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[1] Julius Kühn-Institute (JKI), Federal Research Centre for Cultivated Plants, Institute for Ecological Chemistry, Plant Analysis and Stored Product Protection, Quedlinburg, Germany
[2] Hansabred GmbH & Co. KG, Dresden, Germany
[3] Humboldt-Universität zu Berlin, Albrecht Daniel Thaer-Institute of Agricultural and Horticultural Sciences, Department of Horticultural Plant Systems, Berlin, Germany

A search for the ideal flavor of strawberry – Comparison of consumer acceptance and metabolite patterns in *Fragaria* × *ananassa* Duch.

Detlef Ulrich[1,*], Klaus Olbricht[2,3]

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Summary

Until today, there is no valid definition of the ideal flavor pattern in strawberry. Despite numerous investigations of the metabolic composition of strawberries, the description of the relationship between flavor pattern and consumer acceptance is inconsistent.

The aim of the present study was to correlate overall liking (acceptance), the intensity of important sensory parameters, which were evaluated by a consumer panel, and data of instrumental analyses like soluble solids content, titratable acidity and volatile organic compound patterning. The data were collected over a period of three harvest years. They are suitable to reveal the relationships and interactions between the metabolite patterns of strawberry and the sensory properties due to the use of a high diversity of the gene pool and due to a special sample preparation with representative sample sizes for both human sensory and instrumental analysis. A high genetic diversity was considered including genotypes from cultivar crossing and from wild species introgression. It was found that the volatile compounds methyl 2-methylbutanoate, (*Z*)-3-hexenyl acetate, linalool and decanoic acid correlate positively with the attribute 'sweet' and, therefore, can act as sweetness enhancers. Furthermore, compounds were identified with positive (linalool, lactones) and negative impact (some esters, furanones) on the sensory quality. From these findings, strategies towards improved, sensorially valuable strawberry cultivars with a high consumer acceptance can be deduced.

Abbreviations

immSBSE, immersion stirbar sorptive extraction; HS-SPME, headspace solid phase microextraction; qMS, quadrupol mass spectrometry; PCA, principal component analysis; PDMS, polydimethylsiloxane; SSC, soluble solids content; TA, titratable acid; TIC, total ion chromatogram; VOCs, volatile organic compounds

Introduction

Strawberry is the most important berry fruit worldwide. The genus *Fragaria* comprises about 25 species, whereas the majorities of fruit consumed today belong to the so-called garden or cultivated strawberry (*F.* × *ananassa* Duch.) which is a hybrid of the two American species *F. chiloensis* (L.) Miller and *F. virginiana* Miller. In the past, wild species or selected and cultivated wild-types of *F. vesca* L., *F. moschata* Weston, *F. viridis* Weston and *F. virginiana* were traded and consumed in significant quantities, too. However, after the 1750's these types were replaced by cultivars of the garden strawberry with its bigger fruits and a pleasant flavor. Then as now, strawberries were purchased by consumers because of their unique flavor. This is in agreement with studies of food psychologists who pointed out that flavor is the essential quality attribute of food for the decision to consume (Ellrott, 2012; Pudel, 2003). In the context of consumers' choice, characteristics like fruit size, color and vitamin content rank behind flavor (Bhat et al., 2015).

Nevertheless, for decades consumers complain about fruit with poor flavor especially those which are offered from supermarkets. Already Alston (1992) pointed out that "most of the flavors appreciated today in plant products were recognized many years ago and are often best represented in old varieties unsuited to large scale commercial production". Modern high-yield cultivars are lacking of pleasant flavor attributes. Ulrich et al. (1997) published a comparative study of aroma profiles of old and new strawberry cultivars and wild species. This study demonstrated losses of volatile organic compounds (VOCs) caused by domestication and breeding which is known as the so-called domestication effect, funnel effect or genetic bottleneck. These findings on the metabolite level were confirmed by subsequent studies on strawberry (Aharoni et al., 2004) and for other cultivated species like tomato (Goff and Klee, 2006). In parallel, a loss of allele diversity on the genomic level was pointed out for strawberry by Gil-Ariza et al. (2009) and Horvath et al. (2011). Therefore, flavor improvement has become a main target in breeding of new consumer-preferred cultivars (Ulrich and Olbricht, 2011).

In contrast to other important traits like sugar content, yield and resistance, which are more or less easy to quantify, flavor results from the complex interaction of hundreds of chemicals that originate from a plenty of biosynthetic pathways. Flavor is regulated by an unknown number of genes and hence the selection of flavor-rich genotypes is a highly complex matter. As a consequence for practical breeding, limited attention is paid to sensory quality apart from off-flavor types. Furthermore, sensory quality is mostly evaluated in very late stages when more easily assessable characteristics have already been defined (Alston, 1992).

Additionally, the inclusion of objective methods for assessing flavor quality in plant breeding is problematic because of practical constraints: Objective human sensory methods like quantitative descriptive methods (analytic) or consumer tests (hedonic) demand a large sensory panel and require big fruit samples. Both of these conditions are difficult (almost impossible) to implement in practical cultivar breeding programs that often deal with single plants and with a huge number of progenies.

To overcome these constraints instrumental methods were used to replace or complement human sensory. In strawberry breeding research the use of soluble solids content measurement (SSC or brix) for sugars ('sweet') and titratable acids (TA) or pH ('sour') are common (Mathey et al., 2013; Skrede et al., 2012). More sophisticated methods like HPLC (Pelayo-Zalvidar, 2007) or biochemical kits for sugar and acid profiles (Schwieterman et al., 2014) are rarely applied. In contrast, gas chromatographic analyses for VOC patterns (aroma) were used frequently and published in a

* Corresponding author

large number. Nonetheless, until now no agreement has been reached about the chemical constituents of strawberry flavor (Schwieterman et al., 2014). In particular, the data of VOC patterns reported in the literature are highly heterogeneous.

In a detailed two-year study, Schwieterman et al. (2014) estimated seasonal influences, the relationships between sensory parameters (intensity of sweetness, sourness, flavor), hedonic responses (texture and overall liking) as well as VOC patterns. Thirty-five current commercial cultivars and selections from the North American and the European gene pool were used. The authors revealed correlations between sugar content and sweetness, titratable acidity and sourness, total and specific VOC content and flavor intensity. The overall liking of strawberry was mainly subjected to the sensory parameters sweetness and flavor. The authors argued that a more powerful correlation between instrumental values and hedonic characters was undermined by co-activation of taste and retronasal olfaction which may lead to enhancement and/or depression of distinct sensory sensations.

Consumer liking or acceptance of food underlie parameters like gender, age, cultural background and habituality. However, some cultivars possess appreciation over a long period, for example, cv. 'Frau Mieze Schindler' (Germany, 1933) (Olbricht et al., 2011), cv. 'Mara de Bois' (France, 1991), cv. 'Gariguette' (France, 1976) (Marionnet, 1993; N. N., 2016; Vaysse et al., 2012), and cv. 'Ottoman' (Turkey, before 1900) (Karacam et al., 2015). Obviously, there are generally accepted flavor archetypes that are rather stable over long periods and that can serve as orientation guides for plant breeding.

The aim of the present study was to correlate overall liking (acceptance) and the intensity of important sensory parameters evaluated by a consumer panel with data of instrumental analyses like SSC, TA and VOC patterning. Special attention was given to two prerequisites that are essential for the determination of meaningful results in a consumer study. Firstly, genotypes with a high genetic diversity were used to guarantee a wide range of variation in the considered fruit characteristics. For this purpose, old and new common commercial cultivars and breeding clones originated from cultivar crossing and from wild species introgression were used. Secondly, it was ensured that every member of the consumer panel received a representative sample from a carefully mixed berry batch. Fruit material for sensory testing and instrumental analysis were taken from the identical batch. The experiment was conducted repeatedly over a time span of three years. By this approach statistically significant data can be expected.

Materials and methods

Plant material

Sixteen cultivars and breeding clones of *F. × ananassa* were planted in rows as fresh plants in August 2012, 2013, and 2014 in the open field on sandy loam on gravel ground at Dresden-Weixdorf, Germany (elevation 188 m N.N., Lat: 51.142703, Lon: 13.772751). The plant material is characterized in Tab. 1. Besides standard cultivars with good and medium flavor also modern cultivars with poor sensory quality and breeding clones with very intense typical and untypical flavor (off-flavor types) were used.

Fruit material

The whole test comprises sixteen cultivars and breeding clones with nineteen test samples, respectively. Fully ripe and typical fruits of one-year-old plants were harvested in 2013, 2014, and 2015. The day before testing, the fruits were harvested and were stored overnight in a chilling chamber at 4 °C. After warming to room temperature and immediately before testing, approximately 7 kg of fruit from at least 50 plants per genotype were cut into quarters and carefully mixed to ensure a representative sample batch. The time-consuming preparation was conducted because the homogeneity of the samples is important since a significant fruit-to-fruit variability is known (Vitten, 2008). This procedure, which required the fragmentation of the fruits, avoids the judgment of fruit appearance and deliberately omitted the assessment of texture and favors the homogeneity of the batch sample. Thus, it could be ensured that at the test dates all samples (sensorial and instrumental) derived from the same population mean. The portions of minimal 70 grams were served in plastic cups covered with aluminum foil. Assuming an average weight per fruit of 20 g it was assured that a mixture of at least fourteen single fruits was served per panelist and genotype. A 1000 g fraction of each 7 kg sample batch was used for the analysis of soluble solids, acidity and VOC patterns.

