

Supplementary Material

Table S1. Amounts of esters, alcohols, terpenes (equivalent $\mu\text{g/L}$) and their odour and threshold values. The numbers in the column “code” are those used as symbol of the molecules in the PCA (Figures 3 and 4). In a row, values with different letters are significantly different (one-way ANOVA and LSD test, $P < 0.05$).

Volatile aromatic compounds	Code	Odour	Aroma Threshold (mg/L)	Sc7	Sc22	Sc34	Sc41	Sc48	Sc65	Sc70
ESTERS										
Ethyl propanoate	1	Pineapple	2.1	109.35 B,C	85.86 B	130.89 C	0.00 A	0.00 A	79.89 B	123.63 C
Ethyl isobutyrate	2	sweet, fruity, ethereal	0.6	50.87 B	164.04 E	87.04 C	0.00 A	0.00 A	40.97 B	120.28 D
Ethyl butanoate	3	Floral, fruity	0.6	0.09 A	1.00 A,B	0.05 A	10.53 D	0.00 A	3.32 B,C	4.62 C
Propyl acetate	4	Pears	0.2	42.79C, D	38.34A,B,C	28.52 A,B	25.81 A	42.38B,C,D	52.82 D	30.11A,B,C
Isobutyl acetate	6	Banana, fruity	1.9	90.30 B	64.89 A	98.31 B	125.88 C	61.25 A	124.37 C	90.87 B
Ethyl butyrate	7	Floral, fruity	0.02	82.85A ,B,C	69.91 A,B	68.16 A	97.95 C	59.01 A	100.71 C	94.31 B,C
Ethyl 2-methylbutyrate	8	Fruity, apple peal	5.6	1.06 B,C	0.07 A	0.62 B	1.40 C	0.70 B	1.92 D	2.16 D
Ethyl isovalerate	9	Fruity-buttery	3.9	0.66 B	0.60 A,B	0.43 A,B	1.04 C,D	0.25 A	0.73 B,C	1.22 D
Butyl acetate	10	Fruity	1.8	1.19A, B,C,D	0.96 A,B,C	1.49 C,D	1.74 D	0.62 A	1.28 B,C,D	0.89 A,B
Isoamyl acetate	11	Banana, pear	0.03 ^a	437.33 A,B	358.98 A	497.94 B	609.96 C	355.97 A	458.12 A,B	334.18 A
Ethyl valerate	12	Pleasant odour	-	0.92 A,B	0.69 A	0.63 A	1.15 B	0.53 A	1.13 B	0.93 A,B
Methyl hexanoate	13	Pineapple	0-3	1.39 A	1.09 A	1.50 A,B	2.06 C	1.38 A	1.99 B,C	1.07 A
Ethyl hexanoate	14	Fruity	0.05 ^a	126.39 A,B	69.88 A	308.79 E	188.47 C,D	91.22 A,B	140.69 B,C	247.15 D,E
Isoamyl butyrate	15	Fruity (pear-like)	0.02 ^a	3.44 B,C	2.08 A,B	1.48 A	4.26 C,D	1.08 A	1.93 A,B	5.01 D

