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Communication

BIOPEP-UWM Virtual—A Novel Database of Food-Derived Peptides with In Silico-Predicted Biological Activity

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Abstract: The novel BIOPEP-UWM Virtual database is designed as a repository of peptide sequences whose bioactivity or taste information was the result of in silico predictions. It is a tool complementary to the existing BIOPEP-UWM database summarizing the results of experimental data on bioactive peptides. The layout and organization of the new database are identical to those of the existing BIOPEP-UWM database of bioactive peptides. The peptide data record includes the following information: name; sequence and function information (understood as information about the predicted target biomacromolecule); bibliographic data with the reference paper describing the peptide; additional information, including the peptide structure, annotated using chemical codes as well as the specification of the method used for bioactivity prediction; information about other activities discovered experimentally or predicted using computational methods; peptide taste (if available); and a database reference tab providing information about compound annotations in other databases (if available).

Keywords: peptides; bioactivity; taste; molecular docking; in silico predictions; database

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1. Introduction

Bioinformatics represents a set of standard methods applied in research on peptides, including those of food origin [1–3]. Recently, the importance of the computational approach has been highlighted in, for example, the search for anti-SARS-CoV2 peptides [4–6]. The in silico approach includes molecular docking studies of peptides, which appear to be an emerging tool for predicting the bioactivity of food peptides [4,6–9]. Its application for educational purposes has been recently described by Khan and coworkers [10]. Molecular docking is usually deployed together with experimental confirmation of biological properties of molecules, e.g., enzyme inhibition potential, but there are also investigations restricted to computational predictions. Another experimental model includes the in silico screening of many compounds, of which only one or a few of the most promising are then subjected to laboratory testing. Although in silico predictions are not fully equivalent to experimental works, they provide valuable information about the biological functions of compounds. However, critical interpretation of such results is always necessary. Strong and weak points as well as opinions concerning computational predictions of bioactivity of chemical substances have been recently discussed by Medina-Franco et al. [11]. Taking into account the pros and cons of in silico predictions concerning bioactive peptides, they may be annotated in a separate database.

The BIOPEP-UWM database [12] has become a popular information resource in research concerning the bioactivity and taste of peptides, mainly those derived from foods. It is also used for students' education [13]. The existing peptide databases, the BIOPEP-UWM database of bioactive peptides and the BIOPEP-UWM database of sensory peptides and amino acids, contain only data concerning peptides with bioactivity or taste evaluated in vitro or in vivo. The newly launched database provides the results of computational

predictions of the biological activity or the taste of peptides, especially those derived from foods, which have yet not been confirmed in laboratory conditions.

To date, our policy concerning the annotation of peptides in the BIOPEP-UWM database only took into account the compounds with biological properties confirmed experimentally. Submissions of peptides that function was predicted via the in silico method were declined. Thus, the launching of a new database is a result of the change of this policy. Results concerning the bioactivity or taste of peptides, obtained experimentally or predicted in silico and confirmed experimentally, will still be presented in our twin BIOPEP-UWM databases, i.e., of bioactive peptides and of sensory peptides and amino acids, whereas results obtained using computational methods only (considered virtual) will be presented in the new database.

The aim of this publication was to announce and provide a brief description of the new tool serving as a repository of data concerning peptides with the biological activity or taste predicted in silico and other recent changes in the BIOPEP-UWM database.

2. Database Description

The database is freely available without registration. It has been recently moved to a new server. Its current address is the following: https://biochemia.uwm.edu.pl/en/biopep-uwm-2/ (Last accessed on 13 July 2022). A screenshot of the current homepage of the BIOPEP-UWM database is presented in Figure 1, the database organization in Figure 2, a fragment of the list of peptides in Figure 3, a screenshot of individual peptide data in Figure 4, and a screenshot of the "Screen and print peptide data" tab content in Figure 5.

