



BIOPEP database of sensory peptides and amino acids



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ABSTRACT

Peptides and amino acids belong to compounds that influence the taste of foods. The aim of this study was to develop a database of sensory peptides and amino acids. Information about the taste of the analyzed compounds was obtained from sensory studies described in the literature. The database of sensory peptides and amino acids has identical structure to the BIOPEP database of biologically active peptides. The information about sensory peptides and amino acids was inserted into the database using standard BIOPEP layouts for bioactive peptides. Information about the biological activity of sensory peptides was obtained from BIOPEP and other databases.

The information annotated in the BIOPEP database of sensory peptides and amino acids includes: sequence written in a one-letter code, information about taste, reference, structure written with the use of chemical codes (SMILES, InChI and InChIKey), bioactivity data (mainly inhibition of proteolytic enzymes), if applicable, and ID numbers from other biological and chemical databases.

The database contains tools for determining the location of peptides in protein sequences (profiles of potential sensory activity), comparing protein sequences as precursors of sensory peptides based on the frequency of sensory fragments as a quantitative descriptor, simulating proteolysis and calculating novel parameters for quantitative description of simulated proteolysis.

The BIOPEP database of sensory peptides and amino acids is available at <http://www.uwm.edu.pl/biochemia/index.php/pl/biopep>. It is an open access resource that does not require user registration.

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1. Introduction

Humans are capable of identifying five basic tastes: sweet, salty, bitter, sour, and umami. According to other scientific reports, other tastes can also be recognized as a result of fatty acid reactions in fats (Cygankiewicz, Masłowska, & Krajewska, 2014). Peptides and amino acids have various biological functions, and they influence the taste of food products (Temussi, 2012). Sensory (possessing experimentally recognized taste and affecting taste of foodstuffs) peptides and amino acids became an object of scientific inquiry 50 years ago on account of their taste-altering properties (Fujimaki, Yamashita, Okazawa, & Arai, 1968; Kirimura, Shimizu, Kimizuka, Ninomiya, & Katsuya, 1969; Solms, Vuataz, & Egli, 1965). The taste imparted by peptides and amino acids continues to be widely researched (Cheung, Aluko, Cliff, & Li-Chan, 2015; Gong, Mohan, Gibson, & Udenigwe, 2015; Kim, Son, Kim, Misaka, & Rhyu, 2015; Kohl, Behrens, Dunkel, Hofmann, & Meyerhof, 2013). Peptides and peptidomimetics were also objects of in silico studies in the context of their bitter taste. Examples of such research are presented in reviews of Udenigwe (2014), Li-Chan (2015)

and Iwaniak, Minkiewicz, Darewicz, Protasiewicz, and Mogut (2015). Computer databases are among the most important tools for in silico analysis. They are repositories of various information about the structure, sequence, nomenclature, properties and function of molecules which play an important role in life sciences. The information collected in Internet databases is a valuable source of knowledge about chemical compounds, including those originating from foods (de la Iglesia et al., 2013; Martinez-Mayorga, Peppard, & Medina-Franco, 2014; Nongonierma & FitzGerald, 2016). Information about peptide properties (for some peptides including their taste, especially bitter) can be found in databases of low-molecular-weight compounds, including PubChem (Kim et al., 2016), ChEMBL (Bento et al., 2014) and BitterDB (Wiener, Shudler, Levit, & Niv, 2012), and in databases of peptides such as EROP-Moscow (Zamyatnin, Borchikov, Vladimirov, & Voronina, 2006).

The BIOPEP database developed by our team contains information about peptides and proteins, and it is addressed to food scientists. BIOPEP groups databases of: proteins, bioactive peptides (Minkiewicz, Dziuba, Iwaniak, Dziuba, & Darewicz, 2008), allergenic proteins and their epitopes (Dziuba, Minkiewicz, & Dąbek, 2013). The database of bioactive peptides is a popular tool in studies of peptides derived from foods. Our previous review cited research studies which relied on the BIOPEP database of bioactive peptides (Minkiewicz, Darewicz, et al., 2015). A database supports the annotation of various peptide properties.

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The aim of this study was to develop a database of peptides and amino acids with experimentally documented taste.

2. Methods

Information concerning the taste of peptides and amino acids was obtained from the literature. The query words in Scopus and Web of Science literature databases were “peptide” combined with taste (e.g. bitter or umami). Only peptides with experimentally detected taste were inserted into our database. Results of taste predictions performed in silico were not taken into account. The preferred information concerned the results of experiments based on taste perception by humans. Information about the biological activity of sensory peptides was obtained from other databases. The list of biological and chemical databases cited in BIOPEP and in this publication is presented in Table 1.

Peptide sequences were annotated in a one-letter code and with the use of chemical codes such as SMILES (Simplified Molecular-Input Line-Entry System) (Weininger, 1988), InChI (International Chemical Identifier) and InChIKey (Heller, McNaught, Pletnev, Stein, & Tchekhovskoi, 2015). Amino acid sequences of peptides were translated from a one-letter code written in the FASTA format (Pearson, 2000), using the Open Babel program, version 2.3.1 (O’Boyle et al., 2011). The resulting codes were verified and modified, if necessary, in the Ketcher molecule editor (Karulin & Kozhevnikov, 2011) available on the ChemSpider website (Williams & Tkachenko, 2014). Details concerning the verification and correction of peptide structures are presented in the Supplement.

