhibitor | renin inhibitor | 1 | YA | [3-4] |

Calculations

| ID | NAME | Activity | A | B |
|---|---|---|---|---|
| --- | ---------- | ACE inhibitor | 0.6000 | 0.069605669692626 |
| --- | ---------- | antioxidative | 0.1000 | |
| --- | ---------- | dipeptidyl peptidase III inhibitor | 0.1000 | |
| --- | ---------- | dipeptidyl peptidase IV inhibitor | 0.6000 | 0.00026096728544077 |
| --- | ---------- | opioid antagonist | 0.1000 | |
| --- | ---------- | regulating | 0.1000 | |
| --- | ---------- | renin inhibitor | 0.1000 | |

Results of enzyme action

KIY - ASDY - IPP

Location of released peptides

[1-3],[4-7],[8-10]

Search for active fragments

| No | Peptide ID | Sequence | Location | Name | Function | Activity | Monoisotopic mass | Chemical mass |
|---|---|---|---|---|---|---|---|---|
| 1 | 3522 | IPP | [8-10] | ACE inhibitor (from bovine b-CN) | | ACE inhibitor | 325.1880 | 325.3940 |

$DH_t$ [%]

22.2222

CALCULATE $A_E$, W, $B_E$ and V

| No | Activity | $A_E$ | W | $B_E$ | V |
|---|---|---|---|---|---|
| 1 | ACE inhibitor | 0.1000 | 0.1667 | 0.02 | 0.28733291538345 |

Protein name: Sequence 3

Protein sequence: WKILGAWGYIPP

Profiles of proteins potential biological activity

| ID | Name of peptide | Activity | Number | Sequence | Location |
|---|---|---|---|---|---|
| 3522 | ACE inhibitor (from bovine b-CN) | ACE inhibitor | 1 | IPP | [10-12] |
| 3532 | ACE inhibitor | ACE inhibitor | 1 | GY | [8-9] |
| 7543 | ACE inhibitor | ACE inhibitor | 1 | AW | [6-7] |
| 7581 | ACE inhibitor | ACE inhibitor | 1 | IP | [10-11] |
| 7598 | ACE inhibitor | ACE inhibitor | 1 | GA | [5-6] |

| | | | | | |
|---|---|---|---|---|---|
| 7613 | ACE inhibitor | ACE inhibitor | 1 | WG | [7-8] |
| 7619 | ACE inhibitor | ACE inhibitor | 1 | LG | [4-5] |
| 7836 | ACE inhibitor | ACE inhibitor | 1 | PP | [11-12] |
| 9079 | ACE inhibitor | ACE inhibitor | 1 | IL | [3-4] |
| 8323 | Glucose uptake stimulating peptide | stimulating | 1 | IL | [3-4] |
| 8460 | Antioxidant peptide from marine bivalve (Mactra veneriformis) | antioxidative | 1 | AW | [6-7] |
| 9082 | Antioxidative peptide | antioxidative | 1 | WG | [7-8] |
| 3201 | chymotrypsin inhibitor | inhibitor | 1 | GAW | [5-7] |
| 2886 | Opioid peptide | opioid antagonist | 1 | YIPP | [9-12] |
| 3170 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | PP | [11-12] |
| 8501 | Dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | IP | [10-11] |
| 8524 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | GA | [5-6] |
| 8676 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | WK | [1-2] |
| 8695 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | AW | [6-7] |
| 8697 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | WG | [7-8] |
| 8788 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | GY | [8-9] |
| 8802 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | IL | [3-4] |
| 8812 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | KI | [2-3] |
| 8938 | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | dipeptidyl peptidase IV inhibitor | 1 | YI | [9-10] |
| 9510 | DPP-III inhibitor | dipeptidyl peptidase III inhibitor | 1 | YI | [9-10] |