Sensory test by a consumer panel

The sensory evaluation was performed by a consumer test (affective or hedonic test) with a consumer panel at three days in three years in total. A sensory evaluation form was filled by all members of the consumer panel including an acceptance test by hedonic rating as well as attribute diagnostics (Kemp and Hollowood, 2009). The consumer panel comprised a total number of 237 individuals throughout the three harvest years.

The acceptance was measured on a 7-point facial expression scale (smileys) with the following acceptance values: 0 – dislike very much; 1 – dislike moderately; 2 – dislike slightly; 3 – neither like nor dislike; 4 – like slightly; 5 – like moderately; 6 – like very much.

The sensory attribute diagnostics comprises the quality parameters 'sweet', 'sour', 'aromatic' and 'untypical' flavor. The intensity of these quality parameters was recorded on a 7-point scale with the endpoint values from 0 to 6. Regarding untypical flavor the panelists had the possibility for verbal comments. In addition, the following demographic specifications of the panelists were retrieved: gender, age, smoker/non-smoker, profession and hobby. The sensory test was performed by altogether 237 individuals (Caucasian) consisting of 137 females and 100 males in the age from 8 to 84 years. The average age of the panelists was 33.7 years. A fraction of 92.8% of the panelists were non-smokers. The professions and hobbies were specified in a wide range between scientific/technical and artistic topics.

Estimation of aggregate parameters soluble solids content (SSC in °Brix) and titratable acidity (TA in % of citric acid equivalent)

The brix value was measured using a digital refractometer (Quick-Brix®, Mettler Toledo, Schwerzenbach, Germany), TA was determined with a titrator (716DMS-Titrino-Serie-06® (Metrohm, Filderstadt, Germany) taking the juice from the representative 1000 g fraction of each 7 kg sample batch.

Immersion stir bar sorptive extraction-gas chromatography-quadrupol mass spectrometry (Imm-SBSE-GC-qMS)

A minimum of 1000 g quartered fruits were separated from the 7 kg sample batch. To prepare an enzyme inhibited strawberry juice, one mass part of fruits without sepals were homogenized in one volume part of a solution of 18.6% (m/v) NaCl using a household mixer (Bosch professional MSM 71.) for 2 min. The homogenate was centrifuged 4000 rpm for 30 min. One hundred milliliter of the supernatant were mixed with 10 µl internal standard (0.1% (v/v) 2,6-dimethyl-5-hepten-2-ol dissolved in ethanol). For each sample, three head-space vials containing 3 g NaCl each for saturation were filled with 10 ml of the supernatant, sealed with magnetic crimp caps including septum, and stored at 4 °C.

Tab. 1: Fruit material and characteristics of the genotypes

Genotype	*Abbreviation*	*Harvest year*	*Release/Country*	*Comments*	*Genetic background*
'Daroyal'	dar.13	2013	2006*, FR	early cultivar	
'Rumba'	rum.13	2013	2011*, NL	early cultivar	
'Honeoye'	hon.13 hon.15	2013 2015	1979**, US	early cultivar, sour	'Vibrant' × 'Holiday'
'Evie2'	evi.13	2013	2006**, UK	everbearer, poor flavor	'Everglade' × J92D12
'Elsanta'	els.13	2013	1975**, NL	midseason standard cultivar	'Gorella' × 'Holiday'
P-725	p725.14 p725.15	2014 2015	breeding clone	high-aroma type under application for PBR	introgression with *F. chiloensis*
P-326	p326.14	2014	breeding clone	medium flavor	cultivar cross-breeding
'Sonata'	son.14	2014	1998**, NL	main harvest	'Elsanta' × 'Polka'
'Elianny'	eli.14	2014	2010**, NL	mid season cultivar	
'Frau Mieze Schindler'	ms.14	2014	1933**, DE	late harvest, with excellent flavor, MA type	'Lucida Perfecta' × 'Johannes Müller'
P-565	p565.14 p565.15	2014 2015	breeding clone	off-flavor type	cultivar cross-breeding
P-713	p713.14	2014	breeding clone	off-flavor type	introgression with *F. chiloensis*
P-622	p622.15	2015	breeding clone	high-aroma-type	introgression with *F. chiloensis*
P-709	p709.15	2015	breeding clone	medium flavor	'Roxana' × 'Darlisette'
'Clery'	cle.15	2015	2006*, IT	early standard cultivar	
'Elegance'	ele.15	2015	2009*, UK	perfect fruits, low-flavor type	EM834 × EM1033

* Granted Community Plant Variety Right EU; ** on the market.
Sources: https://cpvoextranet.cpvo.europa.eu; https://en.wikipedia.org/wiki/List_of_strawberry_cultivars;http://strawberryplants.org/2010/05/strawberry-cultivars.

An aliquot of 8 ml of the saturated homogenate but without the solid NaCl deposit was transferred in an empty glass vial for volatile isolation by immersion SBSE. A stir bar with 0.5 mm film thickness and 10 mm length coated with polydimethysiloxane (PDMS) was placed in the liquid (Gerstel, Mülheim an der Ruhr, Germany). The stir bar was moved at 350 rpm at room temperature for 45 min. After removal from the strawberry juice, the stir bar was rinsed with purified water, gently dried with a lint-free tissue and then transferred into a glass tube for thermal desorption and subsequent GC analysis.
The parameters for the thermal desorption unit (TDU, Gerstel) and the cold injection system (CIS4, Gerstel) were the following: thermal desorption at 250 °C, cryo-trapping at -150 °C. The TDU-CIS4 unit was used in Gerstel-modus 3: TDU splitless and CIS4 with 15 ml/ min split flow. The analyses were performed with an Agilent Technologies 6890N gas chromatograph equipped with an Agilent 5975B quadrupol MS detector. Compounds were separated on a polar column ZB-Wax plus 30 m length × 0.25 mm ID × 0.5 µm film thickness. Helium was used as a carrier gas with a column flow rate of 1.1 ml/min. Temperature program: 45 ºC (3 min), temperature gradient 3 K/min to 210 ºC (30 min). The mass spectrometer was used with electron ionization at 70 keV in the full scan mode. All samples were run with three analytical repetitions from an identical part of the same supernatant.
The commercial software ChromStat2.6 (Analyt, Müllheim, Germany) was used for data processing (Ulrich et al., 2008; Olbricht et al., 2008). Data inputs for ChromStat2.6 were raw data from the TIC percentage reports (retention time/peak area data pairs) performed with the software package Chemstation (version Rev.B.02.01.-SR1 [260]) by Agilent. Using ChromStat2.6, the chromatograms were divided in up to 200 time intervals, each of which represented a peak (substance) occurring in at least one chromatogram of the analysis set. The peak detection threshold was set on the 10-fold value of noise. The values are given as raw data (peak area in counts), which also can be described as relative concentration because of the normalized sample preparation. Statistical tests were performed using the software STATISTICA 7.1 by Statsoft.

Results

Sensory test

The ranking of the sensory attribute acceptance over nineteen test samples in three years was found as follows: p725.14 > p622.15 > p709.15 > p326.14 > dar.13 > son.14 > p725.15 > hon.15 > eli.14 > rum.13 > ms.14 > p565.14 > hon.13 > evi.13 > p565.15 > els.13 > cle.15 > ele.15 > p713.14. The absolute values are located between 4.73 (p725.14) and 2.78 (p713.14) on the 7-point scale from 0 to 6.
Fig. 1 displays results of a principal component analysis (PCA) of nineteen test samples from three seasons examined for 'acceptance' and the sensory attributes 'sweet', 'sour', 'aromatic' and 'untypical'. The sensory data were used as the mean values of all panelists who took part in every harvest year (82, 84 and 71 in 2013, 2014 and 2015, respectively). The different samples are spread over the parameter

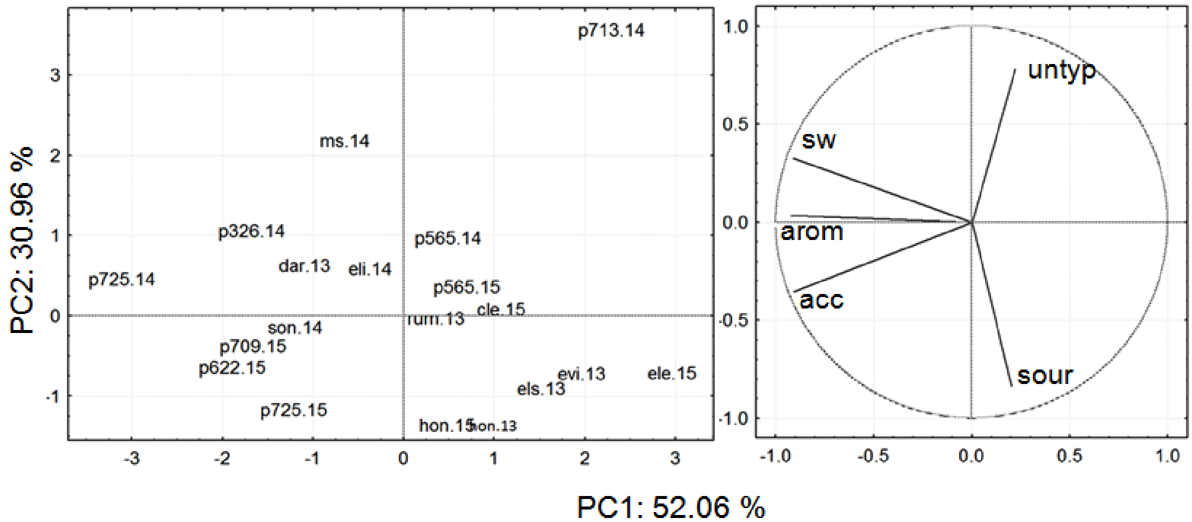

Fig. 1: Principal component analysis (PCA) of the consumer test results with nineteen strawberry samples examined for acceptance and four sensory attributes. Score plot (left) and loadings plot (right). Strawberry samples are named according to Tab. 1.
Abbreviations: sw – 'sweet', arom – 'aromatic', sour – 'sour', untyp – 'untypical', acc – acceptance.