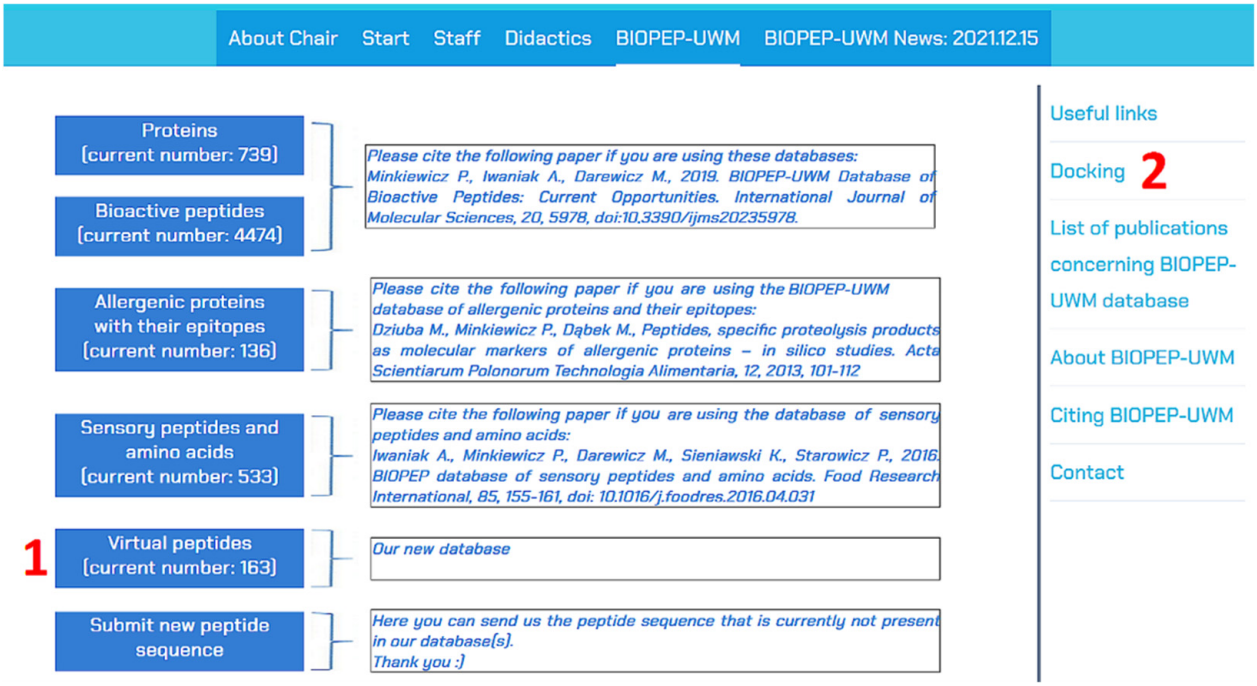


Figure 1. Screenshot of the current homepage of the BIOPEP-UWM database. (**1**) BIOPEP-UWM Virtual tab; (**2**) links to programs for molecular docking.

