Explaining taste association of odorants by multivariate statistical analysis

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Explaining taste association of odorants by multivariate statistical analysis and odour-taste network

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Introduction

Odour taste association relies on a cognitive process based on previous experience and associative memory [1]. This association between odour and taste has been successfully applied to enhance taste perception in foods with low sugar [2] or low salt [3] content. However, the selection of odour-active molecules able to enhance taste perception remains a crucial step.

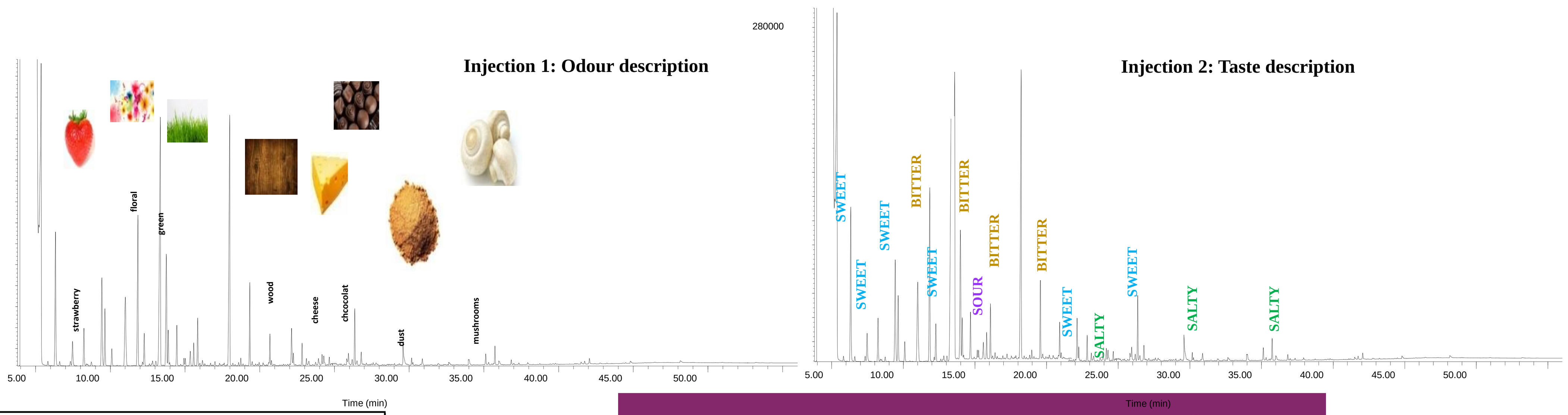
Objective

Search for links between the taste association and the different odorant descriptors given to the different molecules using computational and multivariate analysis.

Experimental procedure and results

GC/O-AT

Sample: dichloromethane extract (3x15mL) of 120 mL commercial multi-fruit juice after SAFE distillation under vacuum (1 Pa) concentrated to 200µL.
GC/O-AT: Agilent HP 6890A, DB-Wax (30m x 0.32mm i.d., 0.5µm), 35°C (5mn), 5°C/min, 240°C.
12 panellists experienced in GC/O.
Injection 1: indicate odour detection using a buzzer and attribute an odour descriptor
Injection 2: indicate odour detection using a buzzer and attribute (mandatory) one of the four taste descriptors: sweet, salty, sour, bitter.