space without distinct cluster formation (Fig. 1, score plot, left). The corresponding loadings plot (right) shows plausible relations of the sensory attributes. The parameters 'sweet' and 'aromatic' are located nearby the 'acceptance' whereas the attributes 'sour' and 'untypical' are placed more or less in opposite quadrants. This is in accordance with the experience that for strawberries the attributes sweet and aromatic carry positive hedonic connotations in contrast to sour taste and untypical aroma impressions.

In the context of all nineteen test samples the clone p713.14 was characterized by the lowest values for 'acceptance' (2.78) and 'sour' (1.47) and the highest untypical aroma impression (2.11). Because of the special sensory characteristics this sample is located in the low-acceptance area far away from the main cluster. For the test sample p725.14 the highest values for 'acceptance' (4.73), 'sweet' (3.74) and 'aromatic' (3.84) were assessed which may explain the close correlation of this genotype with the position of 'acceptance' in the left side of the congruent loadings plot.

A distinct seasonal influence was found for the genotype P-725 which was tested in 2014 and 2015 whereas the cultivar Honeoye (hon.13 and hon.15) and the clone P-565 (p565.14 and p565.15) show more stable results over two harvest years.

In Tab. 2, results of the correlation analysis are summarized. The 'acceptance' positively correlates with high and significant values of both sweetness (0.70) and aromatic sensation (0.81), while sourness (0.12, n.s.) has a minor influence. In contrast, untypical aroma profiles are negatively correlated with 'acceptance' (-0.45 n.s.). Also in-between the sensory attributes significant relations were found. The retronasal sensation 'aromatic' is highly positively related to the sweet taste (0.79). The taste sensation 'sweet' and 'sour' are negatively correlated (-0.48). These findings are in good agreement with experience from breeding practice and the results published by Schwieterman et al. (2014) using berry material from the North American and European gene pool.

Instrumental analysis

a) Aggregate parameters (SSC, TA, quotient SSC/TA). For the determination of the status of fruit ripeness, for making selling and/or purchasing decisions as well as for practical breeding programs, the so-called aggregate parameters SSC and TA are widely used as quality parameters to assess sweetness and sourness (Kleinhenz and Bumgarner, 2015). In this experiment, the values for SSC (in °Brix) vary between 10.7 (son.14) and 6.3 (p565.15) and those for TA (in % citric acid equivalent) between 1.151 (hon.13) and 0.654 (p565.15). The cultivar 'Honeoye', which was tested in two harvest years (hon.13 and hon.15), shows the highest values for TA. This is in agreement with the cultivar description that 'Honeoye' is characterized by a pronounced sourness. As another common quality parameter the quotient of SSC and TA is used as index for a balance in sweetness and sourness. This quotient varies between 14.7 (son.14) and 6.57 (evi.13).

b) VOCs (immSBSE-GC-qMS). Using a non-targeted pattern recognition software (ChromStat2.6) up to 200 peaks were detected in a single chromatogram (TIC from qMS runs). By a manual procedure background peaks (e. g. silicon peaks from the Twister) were eliminated. Altogether 76 peaks were used for further data processing. This compilation comprises 25 fully identified compounds, 39 tentatively identified compounds and 12 unknowns. From the three analytical replicas the mean values were calculated. Altogether, 1444 metabolic data were used for further calculations.

In Fig. 2, results of a PCA are depicted. The nineteen test samples are located in two discrete clusters. Two samples appear as outliers, son.14 in quadrant 3 and p713.14 in quadrant 4. In the corresponding loadings plot some important compound groups are labeled. Accordingly, the sample son.14 is characterized especially by very high amounts of strait chain esters. The most outstanding VOC pattern was found in p713.14, a breeding clone which originates from an introgression with *F. chiloensis*. Compared with the other genotypes this clone contains the highest concentrations of some strait chain esters, branched esters, aromatic esters, methyl thioacetate, eugenol, methyleugenol and especially mesifuran. The latter compound exceeds the level found in the remaining genotypes by one order of magnitude.

The PCA shows that according to the aim of this experiment to study the influence of VOC patterns on sensory sensations and acceptance, the used compilation of genotypes comprises a broad diversity in metabolite concentrations. Altogether 40 out of 76 VOCs show qualitative differences between genotypes and 36 VOCs are compounds that characterize the mutual metabolite pattern of the gene pool used in this experiment. Qualitative differences were defined when distinct metabolites were not detected (concentration below the detection threshold) in one or more samples. The detection threshold was set to $1{\times}10^6$ counts (TIC) which is equivalent to 3 ppb of the internal standard.

Tab. 2: Correlation analysis of VOC data compiled to substance groups with aggregate parameters, sensory attributes and 'acceptance'

	e	eb	earom	t	a	ald	k	lac	phen	acid	fur	o	s	u	sum	sweet	sour	arom	unt	SSC	TA	SSC/TA	acc
e	1.00																						
eb	0.65 *	1.00																					
earom	0.40	0.73 *	1.00																				
t	-0.17	0.17	0.17	1.00																			
a	-0.58 *	-0.24	-0.07	0.24	1.00																		
ald	-0.40	-0.07	-0.08	-0.12	0.07	1.00																	
k	0.07	-0.03	0.04	-0.20	0.18	-0.19	1.00																
lac	-0.09	-0.02	0,00	0.71 *	0.10	-0.02	0.08	1.00															
phen	0.34	0.82 *	0.83 *	0.18	0.08	-0.04	0.04	-0.03	1.00														
acid	0.11	-0.25	-0.39	-0.30	-0.03	-0.13	0.52 *	0.25	-0.28	1.00													
fur	0.37	0.75 *	0.69 *	0,00	0.09	-0.11	0.21	-0.08	0.86 *	0.05	1.00												
o	0.40	0.28	0.35	0.12	-0.04	-0.15	0,00	0.27	0.26	-0.09	0.13	1.00											
s	0.50 *	0.77 *	0.79 *	-0.01	-0.06	-0.19	-0.03	-0.27	0.73 *	-0.30	0.75 *	0.26	1.00										
u	0.36	0.53 *	0.56 *	0.55 *	-0.02	-0.14	0.14	0.73 *	0.54 *	0.11	0.48 *	0.49 *	0.30	1.00									
sum	0.49 *	0.44	0.31	0.53 *	-0.17	-0.22	0.17	0.80 *	0.30	0.31	0.30	0.45	0.15	0.90 *	1.00								
sweet	0.31	0.34	0.12	0.38	-0.32	-0.47 *	-0.31	0.20	0.22	-0.26	0.04	0.10	0.08	0.28	0.30	1.00							
sour	-0.54 *	-0.48 *	-0.39	0.28	0.49 *	0.45	0.15	0.50 *	-0.41	0.29	-0.29	0.01	-0.45	0.04	0.14	-0.48 *	1.00						
arom	0.21	0.09	-0.10	0.49 *	-0.29	-0.48 *	0,00	0.42	-0.09	0.01	-0.17	0.03	-0.13	0.25	0.42	0.79 *	-0.07	1.00					
unt	0.12	0.45	0.45	-0.19	-0.03	0.13	0.20	-0.34	0.50 *	-0.13	0.48 *	-0.38	0.46 *	-0.03	-0.14	-0.01	-0.33	-0.01	1.00				
SSC	0.09	0.31	0.03	0.25	0.15	-0.24	0.21	0.26	0.35	0.29	0.35	-0.30	0,00	0.26	0.34	0.40	-0.13	0.44	0.51 *	1.00			
TA	-0.70 *	-0.33	-0.13	0.51 *	0.46 *	0.29	0.17	0.46 *	-0.19	-0.08	-0.22	-0.22	-0.35	0.05	0.02	-0.06	0.70 *	0.29	0.04	0.15	1.00		
SSC/TA	0.62 *	0.52 *	0.14	-0.20	-0.21	-0.37	0.12	-0.15	0.45	0.33	0.49 *	-0.08	0.29	0.19	0.28	0.30	-0.58 *	0.10	0.39	0.67 *	-0.62 *	1.00	
acc	-0.04	-0.18	-0.42	0.53 *	-0.19	-0.28	-0.32	0.47 *	-0.41	-0.03	-0.48 *	0.03	-0.38	0.11	0.29	0.70 *	0.12	0.81 *	-0.45	0.12	0.27	-0.15	1.00
	e	**eb**	**earom**	**t**	**a**	**ald**	**k**	**lac**	**phen**	**acid**	**fur**	**o**	**s**	**u**	**sum**	**sweet**	**sour**	**arom**	**unt**	**SSC**	**TA**	**SSC/TA**	**acc**

Abbreviations: e – strait-chain esters, eb – branched esters, earoma – aromatic esters, t – terpenoids, a – alcohols, ald – aldehydes, k – ketones, lac – lactones, phen – phenylpropanoids, acid – acids, fur – furanones, o – others, s – sulfur containing compounds, u – unidentified compounds, sum – sum of all 76 peaks, arom – aromatic, unt – untypical, acc – acceptance. Correlation coefficients with asterisk (*) indicate a significant correlation on the level $p < 0.05$.

