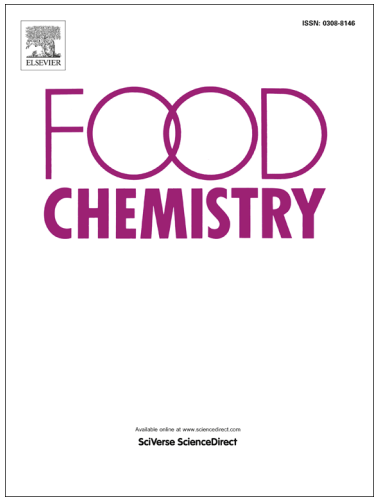

In-silico prediction of sweetness using structure-activity relationship models

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PII: S0308-8146(18)30126-2
DOI: https://doi.org/10.1016/j.foodchem.2018.01.111
Reference: FOCH 22300

To appear in: *Food Chemistry*

Received Date: 13 September 2017
Revised Date: 15 December 2017
Accepted Date: 15 January 2018

Please cite this article as: Goel, A., Gajula, K., Gupta, R., Rai, B., *In-silico* prediction of sweetness using structure-activity relationship models, *Food Chemistry* (2018), doi: https://doi.org/10.1016/j.foodchem.2018.01.111

In-silico prediction of sweetness using structure-activity relationship models

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Abstract

Quantitative structure activity relationship (QSAR) models appear to be an ideal tool for quick screening of promising candidates from a vast library of molecules, which can then be further designed, synthesized and tested using a combination of rigorous first principle simulations, such as molecular docking, molecular dynamics simulation and experiments. In this study, QSAR models have been built with an extensive dataset of 487 compounds to predict the sweetness potency relative to sucrose (ranging 0.2 to 220000). The whole dataset was randomly split into training and test sets in a 70:30 ratio. The models were developed using Genetic Function Approximation (R_{test}^2 = 0.832) and Artificial Neural Network (R_{test}^2 = 0.831). Our models thus offer a convenient route for fast screening of molecules prior to synthesis and testing. Additionally, this study can supplement a molecular modelling approach to improve binding of molecules with sweet taste receptors, leading to design of novel sweeteners.

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