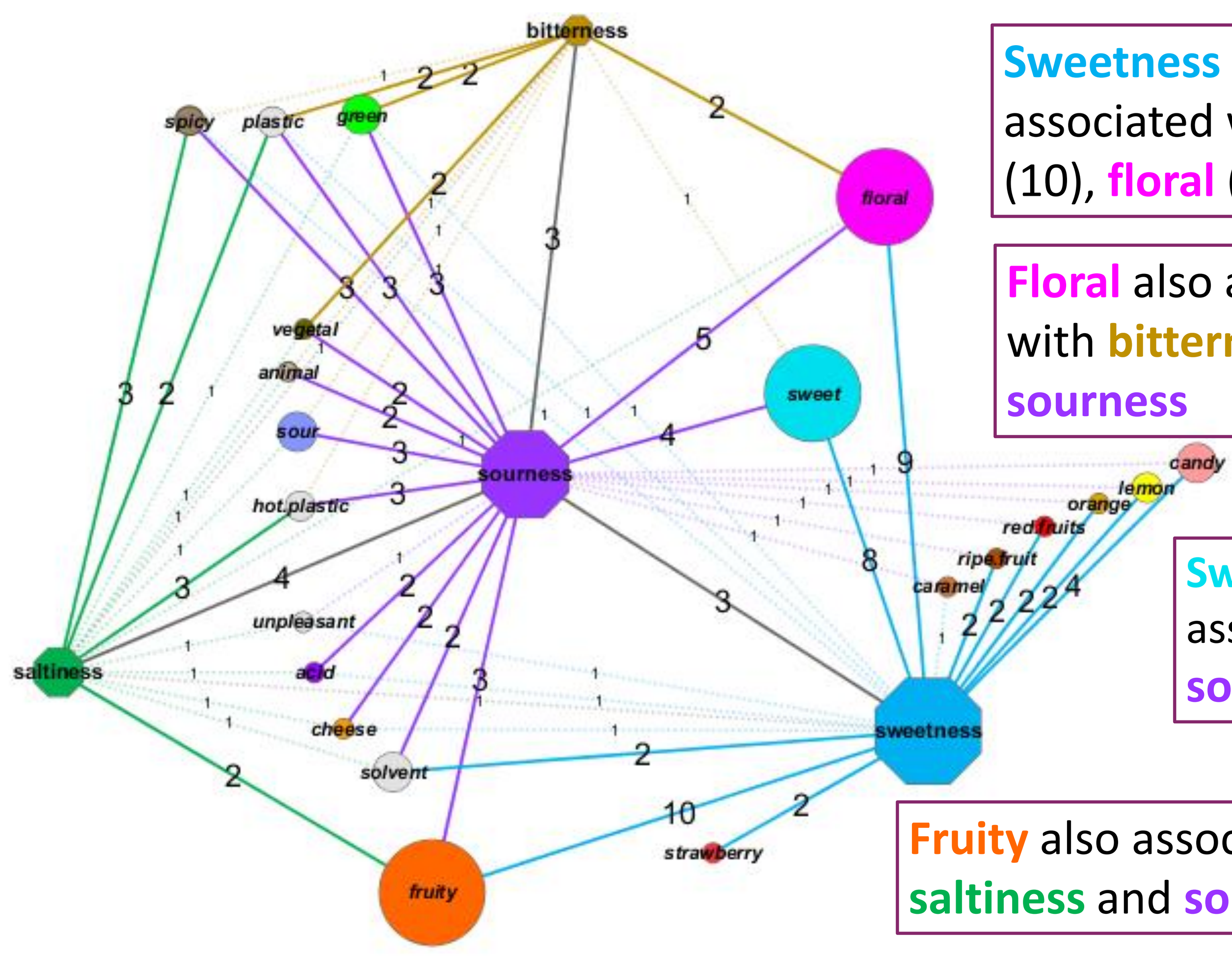


	GC/O: Gas chromatography/olfactometry	GC:O-AT: associated taste			
Compound	Odour attributes	sweetness (%)	sourness (%)	saltiness (%)	bitterness (%)
methyl 2-methylbutanoate (M2MB)	fruity, banane, sweet, bonbon, acid, floral,	58	17	0	0
ethyl butanoate (EB)	fruity, orange, floral, sweet, cheese, red fruits, ripe fruits, transpiration	50	17	0	8
ethyl 2-methylbutanoate (E2MB)	fruity, apple, strawberry, bonbon, sweet, lemon, fusil	58	8	0	8
(E)-β-ocimene	fruity, strawberry, floral, lemon, ripe fruit, solvent	75	0	0	0
linalool	floral, pleasant, fruity, sweet, pineapple, apricot, cake, bonbon, butter	67	8	0	0
β-damascenone	fruity, sweet, peach, floral, old fruit, cherry, red fruits	50	0	0	0
phenylmethanol	sweet, candy, floral, fruity, fresh, green, orange	42	0	0	0
2-phenylethanol	fruity, floral, rose, mushroom	58	0	8	0
(E)-β-ionone	spicy, cinnamon, roasted, solvent, floral, smoky, plastic, leather, fruity	42	17	33	0
furaneol	caramel, cotton candy, sweet, sugar, jam	42	0	0	0
γ-decalactone	floral, menthol, fruity, unpleasant, sweet, citrus	42	8	0	8
isobutyl alcohol	spicy, vegetal, wood, plastic, glue, hot plastic, burnt	0	17	17	50
allo-ocimene	green, metallic, aldehyde, floral, animal, plastic, bitter, sour, vegetal	0	25	8	50
furfural	toasted, fruity, potatoe, mash potatoes, exotic fruit intense, sulfur	0	0	58	8
butyl acetate	lemon, solvent, alcohol, vinegar, sweet, caramel	8	42	8	8
β-myrcene	herb, green, sour, floral, sweet	0	42	0	25
propyl octanoate	green, land, paper, hot plastic	8	42	25	0
pentanoic acid	acid, sharp, cheese, animal, unpleasant, vomit, spice, hot warm	0	42	25	0

A total of 18 molecules from a multifruit juice extract have been described with odour descriptors by classical GC/O and then with taste associated descriptions (sweetness, sourness, saltiness, bitterness) by GC/O-AT, with their detection frequencies (DF%) [2]. Eleven molecules were associated to sweetness perception (DF>10%). Most of them are also described with "sweet" odour descriptors but not all and 2 molecules (butyl acetate and β-myrcene) described with a "sweet" odour are not associated with sweetness.

Computational analysis

A co-occurrence matrix of the different odour descriptors and taste association percentages was realised and a computational analysis [4] allowed to build a network representing the relationships between odours and tastes.



Sweetness mainly associated with fruity (10), floral (9), sweet (8)