Calculations

| ID | NAME | Activity | A | B |
|---|---|---|---|---|
| --- | ---------- | ACE inhibitor | 0.7500 | 0.027619641874223 |
| --- | ---------- | antioxidative | 0.1667 | |
| --- | ---------- | dipeptidyl peptidase III inhibitor | 0.0833 | |
| --- | ---------- | dipeptidyl peptidase IV inhibitor | 0.8333 | 0.0022700178938607 |
| --- | ---------- | inhibitor | 0.0833 | |
| --- | ---------- | opioid antagonist | 0.0833 | |
| --- | ---------- | stimulating | 0.0833 | |

Results of enzyme action

W - KIL - GAW - GY - IPP

Location of released peptides

[1-1],[2-4],[5-7],[8-9],[10-12]

Search for active fragments

| No | Peptide ID | Sequence | Location | Name | Function | Activity | Monoisotopic mass | Chemical mass |
|---|---|---|---|---|---|---|---|---|
| 1 | 3201 | GAW | [5-7] | chymotrypsin inhibitor | | inhibitor | 332.1370 | 332.3440 |
| 2 | 3522 | IPP | [10-12] | ACE inhibitor (from bovine b-CN) | | ACE inhibitor | 325.1880 | 325.3940 |
| 3 | 3532 | GY | [8-9] | ACE inhibitor | Inhibitor of Angiotensin-Converting Enzyme (ACE) (EC 3.4.15.1) (MEROPS ID: XM02-001) | ACE inhibitor | 238.0840 | 238.2220 |
| 4 | 8788 | GY | [8-9] | dipeptidyl peptidase IV inhibitor (DPP IV inhibitor) | Inhibitor of Dipeptidyl Peptidase IV (EC 3.4.14.5) (MEROPS ID: S09.003) | dipeptidyl peptidase IV inhibitor | 238.0840 | 238.2220 |

$DH_t$ [%]

36.3636

CALCULATE $A_E$, W, $B_E$ and V

| No | Activity | $A_E$ | W | $B_E$ | V |
|---|---|---|---|---|---|
| 1 | inhibitor | 0.0833 | 1.0000 | 0 | |
| 2 | ACE inhibitor | 0.1667 | 0.2223 | 0.033730158730159 | 1.2212380914916 |
| 3 | dipeptidyl peptidase IV inhibitor | 0.0833 | 0.1000 | 0 | 0 |

