Identifying the interactions between natural, non-caloric sweeteners and the human sweet receptor by molecular docking

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Abstract

Natural sweeteners, such as stevia and thaumatin, exert their sweet taste by specifically binding to sweet taste receptors. However, the molecular basis of their sweetening power remains to be ascertained. In the present study, we built a comparative model of the hT1R2 and hT1R3 subunits in order to characterize their interactions with natural, non-caloric sweeteners – from glycosylated terpenoids to sweet proteins – at the molecular level. The binding free energy between hT1R2-hT1R3 and sweeteners of different families shows a strong correlation with their sweetness intensity for both, small sweeteners (r = −0.89) and sweet proteins (r = −0.97). The correlation is further improved and generalized throughout all families of sweeteners evaluated, when EC50 values are used instead of relative intensities (r = −0.91). Altogether, these results contribute to a better understanding of the sweetness perception of these sweeteners, and promote the use of docking for better prediction of resulting sweetness.

Keyword

Small sweeteners||Sweet protein||Sweet taste receptor||Sweetness intensity||EC50||Molecular docking