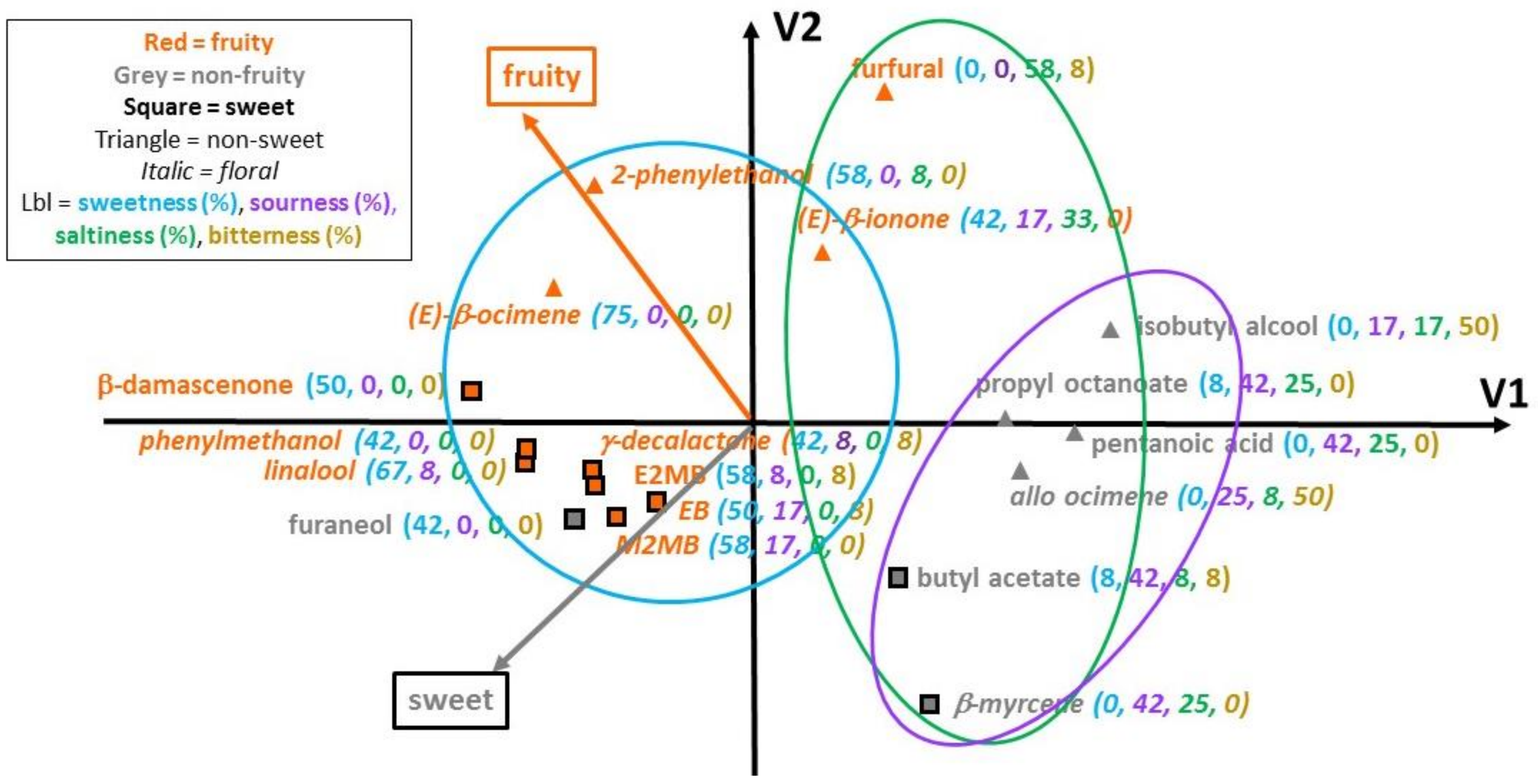
Floral also associated with bitterness and sourness