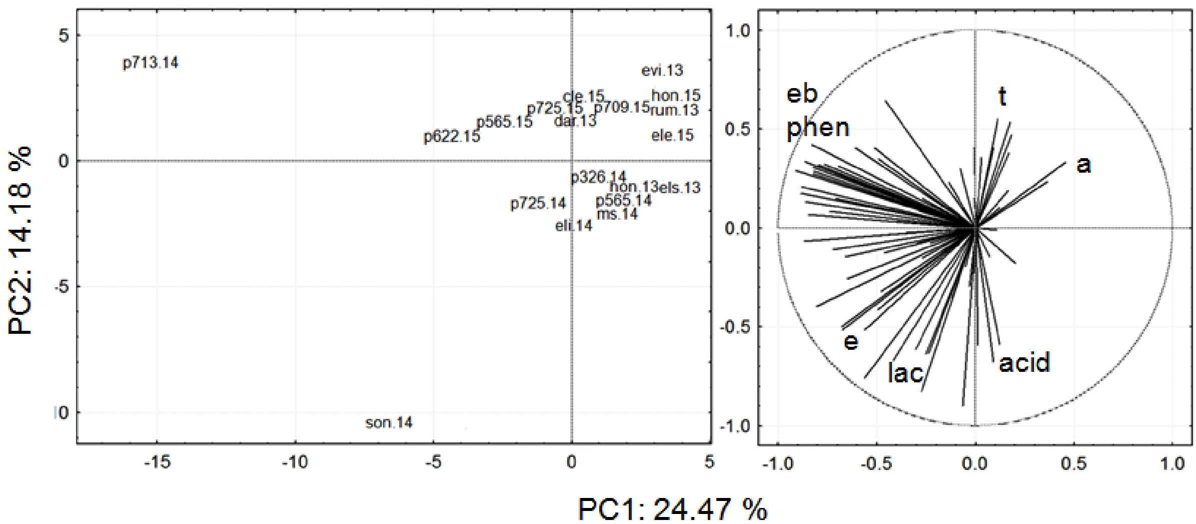

Fig. 2: Principal component analysis (PCA) of results of gas chromatographic analysis of nineteen strawberry samples examined for 76 VOCs. Score plot (left) and loadings plot (right). Strawberry samples are named according to Tab. 1.
Abbreviations: eb – branched esters, e-strait – chain esters, a – alcohols, lac – lactones, t – terpenoids, phen – phenylpropanoids, acid – acids.

Correlations between sensory and instrumental data

a) Aggregate parameters (SSC, TA, quotient SSC/TA). Altogether nine significant correlations were found (Tab. 2). Included are three significant correlation factors between instrumental and sensory data. Sourness is highly positively correlated with TA (0.70) and negatively with SSC/TA (-0.58). The SSC value correlates positively with the sensory sensation 'untypical' (0.51).

b) Volatile compounds. Among the 76 VOCs, three aggregate parameters, four sensory attributes and 'acceptance', altogether 634 significant correlations (560 positive and 73 negative ones) were found. Compounds with generally positive correlations to 'acceptance' belong to the compound groups of terpenes ((*Z*)-linalool oxide (0.50), linalool (0.56)), lactones (γ-decalactone (0.47), γ-dodecalactone (0.61)) and the unknown compound u19 (0.47). Negative coefficients occur with esters (ethyl 2-methylbutanoate (-0.57); ethyl 3-methylbutanoate (-0.59); butyl acetate (-0.56); pentyl acetate (-0.59), 3-methylbutyl butanoate (-0.58) and methyl salicylate (-0.58)), furanones (mesifurane (-0.50)) and phenylpropanoids (methyleugenol (-0.51)). The taste sensation 'sweet' is correlated positively with methyl 2-methylbutanoate (0.47), (*Z*)-3-hexenyl acetate (0.55), linalool (0.49) and decanoic acid (0.56) as well as negatively with 2-pentanone (-0.52) and (*E*)-2-hexenal (-0.47). The relationship of the retronasal sensation 'aromatic' shows some similarities to those with the acceptance (positive correlations with linalool (0.50), δ-decalactone (0.49), decanoic acid (0.51), γ-dodecalactone (0.69) and one unknown compound u19 (0.48); negative correlations with (*E*)-2-hexenal (-0.49), acetic acid (-0.49), 3-furanmethanol (-0.46), methyl salicylate (-0.51)). The quality of correlation is depicted in Fig. 3 as scatterplot for a selection of important correlations. Positive correlations are depicted for 'acceptance' with the sensory parameters 'sweet' and 'aromatic'. The sensory sensation 'untypical' correlates negatively with 'acceptance' (not significant). Further, a positive correlation was found between 'sweet' and 'aromatic' as well as between 'acceptance' and the metabolites linalool, (*Z*)-linalool oxide, γ-decalactone and γ-dodecalactone. The sensory impression 'sour' has no significant influence on 'acceptance'. As examples for negative relations between 'acceptance' and VOCs the compounds mesifuran and butyl acetate were selected. Hereby, the influence of the clone p713.14 on statistical results can be seen. Only with this clone with its extraordinary volatile pattern an influence of mesifurane and butyl acetate on 'acceptance' was found.

To obtain a more simplified arrangement with the multitude of parameters, the 76 VOCs were compiled to 14 compound groups. Results from statistics using data of these compound groups instead of individual VOCs are depicted in Tab. 2. Out of 55 significant correlation coefficients, a number of 46 show positive values and nine negative ones. The hedonic attribute 'acceptance' interacts significantly with three compound groups and two sensory attributes: terpenoids (0.53), lactones (0.47), furanones (-0.48), 'sweet' (0.70) and 'aromatic' (0.81). Several high correlations occur between distinct compound groups and may give insight in relationships of biosynthetic pathways even if this question was not in the focus of this study.

Discussion

Results of the consumer study and correlation between sensory attributes

The evaluation of the consumer study reveals clear differences in the acceptance of the genotypes. As a result of the PCA, no clear clustering occurs. The nineteen test samples are rather evenly scattered over the parameter space (Fig. 1). The five samples with the highest 'acceptance' values include four breeding clones (p725.14, p622.15, p709.15, p326.14) and the cultivar 'Daroyal' (dar.13). The sample with the lowest 'acceptance' was the breeding clone p713.14. The location of the sensory attributes in the loadings plot (Fig. 1, right) demonstrates close correlations between the attributes 'sweet', 'aromatic' and 'acceptance', while the attributes 'sour' and 'untypical' are arranged in distant quadrants of the plot. The results of PCA are confirmed by the correlation analysis. 'Acceptance' is positively correlated with the attributes 'sweet' (0.70) and 'aromatic' (0.81). The perception 'untypical' is negatively correlated (-0.45, n.s.), while the attribute 'sour' has only a small influence on the formation of the 'acceptance' (0.12, n.s.). These relationships are consistent with the earlier work of LOEHNDORF (2000) and the results of recent studies of SCHWIETERMAN (2014) and BHAT (2015). These former studies reported that consumers particularly prefer sweet and aromatic ('intense fruity') strawberries.

The sweetness is negatively correlated with acidity (-0.48) and positively correlated (0.79) with the 'aromatic' perception. The final correlation points to an interaction of taste and smell perceptions (MURPHY and CAIN, 1980; DELWICHE, 2004).