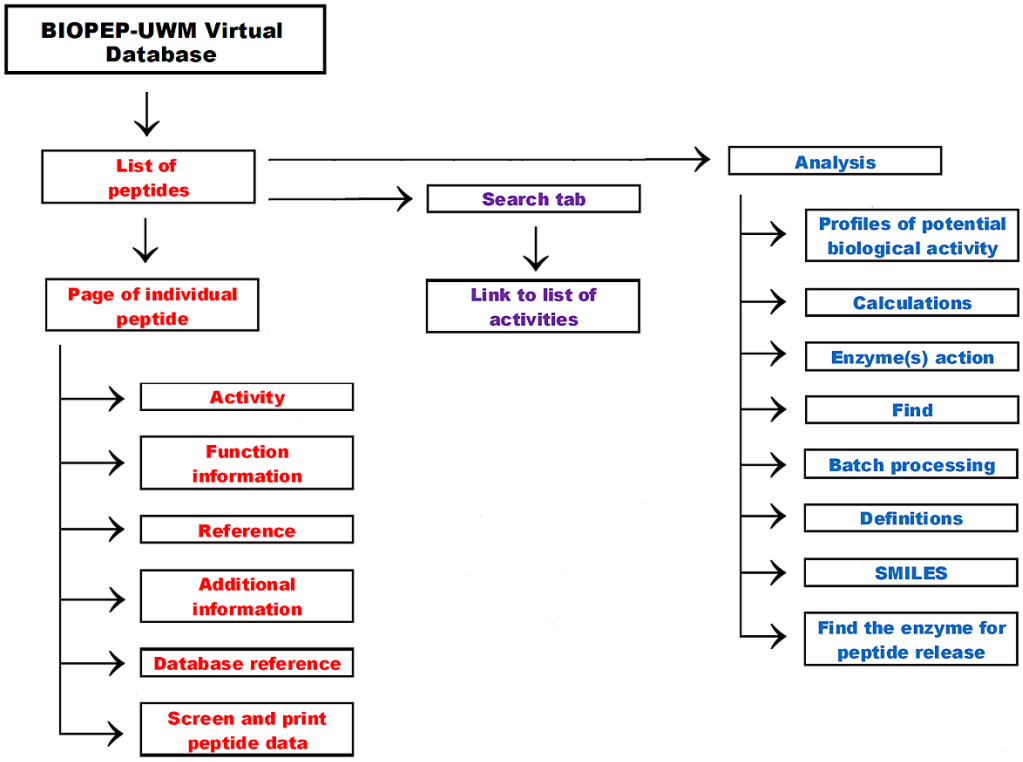


Figure 2. Scheme of the organization of the BIOPEP-UWM Virtual database. Due to the fact that the layout of the new database is identical to the BIOPEP-UWM database of bioactive peptides described in our previous article [12], the Figure is adapted from the above reference.

BIOPEP-UWM: Virtual peptides

ANALYSIS

Number of virtual peptides in database: 163

	ID	Name	Sequence	Chem. mass	Monois. mass	
Virtual Peptide Data	151	ACE inhibitor	PPPVHDFNME	1182.3100	1181.5022	0.00 EC_{50}
Virtual Peptide Data	152	ACE inhibitor	LNFDPNR	874.9390	874.4177	0.00 EC_{50}
Virtual Peptide Data	153	ACE inhibitor	LPQQQAQFK	1087.2310	1086.5670	0.00 EC_{50}
Virtual Peptide Data	154	DPPIV inhibitor	PPPVHDFNME	1182.3100	1181.5022	0.00 EC_{50}
Virtual Peptide Data	155	DPPIV inhibitor	LNFDPNR	874.9390	874.4177	0.00 EC_{50}
Virtual Peptide Data	156	DPPIV inhibitor	LPQQQAQFK	1087.2310	1086.5670	0.00 EC_{50}
Virtual Peptide Data	157	Antiviral peptide	LSTAADMQGVVTDGMASGLDKDYLKPDD	2914.2050	2912.3232	0.00 EC_{50}
Virtual Peptide Data	158	Antiviral peptide	LSTAADMQGVVTDGMASG	1710.8940	1709.7446	0.00 EC_{50}
Virtual Peptide Data	159	Antiviral peptide	VHRKCF	805.8140	805.3890	0.00 EC_{50}
Virtual Peptide Data	160	Antiviral peptide	CQRKTAPY	982.9640	982.4520	0.00 EC_{50}
Virtual Peptide Data	161	Antiviral peptide	YVSSYYHT	1019.0500	1018.4260	0.00 EC_{50}
Virtual Peptide Data	162	Antiviral peptide	PKWF	576.6810	576.2930	0.00 EC_{50}
Virtual Peptide Data	163	Antiviral peptide	AEYCIKR	898.8870	898.4210	0.00 EC_{50}

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Search: by: ID GO exact

ID (e.g. 2572)
Name (e.g. lactorphin)
Activity (e. g. antioxidative) List of activities
Mass (e.g. 700-1200)
Reference (e.g. Meisel)
Sequence (e.g. IPP)
Number of amino acid residues (e.g. 2)
InChIKey (e.g. JNTMAZFVYNDPLB-PEDHHIEDSA-N)

Figure 3. Screenshot of a fragment of the peptide list in the BIOPEP-UWM Virtual database with search options. Links to individual peptide cards are presented in the left column.

The website including both new and older parts of the BIOPEP-UWM database (BIOPEP-UWM database of proteins; the BIOPEP-UWM database of bioactive peptides, our main database; the BIOPEP-UWM database of allergens and their epitopes; and the BIOPEP-UWM database of sensory peptides and amino acids) has been moved into a new server. Users are redirected to this website automatically when they access the database via the old address, described previously [12].

The BIOPEP-UWM database (providing access to BIOPEP-UWM Virtual together with existing databases of the sequences of bioactive peptides as well as sensory peptides and amino acids) is a website constructed using an updated content management system (WordPress). Applications associated with the database are written in the PHP language.

