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

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Introduction

Objective

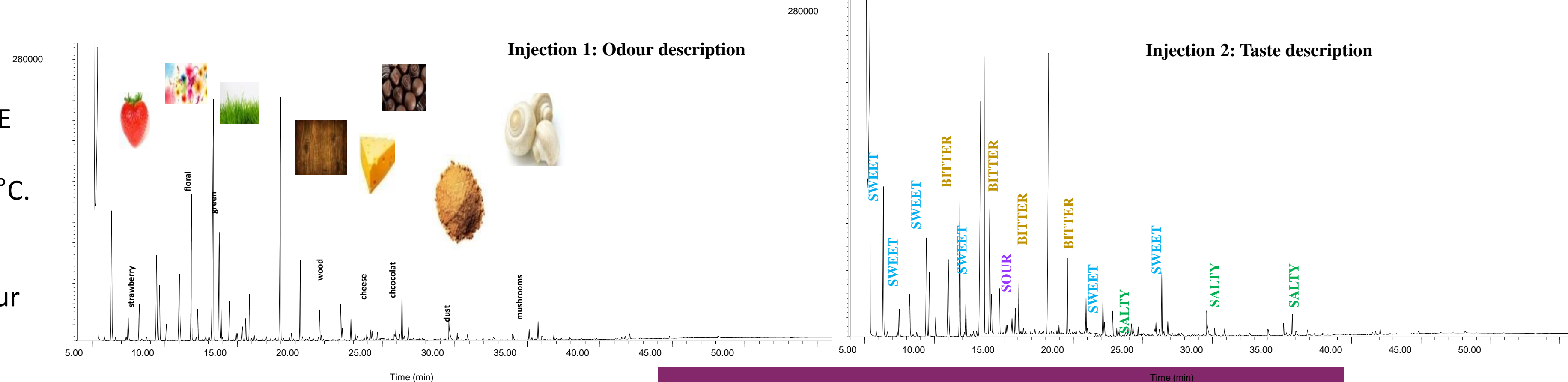
Odour taste association relies on a cognitive process based on previous experience and associative memory [1]. This association between odour and taste has been successfully applied to enhance taste perception in foods with low sugar [2] or low salt [3] content. However, the selection of odour-active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