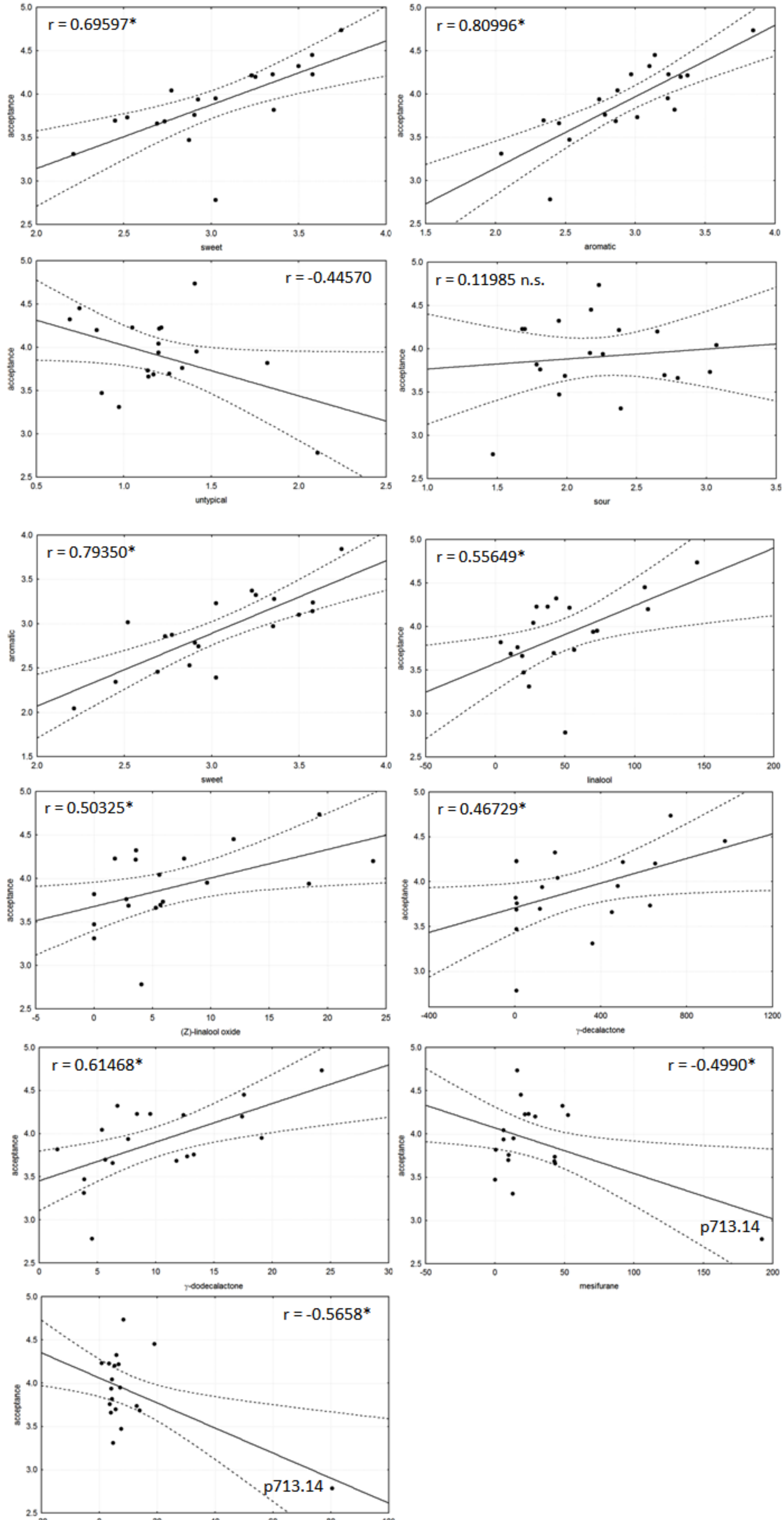

Fig. 3: Selected scatterplots of a linear regression model for analysis. Nomenclature: r – correlation coefficient. Correlation coefficients with asterisk (*) indicate a significant correlation on the level $p < 0.05$. Dotted bands for 95 % confidence.

Correlation between sensory attributes and aggregate parameters

In practice the aggregate parameter SSC (brix value) and TA are often used as convenient index for the sensory attributes 'sweet' and 'sour'. The ratio of these two parameters should enable an assessment of the sweet-sour balance. Both aggregate parameters and their ratio show no significant correlation with 'acceptance' (Tab. 2). Only 'sour' and TA are significantly correlated (0.70). However, the positive correlation between SSC with the retronasal impression 'untypical' is inexplicable in the context of this experiment. These results demonstrate that the widespread aggregate parameters have only limited significance for the quality analysis. In particular, the SSC is not very meaningful because on the one hand the brix value not only considers sugars and on the other hand also other metabolites can cause a sweet impression (Kleinhenz and Bumgarner, 2015). In analogy, this holds true for the ratio SSC/TA. Although the TA parameter correlates with the impression 'sour', this taste parameter does not contribute to the 'acceptance' (0.12, n.s.).

Correlation between sensory attributes and VOC patterns

A number of 76 VOCs (identified, tentatively identified and unknown peaks) was semi-quantified and was used for correlation analysis. In a PCA, two separate clusters occur based on the VOC concentration patterns (Fig. 2). The upper cluster of eleven samples is in particular characterized by higher contents of alcohols, terpenoids, branched esters and phenylpropanoids, while the lower cluster with eight samples represents fruit with higher concentrations of lactones, acids, and straight-chain esters. According to the correlation analysis, these clusters do not directly reflect the sensory properties. Obviously, these properties are the results of more complex relationships. For example, it is known that γ-decalactone increases the sweetness and creaminess of cream (Schlutt et al., 2007). In a previous study it was reported (Schwieterman et al., 2014) that many of the volatiles that are perceived retronasal through the olfactory system correlate with taste parameters that are detected on the tongue as well as with the hedonic parameter 'acceptance'. Using all determined data, 76 VOC concentrations, three aggregate parameters, four sensory attributes and acceptance, i.e. altogether 634 positive and negative significant correlations were found. Importantly, it was determined that the VOCs methyl 2-methylbutanoate, (*Z*)-3-hexenyl acetate, linalool and decanoic acid correlate positively with the attribute 'sweet' and, therefore, they are suggested to act as sweetness enhancers. Recently, Schwieterman et al. (2014) reported a similar relation for the VOCs 1-penten-3-one, γ-dodecalactone, pentyl butanoate, hexyl butanoate, hexyl acetate and 1-methylbutyl butanoate. Amongst others this different compilations may be explained by the different sample preparation methods (cf. section 'Materials and methods').

To obtain a clearer interpretation of the results and to reduce the number of possible correlations, the 76 VOCs were combined into a total of 14 substance groups. A summary of VOCs into substance groups is a compromise, but it can be justified on the basis of similarities in the sensory properties of the members of a group. The relatively clear grouping of samples and loadings after a PCA comprising 14 substance groups, three aggregate parameters, four sensory attributes and 'acceptance' (details not shown) favor this approach (Tab. 2). Thus, the acceptance of a sample is particularly positively influenced by the substance groups of terpenoids (0.53), lactones (0.47) and on weaker extent by the sum of VOCs (0.29, n.s.). Several groups of substances have a negative impact, for example, furanones correlate negatively with 'acceptance' (-0.48).

These relationships indicate the complexity of the sensory perceptions and finally the formation of the impression 'acceptance'. In Fig. 4 these complex dependencies are depicted for three parameters in form of surface plots.

1) 'Acceptance' depending on 'aromatic' and 'sweet' (Fig. 4a): The maximum of 'acceptance' coincides with high values for both, 'aromatic' and 'sweet'. Strawberries with low values for 'aromatic' and/or 'sweet' also show a low value of 'acceptance'. For example, strawberries with a very high sweetness at low flavor levels have low 'acceptance'. This result agrees well with the experience from practical selection work in breeding.

2) 'Acceptance' depending on the concentrations of lactones (lac) and terpenoids (t) (Fig. 4b): The highest values of 'acceptance' were found if the concentrations of both substance groups are high. For the two substance groups decreasing values of 'acceptance' at increasing concentration were found at simultaneously low concentration values of the second group.

3) 'Acceptance' depending on the concentrations of branched ester (eb) and strait-chain ester (s) (Fig. 4c): For these two substance groups and their combination an optimal concentration range exists. As shown for lactones and terpenoids in Fig. 4b very high concentrations lead to lower acceptance.

4) Sweetness depending on the concentrations of lactones (lac), and terpenoids (t) (Fig. 4d):

This function is very similar to that described above for the dependence of 'acceptance' on the concentrations of lactones (lac) and terpenoids (t). A maximum sweetness arises, independently of the SSC value, in combination with high concentrations of both substance groups. Since the sensory impression 'sweet' correlates positively with 'acceptance' (0.70), the influence of these VOC groups can be explained (Fig. 4b).

Environmental influence

It is known that the quality of strawberries is influenced by the genotype (cultivar) and environmental influences such as harvesting day, season (weather) or year (Schwieterman et al., 2014; Ulrich and Olbricht, 2014). In the present experiment, the study of environmental influences was neglected. Clearly, we focused on the correlation of analytical and sensory data. For this purpose the variability of the measurements is crucial in the end, but not the source of this variability. The set of nineteen samples over the test period of three years contains three genotypes ('Honeoye', P-565 and P-725) which were analyzed in two different harvest years, namely, hon.13, hon.15, p565.14, p565.15, p725.14 and p725.15. The sensory and metabolic properties of these genotypes react, as expected, in varying degrees on harvest years (Fig. 1 and 2). This allows an insight in their stability between the two years. Hereby, 'Honeoye' as an established cultivar shows the lowest deviations, followed by P-565. Interestingly, the breeding clone P-725 with its very broad range of VOCs in high quantities shows bigger differences between two harvest years. Compared to stability tests on a model population (Olbricht et al., 2011), it seems plausible that genotypes with a very diverse aroma profile and high concentrations of VOCs exhibit more significant differences between harvest data (days, seasons, years) than genotypes with lower levels caused by the environmental dependency of VOC biosynthesis.

Influence of analytic methods (clean up) on the informational value of results

In the past, numerous studies dealt with VOC analysis leading to very diverse results regarding substance identification (Ulrich et al, 1997; Olbricht et al., 2011; Schieberle and Hofmann, 1997). A cross-comparison of five studies published in the period between 1997 and 2008, which cover up to 50 constituents in each of the single compound lists, results in only seven mutual aroma compounds (Schwieterman et al., 2014). This small subset of VOCs represents the consensus of strawberry aroma compounds.