The graphical layout of the BIOPEP-UWM homepage has been changed as compared to the previous website [12]. As shown in Figure 1, the left column contains tabs of particular databases including the BIOPEP-UWM Virtual and a link to the new peptide data submission form. The middle column contains bibliographic data of articles describing individual parts of the BIOPEP-UWM database [12,14,15]. The right column contains the following tabs: "Useful links", "Docking", "List of publications concerning the BIOPEP-UWM database", "About BIOPEP-UWM", ''Citing BIOPEP-UWM", and "Contact". Among them, the "Docking" tab is new. All other pages existed in the previous version of the BIOPEP-UWM database [12]. The content, layout, and graphics of the old tabs are the same as described in our previous publication [12].

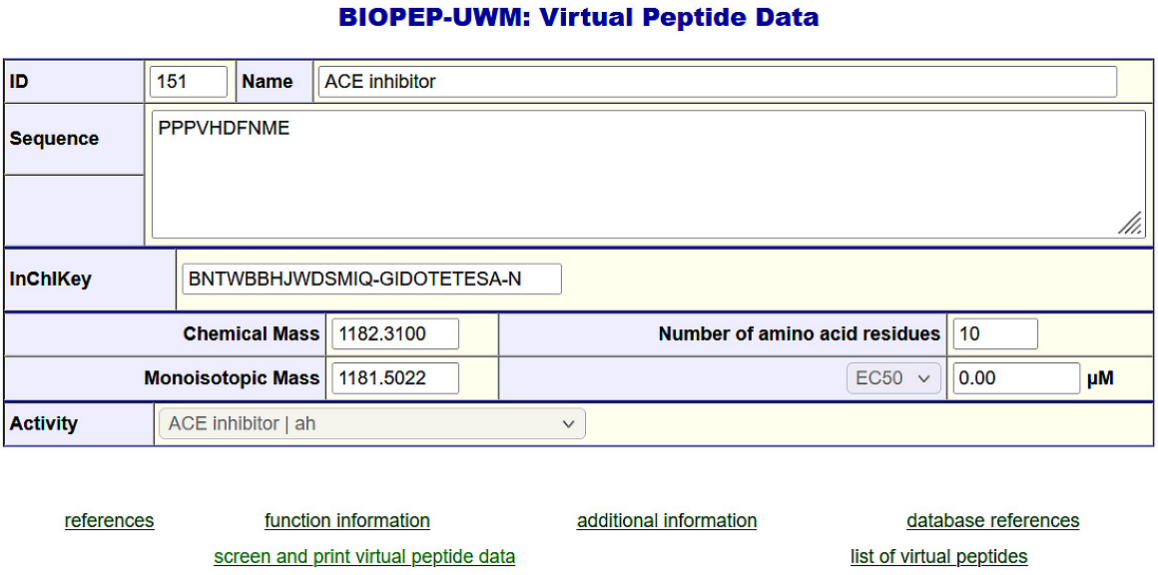
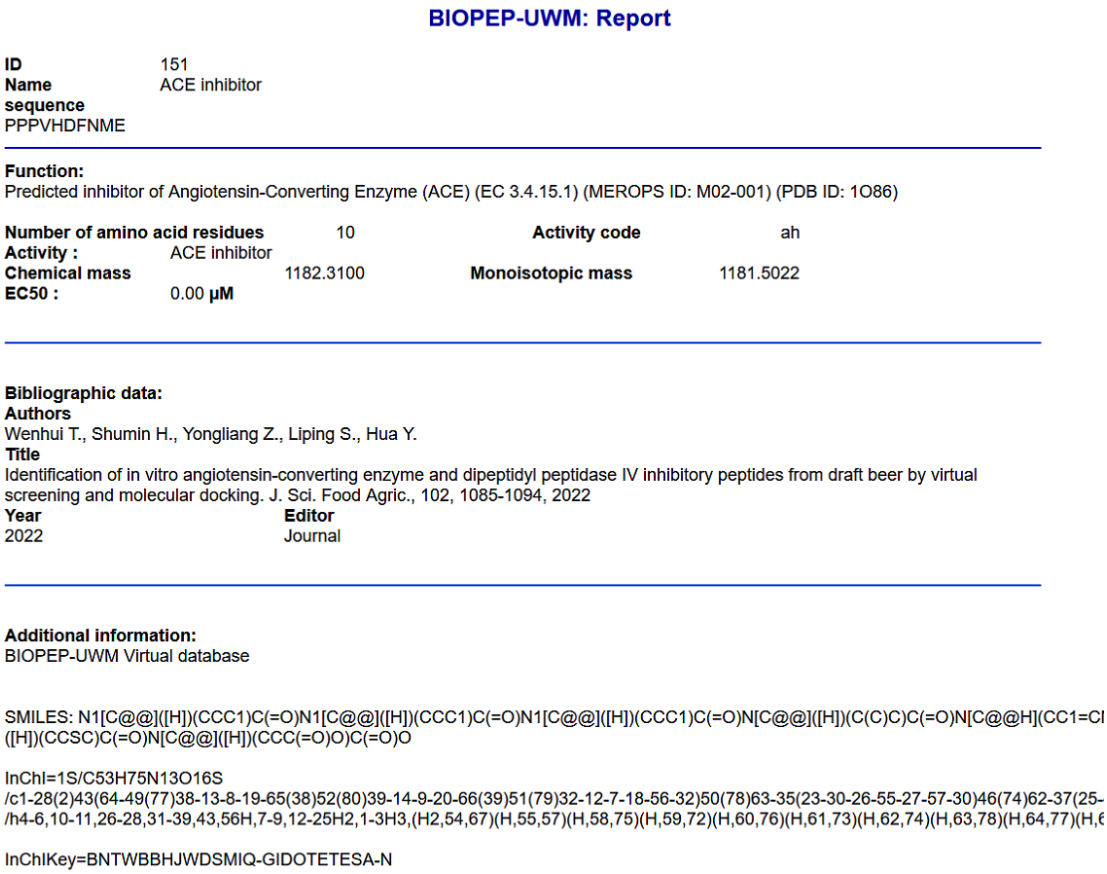