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

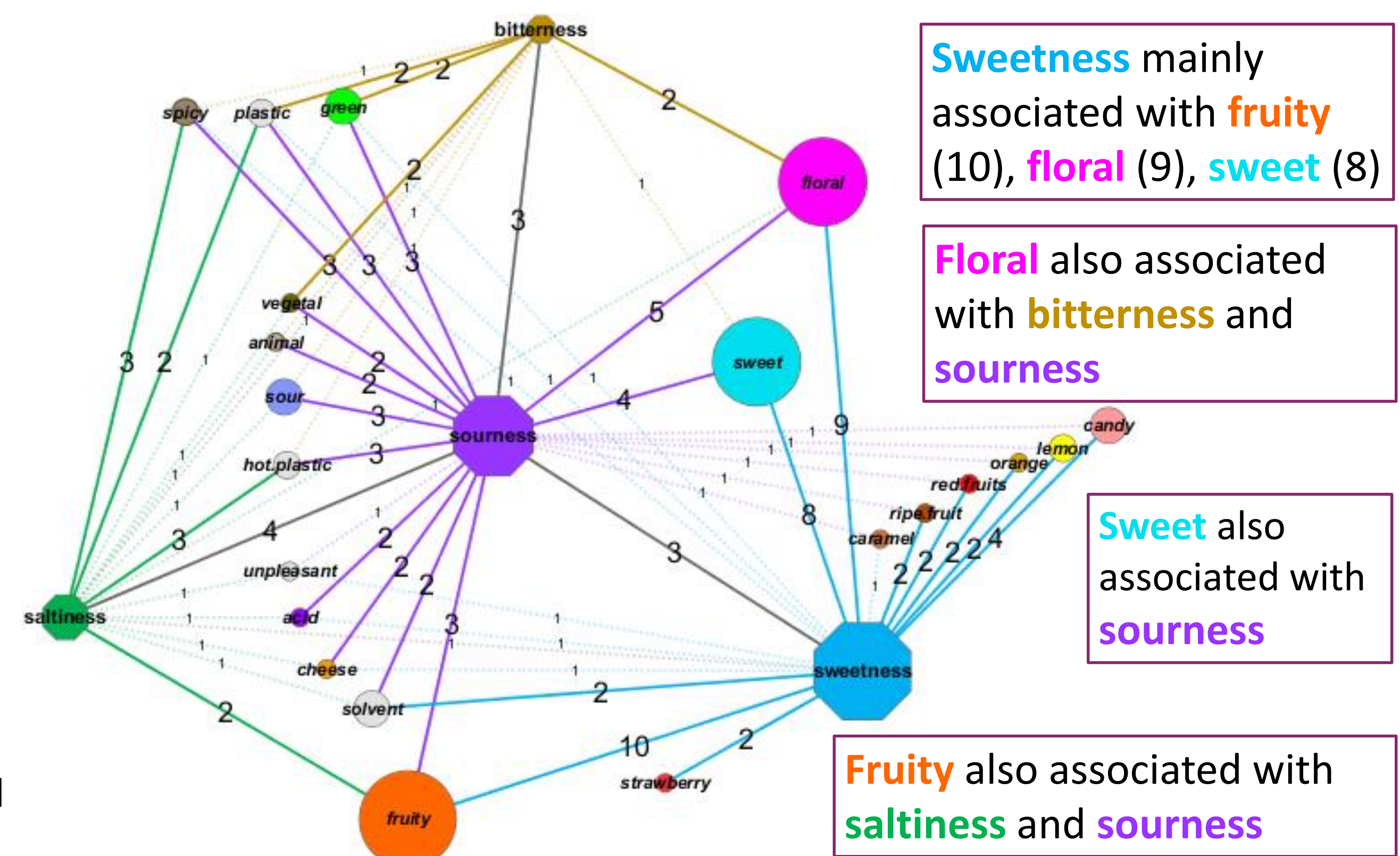
GC/O-AT

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.



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.

