Jan 30, 2022

Dear Editors,

We would like to submit a manuscript entitled “A taste peptide system TastePeptides-Meta including a di/tri-peptide umami/bitter binary classification model Umami\_YYDS, a taste peptide database TastePeptidesDB, and an open-source automatic machine learning package Auto\_Taste\_ML” to be considered for publication in *npj science of food*.

Umami provides amino acid/peptide for animal growth and represents one of the major attractive taste modalities, while bitterness represents a perception that is not conducive to eating. With the development of umami, amino acids, nucleotides, peptides, organic acids and their derivatives are considered to be the major types of umami substances. Thereinto, peptide molecules produced from hydrolysates of fish protein or other foods have become a new interest in the development of umami agent, and their biochemical and umami properties are both important for scientific research and the food industry. However, the identification of flavor peptides in traditional sense is a complex task due to the difficulties in the area of pretreatment, separation, purification, synthesis & characterization and the sensory evaluation of flavor substances. At the same time, the extent to which the umami mechanism of peptide remains incompletely understood because of its multivariate taste characterization (umami, sweet, sour, bitter, salty or kokumi). In terms of the analysis of taste regularity, previous studies have always been restricted by some factors, such as insufficient data size and simplistic models (Scoring Card Method, support vector machine and ridge regression). But, the accuracy and generalization performance of those models are not ideal. Therefore, it is necessary to build a QSAR model with excellent performance and model interpretability to deal with these problems.

With the improvement of computer performance and chemoinformatics, we compiled the information of the reported taste peptide and released it in the form of a database TastePeptidesDB (<http://tastepeptides-meta.com/database/son/1>). In addition, we use the data of umami and bitter peptide to construct an umami-bitterness judgment model Umami\_YYDS (<http://tastepeptides-meta.com/cal>) and encapsulated the modeling process into Auto\_Taste\_ML (<https://pypi.org/project/Auto-Taste-ML/>) as an Auto-Modeling Helper. This model will provide computational support for future high-throughput and fast screening of umami peptides, and can be used as a base learner of the future high-performance ensemble model to improve the screening performance. This is also essential for better understanding the umami mechanism of peptides and may open new possibilities for development of umami industry.

All the authors have reviewed the final version of the manuscript and approved it for publication. We declared that this manuscript has not been published in whole or in part nor is it being considered for publication in other Journals. We look forward to hearing from you when the review process is complete, and we will be pleased to provide any additional materials or information that you require.

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