The origin of unpleasant aftertastes in synthetic sweeteners

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SUPPLEMENTARY MATERIAL

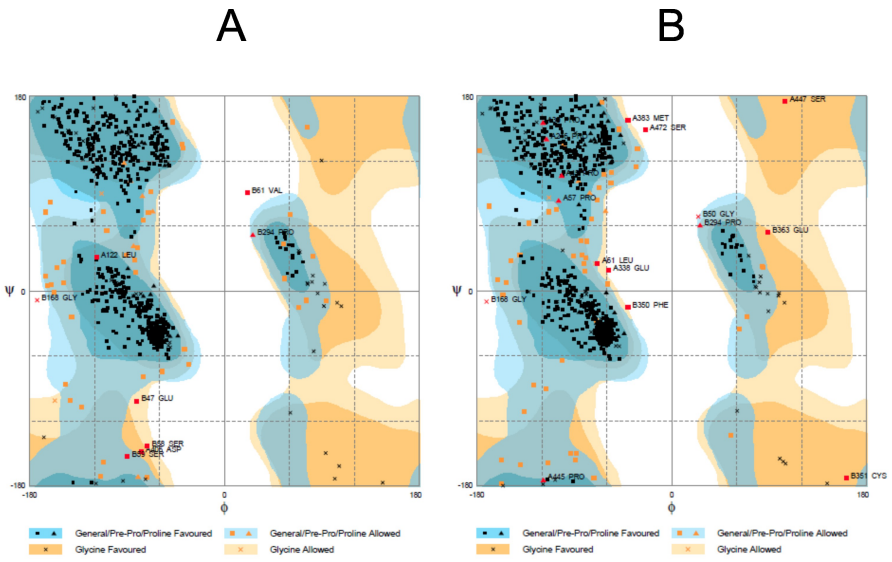

Figure S1. Ramachandran maps of the homology models for the sweet (A) and umami (B) receptors. Ramachandran plots indicate that 92.0% of the residues are in favoured regions, 6.2% in allowed regions and 1.9% in outlier regions for umami receptor; whereas 93.1% of the residues are in favoured regions, 5.9% in allowed regions, and 1.0% in outlier regions for sweet receptor. PROCHECK analyses of the umami and sweet models yielded overall average G factors of -0.37 and -0.32, respectively, which suggest that the conformations both, of main and side chain of the models, are reasonable. The value of QMEAN score for the umami and sweet receptor were -3.35 and -1.82, respectively, pointing that the resulting models were close enough to a set of experimental protein structures from the PDB database.

Table S1. Interaction Energies and Potential Binding Sites for T1R3 protomers of Sweet and Umami Taste Receptors.

ligand	**HT1R3 (sweet)**		**HT1R3 (umami)**	
	$\Delta G_{binding}$/ kcal $mole^{-1}$	lining residues	$\Delta G_{binding}$/ kcal $mole^{-1}$	lining residues
saccharin	-5.8	H145, S146, G168, Y218, S276, V277, A302	-5.8	H145, S146, G168, Y218, S276, V277, A302
acesulfame	-5	H145, S146, Y218, S276, V277, A302	-5	H145, S146, Y218, S276, V277, A302
2_Benzoylbenzoic acid	-6.7	P42, E45, W72, H145, G168, Y218, S276, V277, A302	-6.7	P42, E45, S66, W72, H145, S146, G168, Y218, S276, V277, A302
2-(4-methylbenzoyl) benzoic acid	-6.9	S66, W72, H145, S146, S147, G168, Y218, S276, V277, A302	-6.8	E45, S66, W72, H145, S146, S147, G168, Y218, S276, V277, A302
2-(4-methoxybenzoyl) benzoic acid	-6.8	P42, E45, S66, W72, H145, S146, S147, G168, Y218, S276, V277, A302	-6.7	P42, E45, S66, W72, H145, S146, S147, G168, Y218, S276, V277, A302