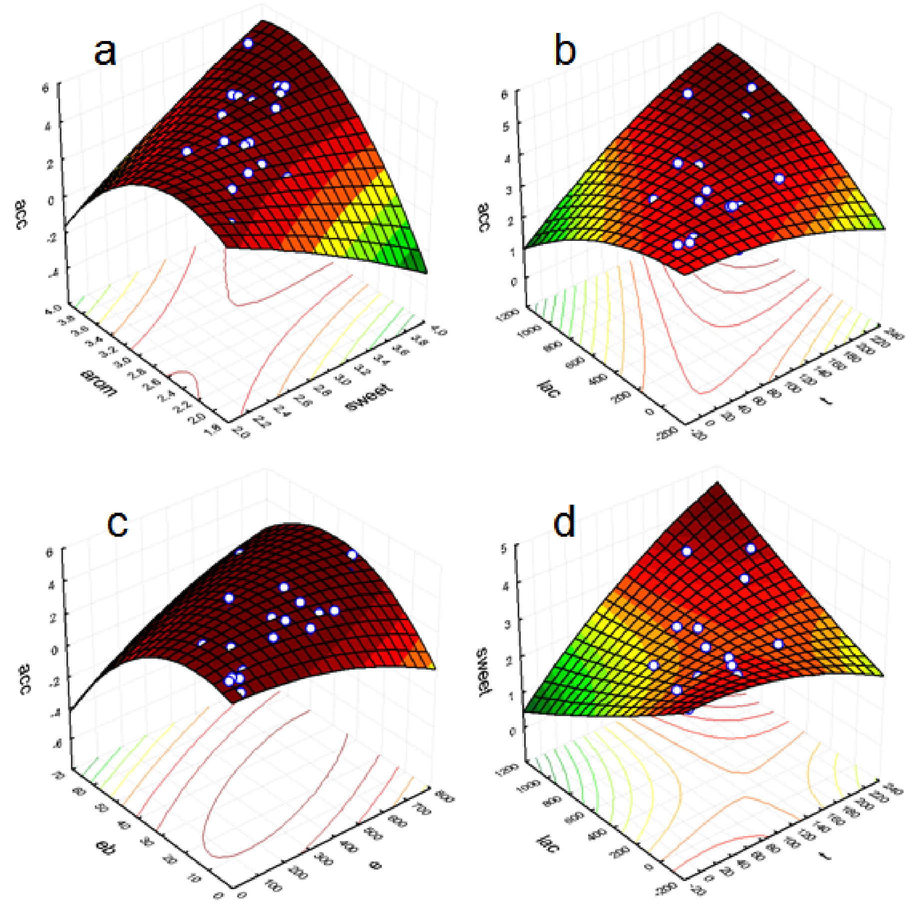

Fig. 4: Surface plot of selected relationships between instrumental and sensory parameters. The relative concentration values are color-coded with red for high and green for low values.

Besides genotypic diversity in metabolite patterns, differences in the characteristics of the used GC methods are the obvious reason for this non-conformity. The comparison between this study (HS-SBSE) and the recent reports by Schwieterman et al. (2014) (dynamic headspace collection) reveals that only 28 out of 116 VOCs are found in both investigations. Obviously, the selection of the extraction method for VOCs is the critical point (Komes et al., 2005). Between different VOC collection methods like liquid extraction (LE), HS-SPME and Imm-SBSE quantitative and qualitative differences occur which result in the above mentioned low degree of consensus in aroma compound research. In the context of correlation analyses qualitative differences between independent studies like those found for sweetness enhancers may be explained.

Do the present results contradict the aroma value concept?

Only a small number of chemicals are concordantly reported in the literature, too, using either the identification of character impact compounds by gas chromatography-olfactometry or the aroma value concept (Ulrich et al., 1997; Schieberle and Hofmann, 1997; Cannon et al., 2015; Du et al., 2011). For the strawberry aroma, consensus has apparently been reached on furanones (DMHF, DMMF), 2-methylbutanoic acid, short chain esters (e. g. butanoates and hexanoates), linalool and γ-decalactone.

In the present study, the correlation analysis between VOCs and 'acceptance' results in negative coefficients, for example, for some esters (ethyl 2-methylbutanoate (-0.57); ethyl 3-methylbutanoate (-0.59); butyl acetate (-0.56); pentyl acetate (-0.59), 3-methylbutyl butanoate (-0.58), methyl salicylate (-0.58)) and mesifurane (-0.50). The negative correlation between VOCs which were appointed as important character impact compounds and the hedonic parameter 'acceptance' constitutes no discrepancy. Of course, esters and furanones belong to the key compounds of typical strawberry flavor and contribute to a significant part to the odorant space coverage (OSC) (Dunkel et al., 2014) but obviously an optimum concentration – or more exactly speaking an optimum odor activity value (OAV) – exists for individual compounds in the complex strawberry matrix. This can explain why negative relationships between aroma compounds and 'acceptance' were found in this study (Fig. 4) if optimal values for a pleasant perception are exceeded. These results correspond to those found for β-damascenone, a character impact compound of tomato flavor with extremely low odor threshold, which was, however, not associated with tomato flavor intensity in a consumer test (Tieman et al., 2012).

Implementation for breeding

The domestication process of food plants is characterized by the search for sweet, non-sour, non-bitter, non-astringent edible parts of a plant. Genotypes were selected for pleasant sensory characteristics as an example of co-evolution and the positive aspect of domestication (Diamond, 2002). As a negative effect, domestication often results in a decline of volatile and non-volatile secondary metabolites coinciding with loss of resistance, which has been demonstrated for intensively bred horticultural and agricultural crops (Meyer et al., 2012; Pickersgill, 2007).

a) Breeding goal 'sweetness'. It was confirmed that sweetness is a main criterion for the acceptance of a fruit. In the plant improvement process, however, sugar and yield are competing breeding goals because sugar content (strictly speaking dry matter) is negatively correlated with yield (Vitten et al., 2009). Consequently, most high performance cultivars in strawberry are large fruited with high yield but with low sugar contents, respectively low dry matter and SSC. Likewise, the selection for low-acidity genotypes took place to avoid an imbalance between sugars and acids (example 'Clery' in this study). However, an increase of sugar content and a simultaneous decrease of acidity coinciding with higher yield are limited. In contrast, low sugar-acid ratios reduce the perception of aroma compounds (Baldwin et al., 2008). Our present results underline that volatiles significantly contribute to sweetness which supports the findings by Schwieterman et al (2014). In particular, this correlation opens new ways to select sweet and high-yielding and aromatic strawberry cultivars. Comparative studies of old and modern cultivars reveal that modern cultivars are continuously containing considerable amounts of linalool whereas several old cultivars are lacking this volatile (unpublished data and Olbricht et al. (2008)). This result can be interpreted as an unconscious result of the domestication caused by selection for sweetness.

b) Breeding goal 'aroma/flavor'. In the recent history of strawberry breeding, aroma profiles played only a role in the sense of avoiding untypical flavor impressions. Unlike firmness and yield, aroma has been clearly underestimated as breeding goal. For decades, results of VOC analyses of wild and cultivated strawberry fruits have been published (Ulrich and Olbricht, 2014; Drawert et al., 1973; Staudt et al., 1975; Pyysalo et al., 1979; Hirvi and Honkanen, 1982) including the definition of chemotypes, discriminated by ester and methyl anthranilate contents (Ulrich et al., 1997). In addition, detailed investigations were conducted to define character impact compounds using gas chromatography olfactometry and/or the aroma value concept (Ulrich et al., 1997; Schieberle and Hofmann, 1997; Cannon et al., 2015; Du et al., 2011). Despite of these numerous investigations of the chemical foundations of strawberry aroma, until now there is no clear definition of the ideal aroma pattern in strawberry.

A consumer study aiming at the correlation of sensory perception with analytical data offers the possibility to discover correlations in this complex parameter system. As a result, single aroma compounds or compound groups should be considered to be important for selection. Consequently, instrumental analysis for VOCs will advance as a selection tool in practical strawberry breeding and will provide an orientation to the balance of different metabolites. Besides the groups of esters with positive or negative correlation to acceptance, some other compounds are obviously important for breeding.

For example, the terpenoid linalool is positively correlated with 'acceptance' as well as to the sensory impression 'aromatic'. It also correlates positively with sweetness. This underlines former reports on linalool as valuable compound for selection of strawberry (Chambers et al., 2012), tomato (Lewinsohn et al., 2001) and numerous other crops (Bernreuther and Schreier, 1991). It is important for a successful selection work that linalool is an environmentally stable synthesized VOC (Olbricht et al., 2011; Olbricht et al., 2008).

