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THE INVESTIGATION OF DETECTION AND SENSING MECHANISM OF SWEETNESS MOLECULES

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Polyelectrolyte assemblies are promising systems for creating electrochemical biosensors. There are fundamental scientific studies that suggest the use of sequentially adsorbed polyelectrolyte layers as a method of immobilization of biologically sensitive molecules on the substrate surface. We offer an electrochemical biosensor for detecting sweet molecules using a specific taste receptor TAS1R3. An electrochemical sensor developed using a simple functionalization protocol can then be used to detect other flavor molecules. In addition, we propose to use molecular docking modeling to understand how sweet molecules can interact with taste receptors [1]. The scientific novelty is in automating the process of determining sweetness without using the traditional method of organoleptic analysis, thereby in the future the formation of a database of sweet molecules will follow, as well as the resulting structures and transformations can become the basis for the development of new sweeteners with higher activity.

The sweet ligand interacting with the receptor and thus activating it is the main stage of sweet taste recognition. This interaction is important not only for understanding the structure and functions of sweet taste receptors, but also for the design or modification of various sweeteners and sweet taste regulators based on the structure. Thus, the objectives of the study are to determine sweetness by the QCM (Quartz crystal microbalance – microweights on a quartz crystal) method by creating successive layers of oppositely charged polyelectrolytes with the TAS1R3 receptor as a sensor for identifying molecules. As well as conducting molecular docking to identify beneficial sites for binding sugars (glucose, sucralose and erythritol) to the sweet taste receptor and complex polyelectrolyte(PEI)-TAS1R3.

The QCM method and the molecular modeling method – molecular docking were used in the work. The QCM method was used to measure low mass changes per unit area [2]. The molecular docking method was used to determine the binding sites in which the interaction energies of the protein and ligand are calculated [3].

The polymer matrix of the composition PEI/TAS1R3/PSS was studied. The protein is completely covered with negatively charged polyelectrolyte PSS, forming an oppositely charged layer at the interface. The matrix is not washable and is able to hold sweetness molecules.

It was shown that sweet molecules were added to the polyelectrolyte matrix PEI/TAS1R3/PSS. During the addition of each ligand, adsorption on the surface of the biosensor was observed. The adsorbed mass of the ligands was different, so the sucralose molecule remains more stable after washing. Moreover, molecular docking confirms the QCM experiment that sucralose with a binding energy of -7.1 kcal/mol binds more strongly to protein compared to glucose (-6.3 kcal/mol) and erythritol (-5.0 kcal/mol). Also, the interaction of the taste receptor with the sweet molecule is confirmed by the methods of impedance spectroscopy and HPLC-MS (High-performance liquid chromatography and tandem mass spectrometry).

The results of work will make it possible in the future to obtain the most effective biosensors capable of detecting various taste molecules that can serve as an electronic tongue.

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