

BITS :: Call for Abstracts 2024 - Oral communication

<i>Type</i>	Oral communication
<i>Session</i>	Bioinformatics AI, Models and Tools
<i>Title</i>	FEEDS and CICERON: a computational pipeline for prediction and functional classification of biopeptides
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<i>Motivation</i>	Biopeptides are short amino acid chains with biological activity and physiological effects relevant to human health that are generated from enzymatic fragmentation of proteins (proteolysis) (Zaky et al., 2022). During fermentation processes, fungal and bacterial species play a crucial role in substrate proteolysis. However, the diverse enzymatic capabilities of these species and the variability of the substrates can significantly impact the quality and yield of the biopeptides. At present, there are no existing tools that, starting from a list of microbial species and the protein sequences of the substrate, can predict the biopeptides generated from the fermentation of organic substrates and identify their function.
<i>Methods</i>	To address these challenges, we have developed FEEDS (Food wastE biopEptiDe claSsifier), an innovative biopeptide prediction tool (Borin et al., 2024). This tool can quickly identify the biopeptides produced based on the protease profiles identified in microbial genomes and the protein composition of the substrate undergoing proteolysis. In the second step, FEEDS utilizes the machine-learning approach implemented in CICERON to perform the functional classification of the biopeptides. CICERON (Classification of bioActive pEptides fRom micrObial fermeNtation) was generated by gathering bioactive peptide sequences and functions from various databases to generate a unified collection. This collection was organized into nine functional classes including immunomodulatory, opioid, and cardiovascular peptides. Upon assessing the sequence properties of biopeptides, four alternative encoding methods were tested in combination with many machine learning algorithms, from basic classifiers like logistic regression to advanced algorithms like BERT.
<i>Results</i>	Through in-silico testing conducted on more than 1000 microbial genomes and some selected protein substrates from <i>Hordeum vulgare</i> and <i>Vitis vinifera</i> , we have gained insights into the effectiveness of FEEDS in biopeptide prediction. These findings were compared with data from the literature and with original results obtained from mass spectrometry analysis of real samples, further validating the importance of our prediction. The pipeline can be used for an in-silico preliminary assessment of microbial species to be used for biopeptides generation and for selecting the best substrate. Regarding CICERON, tests performed on 171 models produced the best-tailored models for each functional class. Our tool outperforms state-of-the-art classifiers on a realistic benchmark dataset. Altogether, our work provides tools for real-world peptide classification and can serve as a benchmark for future model development.
<i>References:</i>	Bizzotto E, Zampieri G, Treu L, Filannino P, Di Cagno R, Campanaro S. Classification of bioactive peptides: a systematic benchmark of models and encodings. Computational and Structural Biotechnology Journal (Under review). Centurion VB, Bizzotto E, Tonini S, Filannino P, Di Cagno R, Zampieri G, Campanaro S. FEEDS, the Food wastE biopEptiDe claSsifier: From microbial genomes and substrates to biopeptides function (2024) Current Research in Biotechnology, 7, art. no. 100186 DOI: 10.1016/j.crbiot.2024.100186 Zaky AA, Simal-Gandara J, Eun J-B, Shim J-H, Abd El-Aty AM. Bioactivities, Applications, Safety, and Health Benefits of Bioactive Peptides From Food and ByProducts: A Review. Front Nutr 2022;8:815640. DOI: 10.3389/fnut.2021.815640
<i>Info</i>	-
<i>filename</i>	-
<i>Figure</i>	-
<i>Availability</i>	https://github.com/vborincenturion/feeds
Dissemination Material	

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Summary

Biopeptides are short amino acid chains with biological activity and physiological effects relevant to human health. We have developed a pipeline composed of two software (FEEDS and CICERON) to predict the bioactive peptides generated by the natural proteolysis of a mixture of proteins and to predict their potential bioactive role. These tools can be used to perform predictive analyses of the bioactive peptides obtained from microbial fermentation of natural byproducts.

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