Figure 4. Screenshot of example peptide data: a predicted inhibitor of the angiotensin-converting enzyme (ACE) (BIOPEP-UWM Virtual ID: 151). The above peptide has been described by Wen-hui et al. [16].



BIOPEP-UWM: Report

ID 151
Name ACE inhibitor
sequence
PPPVHDFNME

Function:
Predicted inhibitor of Angiotensin-Converting Enzyme (ACE) (EC 3.4.15.1) (MEROPS ID: M02-001) (PDB ID: 1O86)

Number of amino acid residues 10 **Activity code** ah
Activity : ACE inhibitor
Chemical mass 1182.3100 **Monoisotopic mass** 1181.5022
EC50 : 0.00 **µM**

Bibliographic data:
Authors
Wenhui T., Shumin H., Yongliang Z., Liping S., Hua Y.
Title
Identification of in vitro angiotensin-converting enzyme and dipeptidyl peptidase IV inhibitory peptides from draft beer by virtual screening and molecular docking. J. Sci. Food Agric., 102, 1085-1094, 2022
Year **Editor**
2022 Journal

Additional information:
BIOPEP-UWM Virtual database

SMILES: N1[C@@]([H])(CCC1)C(=O)N1[C@@]([H])(CCC1)C(=O)N1[C@@]([H])(CCC1)C(=O)N[C@@]([H])(C(C)C)C(=O)N[C@@H](CC1=CI
([H])(CCSC)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)O

InChI=1S/C53H75N13O16S
/c1-28(2)43(64-49(77)38-13-8-19-65(38)52(80)39-14-9-20-66(39)51(79)32-12-7-18-56-32)50(78)63-35(23-30-26-55-27-57-30)46(74)62-37(25-
/h4-6,10-11,26-28,31-39,43,56H,7-9,12-25H2,1-3H3,(H2,54,67)(H,55,57)(H,58,75)(H,59,72)(H,60,76)(H,61,73)(H,62,74)(H,63,78)(H,64,77)(H,6

InChIKey=BNTWBBHJWDSMIQ-GIDOTETESA-N

Figure 5. Screenshot of the content from the tab "Screen and print peptide data" (see Figure 3): an exemplary peptide with BIOPEP-UWM Virtual ID: 151.