CALCULATE $a_T$, $a_S$, $A_S$, $a_{TE}$, $a_{SE}$, $A_{TE}$

| ID | Sequence | Activity | $a_T$ | $a_S$ | $A_S$ | $a_{TE}$ | $a_{SE}$ | $A_{TE}$ |
|---|---|---|---|---|---|---|---|---|
| 3522 | IPP | ACE inhibitor | 3 | 1.000 | 0.091 | 6 | 2.000 | 0.182 |
| 3563 | AY | ACE inhibitor | 1 | 0.333 | 0.091 | 0 | 0.000 | 0.000 |
| 7581 | IP | ACE inhibitor | 3 | 1.000 | 0.091 | 0 | 0.000 | 0.000 |
| 7584 | AP | ACE inhibitor | 1 | 0.333 | 0.091 | 0 | 0.000 | 0.000 |
| 7589 | YA | ACE inhibitor | 2 | 0.667 | 0.095 | 0 | 0.000 | 0.000 |
| 7590 | AA | ACE inhibitor | 1 | 0.333 | 0.091 | 0 | 0.000 | 0.000 |
| 7833 | PT | ACE inhibitor | 1 | 0.333 | 0.091 | 0 | 0.000 | 0.000 |
| 7836 | PP | ACE inhibitor | 3 | 1.000 | 0.091 | 0 | 0.000 | 0.000 |
| 7866 | AY | antioxidative | 1 | 0.333 | 0.091 | 0 | 0.000 | 0.000 |
| 8219 | TY | antioxidative | 1 | 0.333 | 0.091 | 0 | 0.000 | 0.000 |
| 2886 | YIPP | opioid antagonist | 3 | 1.000 | 0.091 | 0 | 0.000 | 0.000 |
| 3170 | PP | dipeptidyl peptidase IV inhibitor | 3 | 1.000 | 0.091 | 0 | 0.000 | 0.000 |
| 3177 | AP | dipeptidyl peptidase IV inhibitor | 1 | 0.333 | 0.091 | 0 | 0.000 | 0.000 |
| 8501 | IP | dipeptidyl peptidase IV inhibitor | 3 | 1.000 | 0.091 | 0 | 0.000 | 0.000 |
| 8637 | AA | dipeptidyl peptidase IV inhibitor | 1 | 0.333 | 0.091 | 0 | 0.000 | 0.000 |
| 8765 | AY | dipeptidyl peptidase IV inhibitor | 1 | 0.333 | 0.091 | 0 | 0.000 | 0.000 |
| 8858 | PK | dipeptidyl peptidase IV inhibitor | 1 | 0.333 | 0.091 | 0 | 0.000 | 0.000 |
| 8863 | PT | dipeptidyl peptidase IV inhibitor | 1 | 0.333 | 0.091 | 0 | 0.000 | 0.000 |
| 8914 | TY | dipeptidyl peptidase IV inhibitor | 1 | 0.333 | 0.091 | 0 | 0.000 | 0.000 |
| 8932 | YA | dipeptidyl peptidase IV inhibitor | 2 | 0.667 | 0.095 | 0 | 0.000 | 0.000 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 8938 | YI | dipeptidyl peptidase IV inhibitor | 3 | 1.000 | 0.091 | 0 | 0.000 | 0.000 |