Hexyl acetate	16	Mild sweet odour	0.7	6.40 A	5.33 A	8.17 B	9.63 C	5.44 A	8.86 B,C	9.20 B,C
Ethyl heptanoate	17	Grape like	0.6	0.72 B	0.44 A	0.26 A	1.01 C,D	0.98 C,D	1.12 D	0.83 B,C
Ethyl trans-2-hexenoate	18	Fruity	0.4	1.24 C	0.83 A,B	1.03 B,C	1.69 D	0.58 A	1.19 C	0.74 A,B
Ethyl octanoate	21	Fruity -	0.02 ^a	150.02 A,B	98.30 A	521.30 D	211.86 B	251.46 C	162.88 A,B	215.60 B
Isoamyl hexanoate	22	Fruity	-	2.66 B,C	2.39 B	1.69 A,B	3.48 C	1.93 A,B	1.00 A	2.42 B
Ethyl decanoate	26	Floral, soap	0.2	0.57 B	0.03 A	1.04 C	0.13 A	0.17 A	1.18 C	0.79 B
Isoamyl octanoate	27	Banana, pear	-	1.62 A,B	1.67 A,B	2.00 B	2.12 B	1.09 A	1.99 B	2.12 B
Ethyl phenylacetate	29	Floral, fruity, rose	0.25	3.97 B	4.27 B	5.92 C	5.84 C	2.25 A	4.22 B	7.81 D
3-Phenylethyl acetate	30	Floral, fruity, rose	0.25	15.18 A	50.91 B,C	91.31 D	24.87 A	64.09 C	88.76 D	43.25 B
Ethyl 2-hydroxyhexanoate	36	Fruity	1.8	1.15 B	0.00 A	0.01 A	1.57 B	0.00 A	1.42 B	1.80 B
Ethyl 3-hydroxyhexanoate	37	Fruity	1.1	1.32 B	0.00 A	0.01 A	1.84 B	0.40 A	1.60 B	0.77 B
Methyl 4-hydroxybutyrate	38	Fruity	1.2	2.27 B,C	0.00 A	1.52 B	3.06 C	2.19 B	3.31 C	3.34 C
Ethyl 4-hydroxybutyrate	39	Fruity	1.2	1.15 B	0.00 A	0.68 A,B	1.80 B	0.00 A	0.00 A	1.25 B
Ethyl 6-hydroxyhexanoate	40	Fruity	1.8	1.98 C	0.86 B	1.96 C	2.95 C	0.19 A	0.53 A,B	2.10 C

ALCOHOLS

1-propanol	43	Pungent, astringent	500	229.87 A	180.02 A	197.83 A	341.22 B	341.45 B	167.00 A	217.61 A
1-Butanol	44	Alcoholic	150 ^a	312.47 C	208.22 B	276.08 B,C	423.42 D	120.20 A	108.46 A	304.25 C

3-Methyl-2-butanol	45	Alcoholic	30 ^a	586.56 C,D	478.88 B,C	353.99 A,B	702.76 D	526.19 C	294.37 A	502.02 C
1-Pentanol	46	alcoholic	80	1.20 C	1.51 D	0.90 B	1.69 D,E	0.89 B	0.24 A	1.97 E
4-Methyl-1-pentanol	47	alcoholic	50	0.80 A,B	0.64 A	1.02 B,C	1.15 C	1.13 C	0.71 A	1.42 D
2-Heptanol	48	alcoholic	0.07	0.78 C	0.46 A,B	0.89 C	1.11 D	0.51 B	0.29 A	1.21 D
1-Hexanol	49	Herbaceous	4	128.35 C	63.69 A	108.03 B,C	174.85 D	51.50 A	96.30 B,C	79.33 A,B
cis-3-Hexen-1-ol	50	Herbaceous	0.4	122.01 B,C	72.18 A	95.05 A,B	145.87 C	87.91 A	133.10 C	85.59 A
1-Octen-3-ol	53	pungent	0.020	0.26 A	0.22 A	0.30 A	0.57 A	0.10 A	0.17 A	0.23 A
1-Heptanol	54	alcoholic	1.0	0.25 A	0.14 A	0.28 A	0.38 A	0.30 A	0.20 A	0.14 A
Benzyl alcohol	56	Floral rose	-	108.08 A,B	90.99 A,B	132.09 B	133.77 B	71.34 A	117.81 A,B	91.43 A,B
2-Phenylethanol	57	Rose	0.75	334.47 C,D	291.64 A,B,C	394.97 D,E	447.81	211.42 A,B	204.49 A	306.29B,C, D
TERPENES										
Linalool	59	Rose	0.025	8.26 B	8.20 B	9.26 B,C	11.24 C	5.55 A	14.56 D	9.88 B,C
α -Terpineol	60	Lilac type note	0.4	7.92 A	9.06 A,B	9.85 B	11.82 C	11.79 C	8.42 A,B	12.26 C
β -Citronellol	61	Citronella	100 ^a	4.51 B	5.93 C	7.85 D	6.30 C	4.56 B	3.07 A	6.15 C
Geraniol	62	Rose	0.4	3.59 A,B	4.21 B	5.72 C	5.84 C	4.03 B	2.64 A	7.21 D
β -damascenone	63	Rose like scent	0.004	12.33 B	0.93 A	13.31 B	17.26 C	0.74 A	0.00 A	11.08 B