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Insights into the Structural Determinants of Bitter Taste Receptors from a Combined *In silico* and *In vitro* Study

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Abstract

The ingestion of a large variety of toxic substances has evolutionary been prevented in humans and in other mammals by an unpleasant perception for bitter tasting food. Uncovering the molecular basis of bitter perception is hence crucial for food research. It is known that such perception is achieved by binding of bitter substances to their target membrane receptors located in oral taste bud cells. Here I will present the results of a recent study, aimed at the investigation of the binding and receptor activation of the most commonly studied human bitter receptor, hTAS2R38 by phenylthiocarbamide (PTC). Some predictions are initially formulated based on state-of-the-art structural bioinformatics calculations. These predictions are then validated against extensive molecular biology experiments. In this way, we have identified several receptor positions involved in direct ligand interactions and in receptor activation, providing insights into the bitter taste perception mechanism.