The modified structures were used as queries for the searches in the ChemSpider database. This database contains direct links to most of the databases listed in Table 1. The searches in AHTPDB (Kumar et al., 2015), BIOPEP (Minkiewicz et al., 2008), EROP-Moscow (Zamyatnin et al., 2006) and PepBank (Duchrow et al., 2009) were performed based on amino acid sequences in a one-letter code. The BRENDA database (Chang et al., 2015) was screened using amino acid sequences in a three-letter code. The BitterBD (Wiener et al., 2012) database was used to find sensory peptides based on their structures encoded in

SMILES. Google™ was queried using InChIKeys according to the recommendations of Southan (2013) and Warr (2015).

The BIOPEP layout for annotating biopeptides (Minkiewicz et al., 2008) was also used to annotate sensory peptides/amino acids with modified graphics. The layout allows the annotation of peptides consisting of amino acids occurring in proteins. The information about sensory peptide sequences is linked with calculation options for evaluating proteins as a potential source of sensory peptides. The following quantitative parameters can be calculated when the program is combined with the database:

The frequency of sensory fragments in a protein sequence (A) (Dziuba, Iwaniak, & Minkiewicz, 2003):

$$A = a/N \quad (1)$$

a number of fragments with a given type of sensory activity in a protein sequence
N number of amino acid residues in a protein.

The frequency of release of fragments with a given type of activity by selected enzymes (A_E) (Minkiewicz, Dziuba, & Michalska, 2011):

$$A_E = d/N \quad (2)$$

d number of peptides with a given taste (e.g. bitter) released by a given enzyme (e.g. trypsin)
N number of amino acid residues in a protein.

The relative frequency of release of fragments with a given type of activity by selected enzymes (W) (Minkiewicz et al., 2011):

$$W = A_E/A \quad (3)$$

Table 1

List of bioinformatics and cheminformatics tools cited in the BIOPEP database of sensory peptides and amino acids as well as in this publication.

Name of database or program	Website*	Reference
ACToR	http://actor.epa.gov/actor/faces/ACToRHome.jsp	Judson et al. (2012)
AHTPDB	http://crdd.osdd.net/raghava/ahtpdb/	Kumar et al. (2015)
BindingDB	http://www.bindingdb.org/bind/index.jsp	Liu, Lin, Wen, Jorriksen, and Gilson (2007)
BioDBcore	http://biobdcore.org/	Gaudet et al. (2011)
BIOPEP database of bioactive peptides	http://www.uwm.edu.pl/biochemia/index.php/pl/biopep	Minkiewicz, Dziuba, Iwaniak, Dziuba, & Darewicz (2008)
BitterDB	http://bitterdb.agri.huji.ac.il/dbbitter.php	Wiener et al. (2012)
BRENDA	http://www.brenda-enzymes.org/	Chang et al. (2015)
ChEBI	http://www.ebi.ac.uk/chebi/	Hastings et al. (2016)
ChEMBL	https://www.ebi.ac.uk/chembl/	Bento et al. (2014)
ChemIDplus	http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp	Tomasulo (2002)
ChemSpider	http://www.chemspider.com/Default.aspx	Williams and Tkachenko (2014)
DrugBank	http://www.drugbank.ca/	Law et al. (2014)
EROP-Moscow	http://erop.inbi.ras.ru/	Zamyatnin et al. (2006)
FooDB	http://foodb.ca/	
HMDB	http://www.hmdb.ca/	Wishart et al. (2013)
KEGG	http://www.genome.jp/kegg/	Kanehisa, Sato, Kawashima, Furumichi, and Tanabe (2016)
MEROPS	http://merops.sanger.ac.uk/	Rawlings, Waller, Barrett, and Bateman (2014)
MetaComBio	http://www.uwm.edu.pl/metachemibio/index.php/about-metacombio	Minkiewicz, Iwaniak, et al. (2015)
OMICtools	http://omictools.com/	Henry, Bandrowski, Pepin, Gonzalez, and Desfeux (2014)
Open Babel	http://openbabel.org/wiki/Main_Page	O’Boyle et al. (2011)
PepBank	http://pepbank.mgh.harvard.edu/	Duchrow et al. (2009)
PubChem	https://pubchem.ncbi.nlm.nih.gov/	Kim et al. (2016)
SATPdb	http://crdd.osdd.net/raghava/satpdb/	Singh et al. (2016)
Scopus	http://www.scopus.com/	
Web of Science	http://thomsonreuters.com/en/products-services/scholarly-scientific-research/scholarly-search-and-discovery/web-of-science.html	
ZINC	http://zinc.docking.org/http://zinc15.docking.org/	Irwin, Sterling, Mysinger, Bolstad, & Coleman, 2012; Sterling & Irwin, 2015

* All websites were accessed within the period between March and December 2015.

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