| 9510 | YI | dipeptidyl peptidase III inhibitor | 3 | 1.000 | 0.091 | 0 | 0.000 | 0.000 |
| 9433 | YA | renin inhibitor | 2 | 0.667 | 0.095 | 0 | 0.000 | 0.000 |
| 3383 | IY | ACE inhibitor | 1 | 0.333 | 0.100 | 0 | 0.000 | 0.000 |
| 9072 | DY | ACE inhibitor | 1 | 0.333 | 0.100 | 0 | 0.000 | 0.000 |
| 2749 | DY | regulating | 1 | 0.333 | 0.100 | 0 | 0.000 | 0.000 |
| 7873 | IY | antioxidative | 1 | 0.333 | 0.100 | 0 | 0.000 | 0.000 |
| 8762 | AS | dipeptidyl peptidase IV inhibitor | 1 | 0.333 | 0.100 | 0 | 0.000 | 0.000 |
| 8812 | KI | dipeptidyl peptidase IV inhibitor | 2 | 0.667 | 0.091 | 0 | 0.000 | 0.000 |
| 3532 | GY | ACE inhibitor | 1 | 0.333 | 0.083 | 1 | 0.333 | 0.083 |
| 7543 | AW | ACE inhibitor | 1 | 0.333 | 0.083 | 0 | 0.000 | 0.000 |
| 7598 | GA | ACE inhibitor | 1 | 0.333 | 0.083 | 0 | 0.000 | 0.000 |
| 7613 | WG | ACE inhibitor | 1 | 0.333 | 0.083 | 0 | 0.000 | 0.000 |
| 7619 | LG | ACE inhibitor | 1 | 0.333 | 0.083 | 0 | 0.000 | 0.000 |
| 9079 | IL | ACE inhibitor | 1 | 0.333 | 0.083 | 0 | 0.000 | 0.000 |
| 8323 | IL | stimulating | 1 | 0.333 | 0.083 | 0 | 0.000 | 0.000 |
| 8460 | AW | antioxidative | 1 | 0.333 | 0.083 | 0 | 0.000 | 0.000 |
| 9082 | WG | antioxidative | 1 | 0.333 | 0.083 | 0 | 0.000 | 0.000 |
| 3201 | GAW | inhibitor | 1 | 0.333 | 0.083 | 1 | 0.333 | 0.083 |
| 8524 | GA | dipeptidyl peptidase IV inhibitor | 1 | 0.333 | 0.083 | 0 | 0.000 | 0.000 |
| 8676 | WK | dipeptidyl peptidase IV inhibitor | 1 | 0.333 | 0.083 | 0 | 0.000 | 0.000 |
| 8695 | AW | dipeptidyl peptidase IV inhibitor | 1 | 0.333 | 0.083 | 0 | 0.000 | 0.000 |
| 8697 | WG | dipeptidyl peptidase IV inhibitor | 1 | 0.333 | 0.083 | 0 | 0.000 | 0.000 |
| 8788 | GY | dipeptidyl peptidase IV inhibitor | 1 | 0.333 | 0.083 | 1 | 0.333 | 0.083 |
| 8802 | IL | dipeptidyl peptidase IV inhibitor | 1 | 0.333 | 0.083 | 0 | 0.000 | 0.000 |

