# Decoding sweet taste from chemical structures

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Our brain perceives sweet taste through the activation of a broadly tuned receptor expressed at the surface of taste buds. No experimental structure of the sweet taste receptor is available and ligand-based approaches are relevant to mine the large chemical space and to establish structure-taste relationships. [1,2]

We will present the first online tool able to predict sweet taste perception based on a machine learning protocol. We have updated and curated the previous database of 316 sweet compounds and added new applicability domain metrics to assess the robustness of the predictions. A novel scaffold of natural sweetener that has never been annotated as sweet has been identified by the present approach and was experimentally validated.

Bibliography :

[1] Chéron J.B. et al. Food Chem., 2017, 221, 1421-1425.
[2] Chéron J.B. et al. Encyclopedia of Food Chemistry, 2019, 1, 189-195.