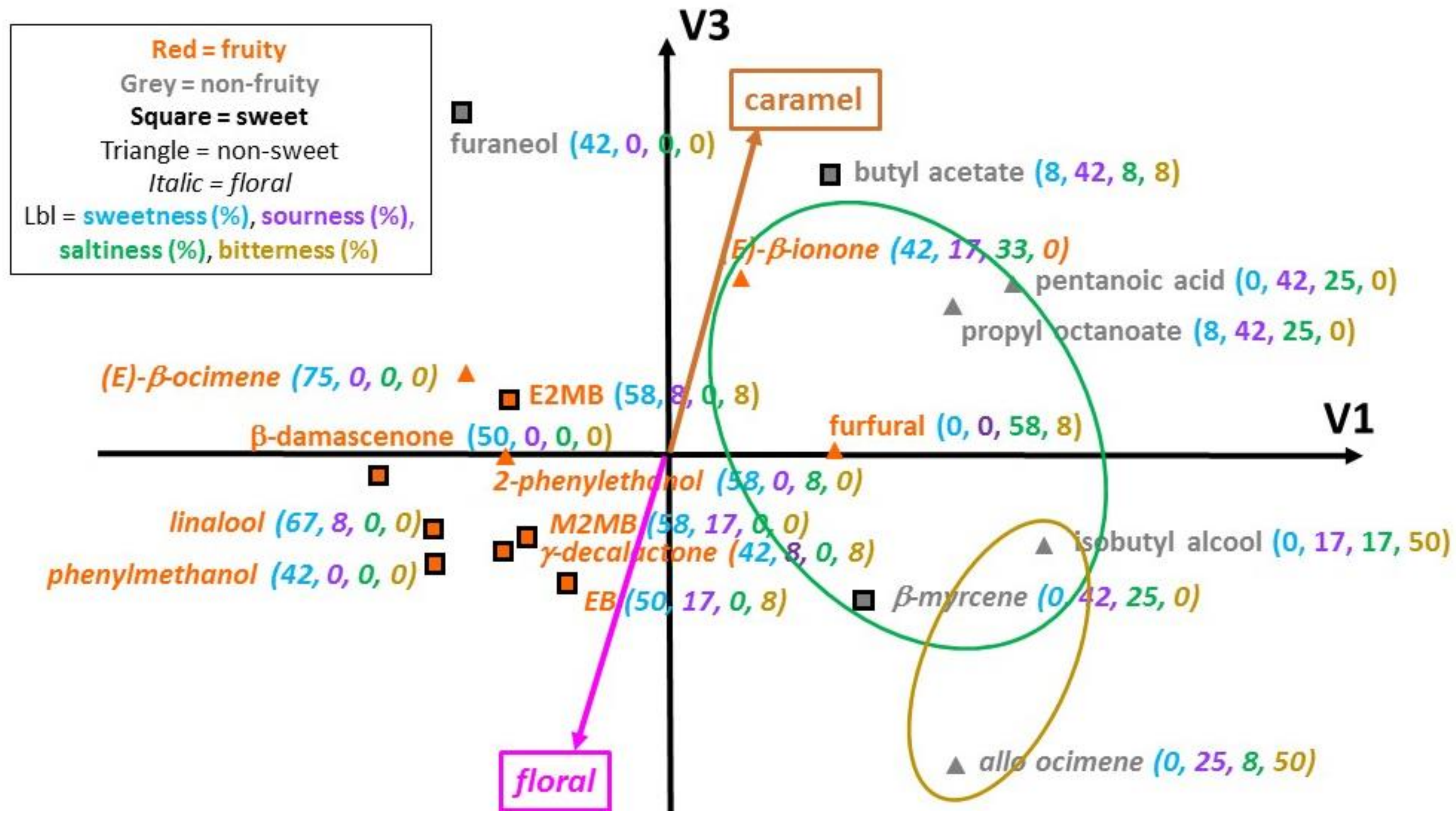
Sweet also associated with sourness

Fruity also associated with saltiness and sourness

Multivariate analysis

As previously developed for odours and odorants [5], a binary matrix was created with the 18 molecules and the binary values for the 21 odours with more than one occurrence and the 4 associated tastes (1: present; 0: absent). We used the Euclidian distance calculated using the Jaccard coefficient to obtain a similarity matrix between odorants and applied a multidimensional scaling (MDS) approach [6].





We used the coordinates of the first three dimensions of MDS to display the odorants in the odour-taste space: the projections on the planes V1V2 and V1V3 showed that V1 separated molecules according mainly to fruity odour/sweetness (negative part) and saltiness/sourness (positive part), V2 according to sweet odour (negative part) and V3 according to floral odour/bitterness (negative part) and caramel odour (positive part).

Among the 11 molecules with the highest DF for sweetness (>42%), located on the negative part of V1, 7 have fruity and **sweet** odours (linalool, methyl-2-methylbutanoate, ethyl-2-methylbutanoate, ethylbutanoate, β-damascenone, phenylmethanol, γ-decalactone) and are close to each other (negative part of V1), 2-phenylethanol, (E)-β-ionone and (E)-β-ocimene are fruity and floral (positive part of V2), furaneol is sweet and caramel (positive part of V3). Molecules associated with saltiness are mainly located on the positive part of V1 and positive part of V3, they have plastic/ spicy odours; those associated with sourness, on the positive part of V1, have sour/green odours and those associated to bitterness, on the negative part of V3, have plastic/green odours.

Conclusion

Our approach provided a visualisation tool for a better understanding of the relationships between odour descriptors and associated taste description and could be used to predict a potential application of odour-active molecules that enhance taste perception.

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