The breeding clones, which were obtained from cross-breeding with wild genotypes, exhibit a high VOC diversity. This is expressed by quantitative and qualitative differences of individual VOCs and significant quantitative differences in the aggregate parameters. Interestingly, the most preferred genotypes P-725 (most appreciated: p725.14) and P-622 show the 37-fold linalool concentration of the cv. 'Frau Mieze Schindler' and the 10-fold one of P-565, respectively. Both breeding clones P-622 and P-725 result from an introgression of *F. chiloensis* ssp. *lucida* (F3) and show the potential of the use of wild germplasm. In contrast, the parallel selection P-713 with the same genetic background and stage of back-crossing demonstrates the danger of such pedigrees. P-713 exhibits a very diverse aroma profile with extraordinary high quantities of some strait-chain esters, branched esters, aromatic esters, methyl thioacetate, eugenol, methyleugenol and especially mesifuran resulting in off-flavor impressions. Comparable positive as well as negative results in the context of such highly diverse aroma patterns were not be reached by cultivar cross-breeding and were not found among cultivars. However, P-725 and P-622 also reached the highest values for γ-decalactone with a 216-fold ratio for p622.14 to ms.14. This lactone is considered as an important key compound for strawberry flavor (Ulrich et al., 1997; Schwieterman et al., 2014; Chambers et al., 2014). Considering that γ-decalactone belongs to the extremely environment-depended volatiles (Olbricht et al., 2011), we continue the discussion with a further important aspect of fruit breeding: the stability of traits.

In our former study (Olbricht et al., 2011) we demonstrated that the highest stability in aroma compounds is reached for genotypes with low or even zero quantities of VOCs. Therefore, the breeding of highly aromatic, but stable strawberry cultivars is a challenge. The stability requirement explains why modern high-performance cultivars are not characterized by high quantities of aroma compounds. On the other hand, the same study showed that a few genotypes with an acceptable stability of high levels of certain aroma compounds can be expected in a progeny, too.

The present study proofs that there is no single optimal pattern of metabolites that cause a high level of acceptance. It rather seems that positive 'acceptance' in strawberries values can be reached with two different types of patterns. One type with high contents of strait chain ester and methyl anthranilate in combination with a balanced sugar-acid ratio was found in old good tasting cultivars like 'Frau Mieze Schindler'. Often the aroma of these old cultivars is characterized as 'wood strawberry-like' because of the pronounced methyl anthranilate note. The second type without methyl anthranilate comprises the majority of common cultivars in which as a subtype the modern cultivars compensate the lack of esters and methyl anthranilate by a pronounced sweet impression caused by sugars and the enhancing effect of some VOCs. Interestingly, the most preferred breeding clone P-725 combines the positive traits of types with a pronounced short chain ester contents, lactones and linalool, but without methyl anthranilate.

In conclusion, beside the sugar-acid balance, the assessment of substances with positive (linalool, lactones) and negative impacts (e. g. branched esters, furanones) on the sensory quality is of particular importance for the breeding of preferred strawberries.

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Associated content

Supporting Information

The supporting material contains a detailed list of semi-quantified VOCs, a complete correlation matrix and the sensory form used in the consumer test.

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Address of the authors:

Detlef Ulrich, Julius Kühn-Institute (JKI), Federal Research Centre for Cultivated Plants, Institute for Ecological Chemistry, Plant Analysis and Stored Product Protection, Erwin-Baur-Straße 27, 06484 Quedlinburg, Germany

E-mail: detlef.ulrich@julius-kuehn.de

Klaus Olbricht, Hansabred GmbH & Co. KG, Radeburger Landstraße 12, 01108 Dresden, Germany / Humboldt-Universität zu Berlin, Albrecht Daniel Thaer-Institute of Agricultural and Horticultural Sciences, Department of Horticultural Plant Systems, Lentzeallee 75, 10115 Berlin, Germany

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Table S1: Chemicals

no	*substance*	*abbreviation*	*CAS*	*identification*	*vendor*
1	methyl acetate	MeOAc	79-20-9	MS	
2	ethyl acetate	EtOAc	141-78-6	MS, RI	1
3	1-methylethyl acetate	1-MeetOAc	108-21-4	MS	
4	ethanol	EtOH	64-17-5	MS, RI	2
5	2-pentanone	2-Pentanone	107-87-9	MS, RI	3
6	methyl butanoate	MeOBu	623-42-7	MS, RI	2
7	methyl isobutyl ketone	Meisobuketon	108-10-1	MS	
8	methyl 2-methylbutanoate	Me2-meOBu	868-57-5	MS, RI	1
9	methyl 3-methylbutanoate	Me3-meOBu	659-70-1	MS	
10	ethyl butanoate	EtOBu	105-54-4	MS, RI	2
11	1-methylethyl butanoate	1-MeetOBu	638-11-9	MS	
12	methyl thioacetate	MethioOAc	16630-66-3	MS	
13	ethyl 2-methylbutanoate	Et2-meOBu	7452-79-1	MS, RI	1
14	ethyl 3-methylbutanoate	Et3-meOBu	108-64-5	MS	
15	butyl acetate	BuOAc	123-86-2	MS, RI	4
16	hexanal	Hexanal	66-25-1	MS, RI	1
17	methyl pentanoate	MeOPent	624-24-8	MS	
18	3-methyl-1-butyl acetate	3-Me-1-ButylOAc	123-92-2	MS	
19	ethyl pentanoate	EtOPent	539-82-2	MS, RI	1
20	butyl propanoate	BuOProp	590-01-2	MS	
21	pentyl acetate	PentOAc	628-63-7	MS, RI	1
22	2-heptanone	2-Heptanone	110-43-0	MS, RI	5
23	methyl hexanoate	MeOHex	106-70-7	MS, RI	1
24	S-methyl butanthioate	S-Me Butanthioate	23747-45-7	MS	
25	3-methylbutanol	3-Mebutanol+	123-51-3	MS	
26	(E)-2-hexenal	E-2-Hexenal+	6728-26-3	MS, RI	5
27	ethyl hexanoate	EtOHex	123-66-0	MS, RI	1
28	3-methylbutyl butanoate	3-MebutylOBu	106-27-4	MS	
29	hexyl acetate	HexOAc	142-92-7	MS, RI	1
30	(Z)-3-hexenyl acetate	Z-3-HexenylOAc	3681-71-8	MS, RI	1
31	2-heptanol	2-Heptanol	543-49-7	MS, RI	1
32	(E)-2-hexenyl acetate	E-2-HexenylOAc	2497-18-9	MS, RI	1
33	1-hexanol	1-Hexanol	111-27-3	MS, RI	1
34	nonanal	Nonanal	124-19-6	MS, RI	4
35	(E)-2-hexenol	E-2-Hexenol	928-95-0	MS, RI	1
36	ethyl methylthioacetate	EtmethioOAc	4455-13-4	MS, RI	4
37	acetic acid	HOOAc	64-19-7	MS, RI	1
38	furfural	Furfural	98-01-1	MS, RI	1
39	(Z)-linalool oxide	Z-Linalooloxid	5989-33-3	MS, RI	2
40	u2S	u2S	u2S		
41	benzaldehyde	Benzaldehyd	100-52-7	MS, RI	1
42	linalool	Linalool	78-70-6	MS, RI	1

43	mesifurane	Methoxyfuraneol	4077-47-8	MS, RI	1
44	u5	u5	u5		
45	acetophenone	Acetophenon	98-86-2	MS	
46	3-furanmethanol	3-Furanmethanol	4412-91-3	MS	
47	2-methylbutanoic acid	2-MeBuOOAc	116-53-0	MS, RI	1
48	u6	u6	u6		
49	u7	u7	u7		
50	α-terpineol	a-Terpineol	98-55-5	MS, RI	2
51	2-methylpropyl butanoate	Et2-meOProp	539-90-2	MS	
52	phenylmethyl acetate	PhenmeOAc	140-11-4	MS	
53	u8	u8	u8	MS	
54	methyl salicilate	MeOSal	119-36-8	MS	
55	hexanoic acid	HexOOAc	142-62-1	MS, RI	1
56	u13	u13	u13		
57	γ-octalactone	g-Octalacton	104-50-7	MS, RI	1
58	metykeugenol	Methyleugenol	93-15-12	MS	
59	γ-nonalactone	g-Nonalacton	104-61-0	MS	
60	furaneol	Furaneol+	3658-77-3	MS, RI	1
61	octyl acetate	OctOAc	124-07-2	MS	
62	u15	u15	u15		
63	α-bisabolol oxideB	a-BisabololoxidB	26181-88-3	MS	
64	γ-decalactone	g-Decalacton	706-14-9	MS, RI	1
65	u17	u17	u17		
66	eugenol	Eugenol	97-53-0	MS, RI	1
67	nonanoic acid	NonaOOH	112-05-0	MS	
68	u18	u18	u18		
69	u19	u19	u19		
70	δ-decalactone	d-Decalacton	705-86-2	MS, RI	1
71	u20	u20	u20		
72	u21	u21	u21		
73	methyl anthranilate	MA	134-20-5	MS, RI	1
74	decanoic acid	DecaOOH	334-48-5	MS	
75	γ-dodecalactone	g-Dodecalacton	2305-05-7	MS, RI	6
76	α-bisabolol oxideA	a-Bisabolol oxideA	22567-36-8	MS	

u* - unknown peaks; u2S – unknown sulfur compound: Identification: MS – library search and RI from literature, RI – RI from co-elution of authentic substance. Vendors: 1 – Sigma-Aldrich Inc.; 2 – Carl Roth GmbH, Karlsruhe,Germany; 3 – Riedel-de Haen, Seelze, Germany; 4 – Alfa Aeser, Karlsruhe, Germany; 5 – Merck KG, Darmstadt, Germany, 6 – Chemos GmbH, Regenstauf, Germany.