The layout of the database "BIOPEP-UWM Virtual" reflects the layout of the BIOPEP-UWM database of bioactive peptides (still considered the main database), described in detail in our previous article [12]. The guide to the database of experimentally discovered bioactive peptides (publication [12] and its supplement) may also serve as a guide to the BIOPEP-UWM Virtual database. A peptide list, opened after clicking the tab of the new database, is arranged as a typical list in the BIOPEP-UWM database [12] (see Figure 3). The value EC_{50} = 0 means that EC_{50} or IC_{50} values were not predicted in the case of enzyme inhibitors presented in Figure 2. Search options are also the same as in the main database of bioactive peptides and enable the search using peptide ID, name, activity (list of activities is available via separate tab), molecular mass range, bibliographic data of reference (e.g., author name), amino acid sequence, number of amino acid residues, and InChIKey. The list of activities attributed to the BIOPEP-UWM Virtual database includes activities from databases of both bioactive peptides and tastes. The list of activities has been updated since 2019. The following activities have been recently added: membrane-active peptides, inhibitors of calpain 2 (EC 3.4.22.53), inhibitors of lipoxygenase, inhibitors of cyclooxygenase-1 (EC 1.14.99.1), inhibitors of cyclooxygenase-2 (EC 1.14.99.1), inhibitors of pancreatic lipase, inhibitors of angiotensin 2-converting enzyme (ACE2) (EC 3.4.17.23), inhibitors of acetylcholinesterase (AChE) (EC 3.1.1.7), inhibitors of butyrylcholinesterase (BChE) (EC 3.1.1.8), and inhibitors of tyrosinase (EC 1.14.18.1). Among them, predicted ACE2 inhibitors and AChE inhibitors are represented in the BIOPEP-UWM Virtual database.

The content of an exemplary peptide record from the BIOPEP-UWM Virtual database is presented in Figures 4 and 5.

The peptide data record includes the following tabs (i.e., cards):

- name (if possible) and sequence;
- function information—information about the predicted target biomacromolecule;

- bibliographic data with the reference paper describing the peptide;
- additional information, including the annotated peptide structure using chemical codes SMILES [17] and InChI [18], InChIKey identifier, specification of the method used for bioactivity prediction (to date, mainly molecular docking), information about other activities discovered experimentally or predicted using computational methods, and/or peptide taste (if available). The last category of content may include information about the main tastes (bitter, umami, sweet, sour, or salty) as well as enhancement or suppression of taste (e.g., bitterness-suppressing or umami-enhancing peptides). This information is taken from the BIOPEP-UWM database of sensory peptides and amino acids [15]. Information about the activity or taste of the peptide cites the database or databases providing this information;
- a database reference tab providing information about compound annotations in other databases (if available). The set of databases cited in this tab is described in our previous article [12]. Information about peptide annotation includes database name and compound ID. This tab also contains information about the annotation of peptides in the BIOPEP-UWM database of bioactive peptides and/or the BIOPEP-UWM database of sensory peptides and amino acids;
- entire peptide data arranged for printing, available via the "Screen and print peptide data". A table screenshot of the content of the above tab is shown in Figure 4.

If the target biomolecule structure mentioned in the "Function information" tab is taken from a database, for example, the Protein Data Bank [19], an ID in the above database is provided. If the target molecule is a proteolytic enzyme, an accession number in the MEROPS database [20] is also provided.

The "Analysis" tab includes all options available in the parent BIOPEP-UWM database of bioactive peptides [12]. It enables finding the location of all virtual bioactive fragments in a protein sequence; calculating quantitative parameters characterizing proteins as potential precursors of bioactive peptides; simulating enzymatic hydrolysis of proteins, followed by finding virtual bioactive fragments among predicted proteolysis products; using a batch processing option, enabling operations on a set of protein sequences without restrictions concerning the number or total length of sequences; converting amino acid sequences into SMILES representations; and finding enzymes potentially hydrolyzing given peptide bonds.

Some changes concerning options available via the "Analysis" tab in all BIOPEP-UWM databases of peptides have been introduced since the publication of our previous article [12]. The first version of batch processing allowed processing a set of protein sequences with a total length of ca. 1500 amino acid residues [12]. This restriction was removed. Profiles of potential biological activity of protein fragments may be sorted according to activity (this version has been available since the launching of the parent database of bioactive peptides) or by fragment sequence. The second option has been added to follow the remarks of users interested in multifunctional peptides. Another modification was the replacement of the "aromatic" version of SMILES representations of aromatic amino acids (fulfilling formal aromaticity rule) by the Kekulé version according to recent recommendations [21,22]. For instance, SMILES strings N[C@@H](Cc1c[nH]cn1)C(=O)O and N[C@@H](Cc1c[nH]c2c1cccc2)C(=O)O were replaced by N[C@@H](CC1=CN=C[NH]1)C(=O)O and N[C@@H](CC1=C[NH]C2=CC=CC=C12)C(=O)O for histidine and tryptophan, respectively. Aromatic SMILES representations of compounds containing heterocyclic (e.g., histidine) and/or conjugated (e.g., tryptophan) aromatic rings are sometimes not accepted by molecular editors or search engines of chemical databases. The PubChem search engine, the biggest database of chemical compounds, converts SMILES representations from the aromatic to the Kekulé version [21]. The change of SMILES representations was expected to improve the interoperability of the BIOPEP-UWM with chemical databases and programs from the approach of cheminformatics.