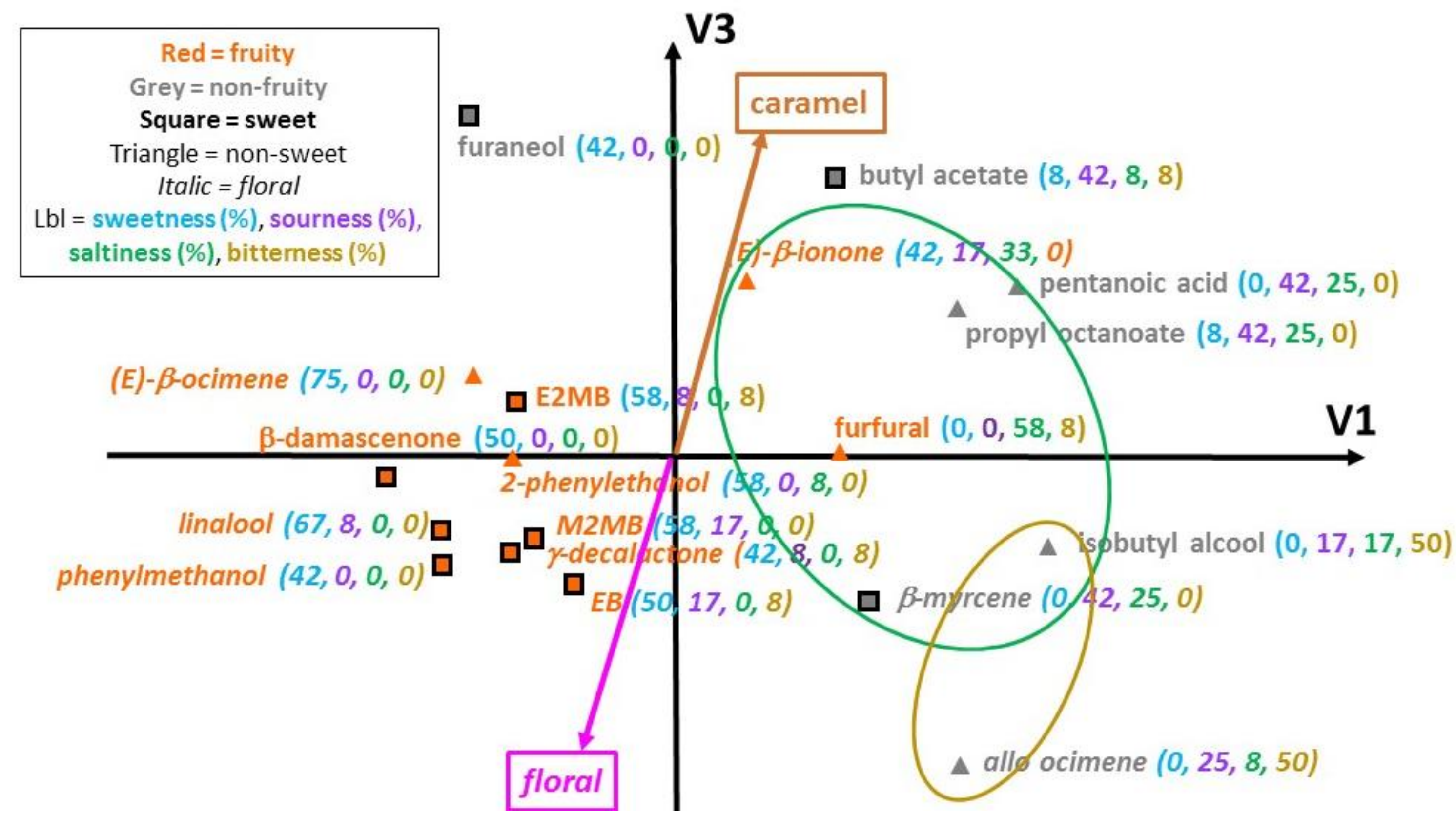
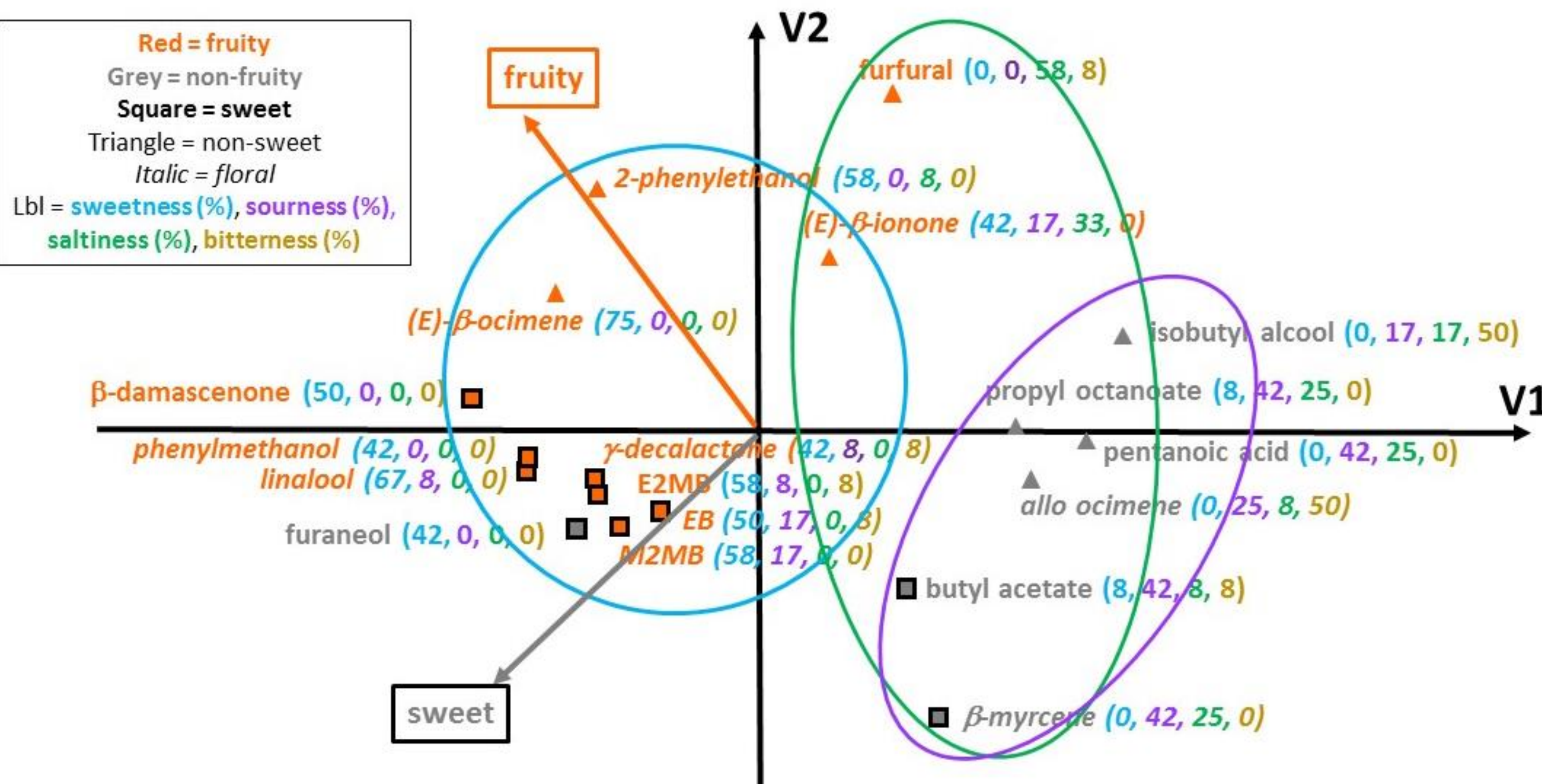


Compound	GC/O: Gas chromatography/olfactometry	GC/O-AT: associated taste			
	Odour attributes	sweetness (%)	sourness (%)	saltiness (%)	bitterness (%)
methyl 2-methylbutanoate (M2MB)	fruity, banane, sweet, bonbon, acid, floral,	58	17	0	0
ethyl butanoate (EB)	fruity, orange, floral, sweet, cheese, red 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.

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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