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Exploring the MSG related metabolic mechanisms through computational docking

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Monosodium Glutamate (MSG), also known as Ajinomoto is a widely used flavour enhancer in various food industries. Glutamate is the major component of the MSG which is produced within the human body. Also, it acts as an excitatory neurotransmitter within the central nervous system. Because of the characteristics of umami taste-producing capability, various foods contain MSG as a food additive. Normally in the market, it is known as E621 flavour enhancer. Among L and D enantiomers only L enantiomer has the flavour enhancing property because of the stimulation of the taste receptors. Even taste-enhancing properties, there are some health problems associated with the monosodium glutamate in the human. Triggering of obesity, diabetes, neurotoxicity (neurological disorders such as Alzheimer, Parkinson, Sclerosis), hepatotoxicity, oxidative kidney damage, headache, sweating, numbness, chest pain, and nausea are mainly associated with the consumption of higher amount of MSG containing foods. Various animal-based trials were performed already to find out the effect of MSG under different laboratory conditions. Computational docking was used to investigate the synergistic effect between monosodium glutamate (MSG) and the receptor proteins and metabolic enzymes. Before the docking step, the glutamate ligand was energetically optimised by using the Gaussian 09 software and the 3D structures of selected receptors and enzyme modeled via the SWISS-MODELER. Also, the proteins were refined by the Galaxy Refiner. The results showed specific changes upon the interaction of MSG with xenobiotic-metabolizing enzymes (CYP2E1), xenobiotic sensing receptor (CAR), GLP-1 receptor, mGlu5 receptor in terms of energy and conformation. The mGlu5 receptor exhibited the most favourable binding interactions with MSG due to the presence of both polar and non-polar amino acids in the binding pocket of receptor. Ser152 tends to form strong hydrogen bonds with the glutamate ligand. Five residues in the binding pocket Ser173, Gly150, Ala174, Tyr223 and Trp100 played critical roles in forming hydrophobic interactions. Also, Gln234, Lys197 and Arg310 was observed as H bond forming amino acids with the glutamate ligand in the GLP-1 receptor. As well as CYP2E1 showed a considerable binding affinity for the glutamate ligand in MSG. The receptor proteins and enzymes, which consisted of non-polar functional groups, demonstrated the lowest docking energy and docking interaction energies. This computational study provides an insight into discovering umami-enhancing compounds and how they may interfere/ interrupt natural metabolisms.

Keywords: CYP2E1, CAR, Docking, Numbness, Umami.