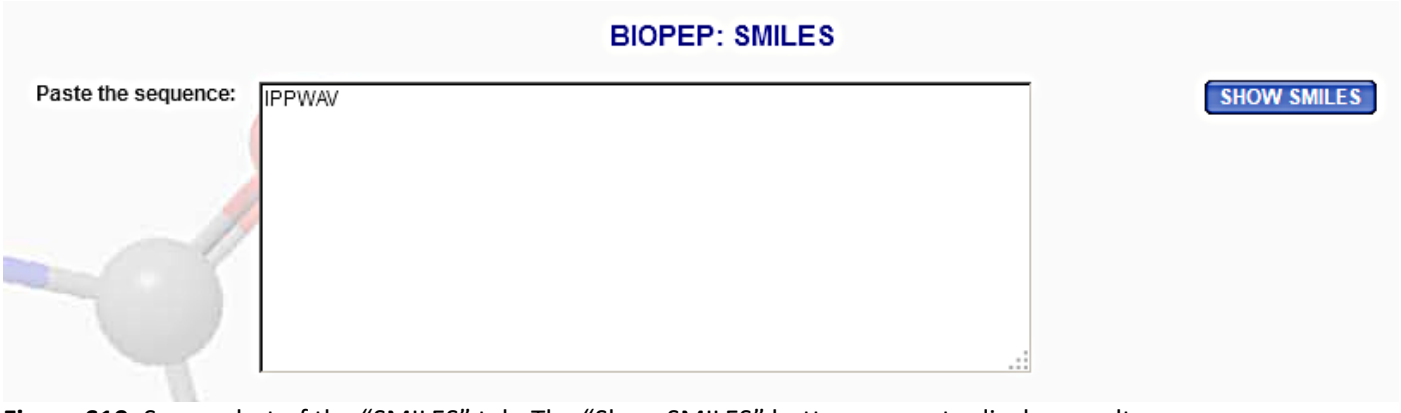



**Figure S19.** Screenshot of the “SMILES” tab. The “Show SMILES” button serves to display result.

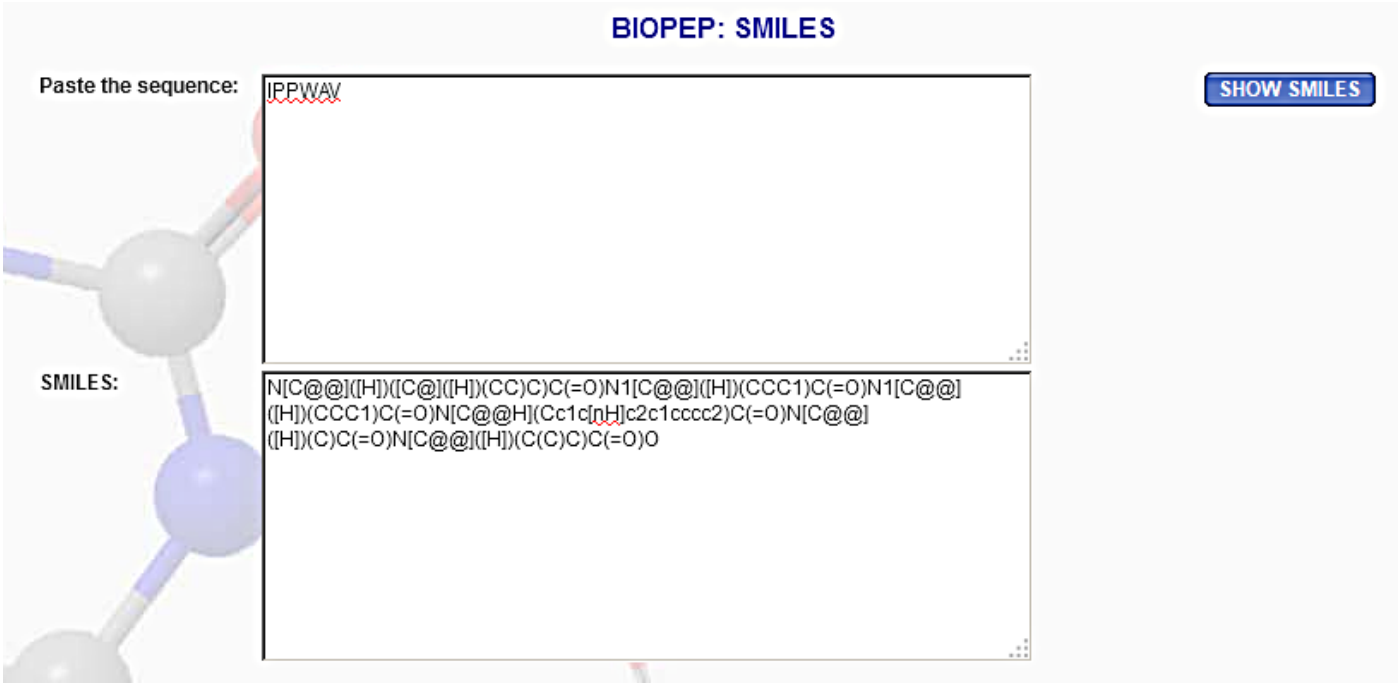



**Figure S20.** Screenshot of the "SMILES" tab with result of conversion of amino acid sequence of peptide IPPWAV into SMILES code.

**Table S10.** Two types of SMILES representations of peptide IPPWAV: aromatic version generated from the amino acid sequence by "SMILES" application in the BIOPEP-UWM database and Kekule version obtained from the previous one using molecule editor of the PubChem database

| Kind of representation | Representation |
|---|---|
| Sequence | IPPWAV |
| Aromatic version of SMILES | N[C@@]([H])([C@]([H])(CC)C)C(=O)N1[C@@]([H])(CCC1)C(=O)N1[C@@]([H])(CCC1)C(=O)N[C@@H](Cc1c[nH]c2c1cccc2)C(=O)N[C@@]([H])(C)C(=O)N[C@@]([H])(C(C)C)C(=O)O |
| Kekule version of SMILES | N[C@@H]([C@H](CC)C)C(=O)N1[C@@H](CCC1)C(=O)N2[C@@H](CCC2)C(=O)N[C@@H](CC3=C[N]([H])C4=CC=CC=C34)C(=O)N[C@@H](C)C(=O)N[C@@H](C(C)C)C(=O)O |