Apart from existing links to bioinformatic tools [12], a new tab has been added that provides access to free access programs for molecular docking, available via the web

servers and not requiring downloading and installation on users' computers (labelled "2" in Figure 1). A screenshot of part of the content of this tab is presented in Figure 5. Information concerning the program includes the name, website, and reference describing the program. Programs are placed on the website in alphabetical order. The first three are shown in Figure 6. Links to some of these programs are also available via the "Useful links" tab (Figure 1) (category: "Bioactivity prediction") and via the MetaComBio website [23] tab named "Programs". The last website also possesses the following new address: https://biochemia.uwm.edu.pl/metachemibio/about-metacombio/ (Last accessed on 13 July 2022).

Program	Website	Reference
B-AceP tool	http://www4g.biotec.or.th/FeptideDB/ligand_docking.php	Panyayai T., Ngamphiw C., Tongsima S., Mhuantong W., Limsripraphan W., Choowongkomon K., Sawatdichaikul O., FeptideDB: A web application for new bioactive peptides from food protein. Heliyon, 2019, 5, e02076.
CB-Dock	http://clab.labshare.cn/cb-dock/php/	Liu Y., Grimm M., Dai W., Hou M., Xiao Z.-X., Cao Y., CB-Dock: a web server for cavity detection-guided protein–ligand blind docking. Acta Pharmacologica Sinica, 2020, 41, 138–144.
ClusPro	https://cluspro.org/login.php?redir=/home.php	Kozakov D., Hall D. R., Xia B., Porter K. A., Padhorny D., Yueh C., Beglov D., Vajda S., The ClusPro web server for protein-protein docking. Nature Protocols, 2017, 12, 255-278.

Figure 6. Screenshot of a fragment of the content of the "Docking" tab (see Figure 1). B-AceP tool [24], CB-Dock [25], and ClusPro [26] programs serve as examples.

We would like to encourage users to submit new information about virtual bioactive peptides to the new database. The above sentence concerns both new peptide sequences, additional information about existing compounds, and correction of errors, if necessary. Although the database's task is to mainly annotate peptides of food origin, submissions of peptides from other sources, synthetic or even in silico, will be accepted as well. The prediction method will be not restricted to molecular docking. Other methods, such as the quantitative structure−activity relationship (QSAR) or machine learning, can also be included. The BIOPEP-UWM database annotates peptides consisting of proteinogenic amino acids and their D-enantiomers. Sequences should be written in a single letter code.

The submission form of new peptide sequences is available on the database homepage (Figure 1) below the tab of the BIOPEP-UWM Virtual database. The submitted information should include the peptide sequence, sender e-mail address for correspondence, name and surname, and full bibliographic data of the article describing a given peptide. We only take into account peptides described in peer-reviewed publications.

3. Conclusions

The BIOPEP-UWM Virtual database is a complementary tool to the existing database of bioactive peptide sequences. It is designed as a repository of peptide sequences whose bioactivity or taste are the result of in silico predictions. The new database provides information about particular compounds and access to a set of tools describing proteins as a potential source of virtual bioactive peptides. It may serve as a guide in further experiments.

Author Contributions: P.M., A.I. and M.D. were the curators of the BIOPEP-UWM database. P.M., M.D. and A.I. designed the new database. P.M., A.I. and M.D. wrote the manuscript. M.D. and A.I. acquired the funding. All authors have read and agreed to the published version of the manuscript.

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Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: The database is freely available without registration at the following website: https://biochemia.uwm.edu.pl/en/biopep-uwm-2/. Individual visits at the BIOPEP-UWM website are not tracked. Users remain anonymous until they publish their results and cite the database name and/or web address.

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Conflicts of Interest: The authors declare no conflict of interest.

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