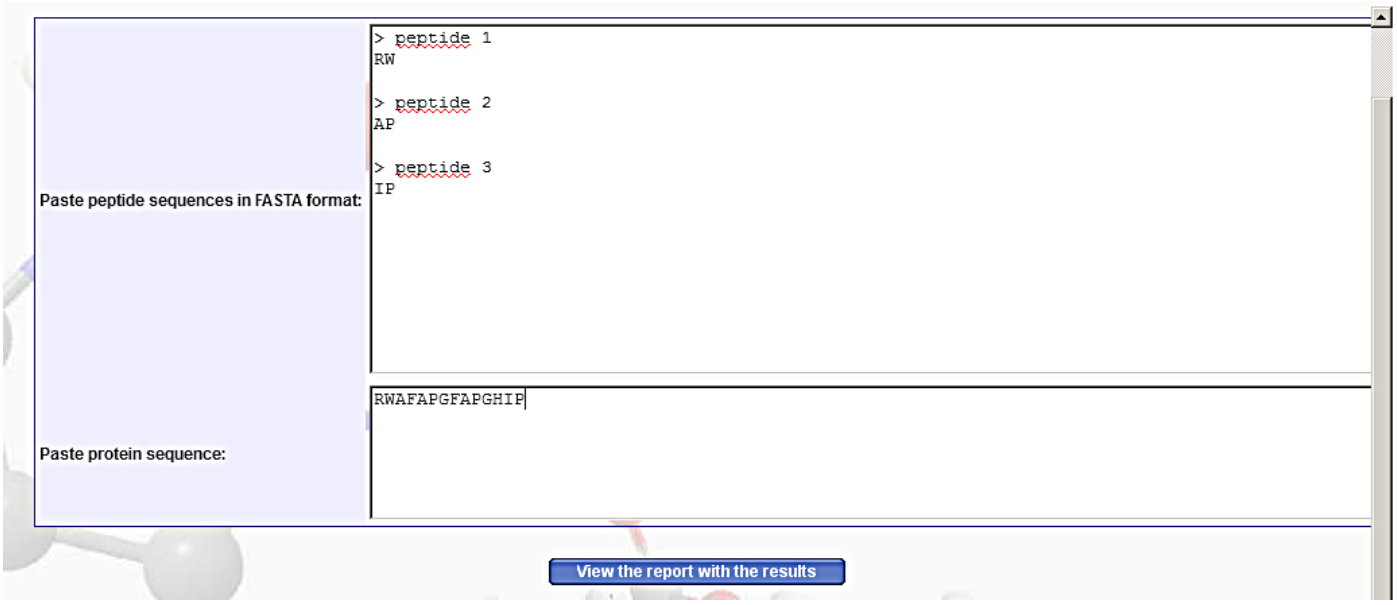



**Figure S21**. Screenshot of the menu of the "Find enzyme for peptide release" tab

**Table S11**. Results of the action of "Find enzyme for peptide release" option. Example covers prediction of release of peptides RW, AP, and IP from the RWAFAPGFAPGHIP sequence.

| **Protein sequence** | **RWAFAPGFAPGHIP** | | | | |
|---|---|---|---|---|---|
| **Peptide sequence** | **RW** | | | | |
| **Location of peptide** | **[1-2]** | | | | |
| **Location of proteolytic events** | **1C: 2-3** | | | | |
| **Displaying of proteolytic events** | **RW-AFAPGFAPGHIP** | | | | |
| ***Proteolytic event*** | ***1C*** | | | | |
| Enzyme Name | EC Number | Enzyme ID | Connection ID | Cutting seqence | Recognition sequence |
| thermolysin | EC 3.4.24.27 | 18 | 49 | A+ | A |
| coccolysin | EC 3.4.24.30 | 40 | 133 | A+ | A |
| chymotrypsin (A) | EC 3.4.21.1 | 11 | 27 | W- | W |
| Proteinase K | EC.3.4.21.67 | 14 | 39 | W- | W |
| chymase | EC 3.4.21.39 | 23 | 64 | W- | W |
| chymotrypsin C | EC 3.4.21.2 | 19 | 87 | W- | W |
| metridin | EC 3.4.21.3 | 27 | 93 | W- | W |
| subtilisin | EC 3.4.21.62 | 41 | 138 | W- | W |
| **Protein sequence** | **RWAFAPGFAPGHIP** | | | | |
| **Peptide sequence** | **AP** | | | | |
| **Location of peptide** | **[5-6],[9-10]** | | | | |
| **Location of proteolytic events** | **1N: 4-5; 1C: 6-7; 2N: 8-9; 2C: 10-11** | | | | |
| **Displaying of proteolytic events** | **RWAF-AP-GF-AP-GHIP** | | | | |
| ***Proteolytic event*** | ***1N*** | | | | |
| Enzyme Name | EC Number | Enzyme ID | Connection ID | Cutting sequence | Recognition sequence |
| chymotrypsin (A) | EC 3.4.21.1 | 11 | 28 | F- | F |
| pepsin (pH 1.3) | EC 3.4.23.1 | 13 | 32 | F- | F |
| Proteinase K | EC.3.4.21.67 | 14 | 34 | F- | F |
| cathepsin G | EC 3.4.21.20 | 21 | 58 | F- | F |
| chymase | EC 3.4.21.39 | 23 | 62 | F- | F |
| papain | EC 3.4.22.2 | 24 | 66 | F- | F |
| ficin | EC 3.4.22.3 | 25 | 73 | F- | F |
| metridin | EC 3.4.21.3 | 27 | 91 | F- | F |
| pancreatic elastase II | EC 3.4.21.71 | 29 | 101 | F- | F |
| oligopeptidase F | - | 36 | 114 | F- | F |
| subtilisin | EC 3.4.21.62 | 41 | 135 | F- | F |
| thermolysin | EC 3.4.24.27 | 18 | 49 | A+ | A |
| papain | EC 3.4.22.2 | 24 | 71 | A+ | A |
| calpain 2 | EC 3.4.22.53 | 33 | 109 | A+ | A |
| coccolysin | EC 3.4.24.30 | 40 | 133 | A+ | A |

| Proteolytic event | 1C | | | | |
|---|---|---|---|---|---|
| Enzyme Name | EC Number | Enzyme ID | Connection ID | Cutting sequence | Recognition sequence |
| Proteinase K | EC.3.4.21.67 | 14 | 40 | P- | P |
| prolyl oligopeptidase | EC 3.4.21.26 | 16 | 47 | P- | P |
| chymotrypsin C | EC 3.4.21.2 | 19 | 85 | P- | P |
| Proteolytic event | 2N | | | | |
| Enzyme Name | EC Number | Enzyme ID | Connection ID | Cutting sequence | Recognition sequence |
| chymotrypsin (A) | EC 3.4.21.1 | 11 | 28 | F- | F |
| pepsin (pH 1.3) | EC 3.4.23.1 | 13 | 32 | F- | F |
| Proteinase K | EC.3.4.21.67 | 14 | 34 | F- | F |
| cathepsin G | EC 3.4.21.20 | 21 | 58 | F- | F |
| chymase | EC 3.4.21.39 | 23 | 62 | F- | F |
| papain | EC 3.4.22.2 | 24 | 66 | F- | F |
| ficin | EC 3.4.22.3 | 25 | 73 | F- | F |
| metridin | EC 3.4.21.3 | 27 | 91 | F- | F |
| pancreatic elastase II | EC 3.4.21.71 | 29 | 101 | F- | F |
| oligopeptidase F | - | 36 | 114 | F- | F |
| subtilisin | EC 3.4.21.62 | 41 | 135 | F- | F |
| thermolysin | EC 3.4.24.27 | 18 | 49 | A+ | A |
| papain | EC 3.4.22.2 | 24 | 71 | A+ | A |
| calpain 2 | EC 3.4.22.53 | 33 | 109 | A+ | A |
| coccolysin | EC 3.4.24.30 | 40 | 133 | A+ | A |
| Proteolytic event | 2C | | | | |
| Enzyme Name | EC Number | Enzyme ID | Connection ID | Cutting seqence | Recognition sequence |
| Proteinase K | EC.3.4.21.67 | 14 | 40 | P- | P |
| prolyl oligopeptidase | EC 3.4.21.26 | 16 | 47 | P- | P |
| chymotrypsin C | EC 3.4.21.2 | 19 | 85 | P- | P |
| Protein sequence | RWAFAPGFAPGHIP | | | | |
| Peptide sequence | IP | | | | |
| Location of peptide | [13-14] | | | | |
| Location of proteolytic events | 1N: 12-13 | | | | |
| Displaying of proteolytic events | RWAFAPGFAPGH-IP | | | | |
| Proteolytic event | 1N | | | | |
| Enzyme Name | EC Number | Enzyme ID | Connection ID | Cutting sequence | Recognition sequence |
| cathepsin G | EC 3.4.21.20 | 21 | 57 | H- | H |
| chymotrypsin (A) | EC 3.4.21.1 | 11 | 142 | H- | H |
| ficin | EC 3.4.22.3 | 25 | 185 | H- | H |

| | | | | | |
|---|---|---|---|---|---|
| thermolysin | EC 3.4.24.27 | 18 | 51 | I+ | I |
| coccolysin | EC 3.4.24.30 | 40 | 175 | I+ | I |
| pepsin (pH > 2) | EC 3.4.23.1 | 39 | 189 | I+ | I |