Table S2: Sensory form

Erdbeer – Verkostung

Glas-Nr. 1

Geschlecht: ☐ w ☐ m   Alter: .... Jahre   Beruf: ....

Raucher: ☐ ja ☐ nein   Hobby: ....

Bitte den Deckel abnehmen und die Erdbeerstücke mit dem Löffel essen. Zuerst wird die Beliebtheit bewertet, dann die Eigenschaften. Bitte ankreuzen.

Beliebtheit

0	1	2	3	4	5	6
missfällt mir sehr	missfällt mir ziemlich	missfällt mir etwas	weder noch	gefällt mir etwas	gefällt mir ziemlich	gefällt mir sehr

Eigenschaften

- süß

☐ .... ☐ .... ☐ .... ☐ .... ☐ .... ☐ .... ☐
wenig   mittel   stark

- sauer

☐ .... ☐ .... ☐ .... ☐ .... ☐ .... ☐ .... ☐
wenig   mittel   stark

- aromatisch

☐ .... ☐ .... ☐ .... ☐ .... ☐ .... ☐ .... ☐
wenig   mittel   stark

- anderes Aroma: ....

☐ .... ☐ .... ☐ .... ☐ .... ☐ .... ☐ .... ☐
wenig   mittel   stark

Danke !

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Table S3: Complete data set

sample	year	meOAc	etOAc	1-meetOAc	etOH	2-pentanone	meOBu	meisobuketone	me2-meOBu	me3-meOBu	etOBu	1-meetOBu	methioOAc	et2-meOBu	et3-meOBu	buOAc	hexanal	meOPent	3-me-1-butylOAc	etOPent	buOProp	pentOAc
dar13	2013	7.51	2.09	2.90	5.06	2.18	294.50	0.33	1.87	5.37	44.76	11.79	1.93	0.56	0.74	3.38	2.61	0.00	4.45	0.00	0.00	0.00
els13	2013	9.83	0.67	19.26	4.58	1.41	17.20	0.00	1.50	0.11	0.94	2.05	0.00	0.00	0.00	4.07	4.08	0.00	6.46	0.00	0.00	0.00
evi13	2013	11.87	2.48	3.09	6.53	0.75	65.17	0.27	0.66	11.10	2.43	0.70	0.41	0.00	0.74	5.71	7.48	0.00	11.31	0.00	0.00	0.00
hon13	2013	0.00	0.13	0.79	7.61	15.88	4.25	4.56	0.00	1.57	1.22	0.00	0.00	0.36	0.57	12.96	4.31	0.00	4.25	0.00	0.00	0.72
rum13	2013	0.00	0.00	0.00	5.98	2.32	1.35	1.45	0.27	0.71	0.13	0.00	0.12	0.14	0.34	4.12	4.11	0.00	3.55	0.00	0.00	0.54
eli14	2014	0.72	2.56	0.48	5.32	1.69	122.59	0.44	0.29	0.00	129.58	0.00	0.00	0.00	0.00	7.20	4.03	0.74	4.75	0.00	0.00	0.00
ms14	2014	1.52	3.83	2.26	3.39	5.05	102.49	1.61	0.42	1.71	22.49	4.89	0.00	0.00	1.13	4.43	2.96	0.00	9.85	0.00	0.00	0.00
p32614	2014	0.24	3.20	0.51	4.06	1.70	45.99	0.83	2.30	0.35	20.84	4.97	0.00	0.00	0.00	0.83	5.07	0.00	10.88	0.00	0.00	0.00
p56514	2014	1.58	3.81	0.00	4.60	3.80	297.00	0.40	0.91	1.71	123.93	0.00	0.00	0.00	0.00	3.63	3.63	1.64	8.62	0.00	0.00	0.00
p71314	2014	0.86	11.00	1.21	12.30	5.01	152.11	3.04	1.17	9.90	242.35	0.00	1.55	2.29	13.88	80.50	3.28	0.00	23.12	1.04	1.98	1.69
p72514	2014	0.82	3.45	0.00	16.04	2.23	146.89	0.39	0.97	1.53	39.63	0.00	0.00	0.00	0.00	8.31	6.15	1.08	21.63	0.00	0.00	0.00
son14	2014	1.64	4.00	1.85	8.17	4.51	295.38	1.11	1.27	2.29	206.58	0.00	0.00	0.00	1.64	6.63	5.45	3.90	5.91	1.78	0.00	0.00
p56515	2015	28.22	0.61	1.14	3.86	6.58	498.65	0.54	2.71	3.63	64.37	32.17	0.00	0.00	0.00	13.98	2.76	2.22	10.55	0.00	0.00	0.00
p62215	2015	30.64	2.63	6.19	4.62	2.61	222.75	0.61	3.17	3.56	48.96	17.11	0.00	0.00	0.45	19.00	4.29	0.88	11.17	0.49	1.53	0.00
p70915	2015	28.04	0.61	0.68	6.20	2.71	249.15	0.84	1.08	3.71	19.20	0.00	0.00	0.00	0.00	5.98	3.00	1.45	5.19	0.00	0.00	0.00
p72515	2015	27.22	1.63	3.06	4.34	1.95	204.29	0.00	1.96	2.63	23.69	1.66	0.41	0.00	0.00	5.24	3.69	0.49	8.86	0.00	0.00	0.00
cle15	2015	47.33	2.00	2.82	13.35	3.09	335.03	0.36	1.69	3.04	12.07	2.02	0.00	0.00	0.00	7.55	4.33	1.09	9.33	0.00	0.00	0.00
ele15	2015	29.66	0.00	0.00	13.56	11.31	2.43	1.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	4.71	5.18	0.00	2.89	0.00	0.00	0.00
hon15	2015	29.75	0.00	0.00	12.60	6.08	3.12	0.70	0.00	0.00	1.46	0.00	0.00	0.00	0.00	4.35	5.09	0.00	3.76	0.00	0.00	0.00

sample	year	2-heptanone	meOHex	S-meButanthioate	3-mebutanol	E-2-hexenal	etOHex	3-mebutylOBu	hexOAc	Z-3-hexenylOAc	2-heptanol	E-2-hexenylOAc	1-hexanol	nonanal	E-2-hexenol	etmethioOAc	HOOAc	furfural	Z-linalooloxide	u2S
dar13	2013	2.11	56.19	1.83	0.00	84.95	6.59	0.37	3.45	1.26	0.00	10.58	3.00	2.18	6.68	0.00	2.70	0.86	7.73	0.00
els13	2013	1.19	28.66	0.00	0.00	131.99	1.97	0.00	4.93	1.21	0.00	14.82	8.32	1.96	15.22	0.00	2.71	0.72	5.29	0.00
evi13	2013	0.00	12.03	0.00	0.00	189.69	0.14	0.00	3.04	0.91	0.00	6.10	3.22	2.02	4.50	0.00	2.98	0.34	5.69	0.00
hon13	2013	11.69	2.32	0.00	0.00	96.11	0.61	0.35	6.72	0.00	0.00	11.24	9.59	1.52	12.92	0.00	2.77	0.52	5.90	0.00
rum13	2013	1.02	0.50	0.00	0.00	92.12	0.00	0.00	8.08	1.47	0.00	18.91	14.94	1.22	16.08	0.00	1.88	0.84	18.40	0.00
eli14	2014	4.30	60.67	0.00	0.00	99.46	35.16	0.00	6.98	2.09	0.00	13.05	1.18	1.89	0.00	0.00	1.48	0.38	9.68	0.39
ms14	2014	8.87	73.19	0.00	1.74	120.33	19.84	0.00	11.03	3.07	1.28	30.41	2.16	1.57	3.10	0.00	1.73	1.11	0.00	0.00
p32614	2014	3.61	14.19	0.00	3.09	104.91	11.62	0.00	7.98	1.37	0.00	11.35	2.47	1.72	2.85	0.00	1.29	0.37	1.80	0.34
p56514	2014	4.86	53.43	1.72	1.47	103.45	22.11	0.00	3.75	0.36	0.00	5.32	0.75	1.41	1.54	0.00	1.61	1.06	2.77	0.00
p71314	2014	5.26	26.99	5.00	5.72	113.06	38.08	1.55	18.02	1.47	1.64	7.44	2.16	2.16	1.99	2.06	1.99	0.74	4.06	2.58
p72514	2014	3.39	27.96	2.08	3.82	76.66	17.90	0.00	9.44	1.29	0.00	8.24	2.35	5.58	1.20	0.00	1.39	0.81	19.28	1.14
son14	2014	12.82	113.40	0.00	1.49	102.25	74.73	0.00	5.14	1.27	1.77	2.91	2.06	1.07	0.36	0.00	1.45	0.00	3.57	0.39
p56515	2015	4.50	44.75	3.71	0.00	82.39	5.34	0.78	4.12	0.00	0.00	10.49	1.79	4.53	3.16	1.14	2.27	1.48	2.97	1.15
p62215	2015	2.30	26.67	0.00	0.00	120.19	5.00	0.00	14.10	4.26	1.32	53.56	3.17	3.31	4.22	0.81	2.63	3.40	11.96	1.59
p70915	2015	1.94	21.56	0.00	0.00	77.40	1.57	0.00	2.91	0.00	0.00	9.38	3.71	3.16	5.54	0.46	2.56	2.34	3.61	1.21
p72515	2015	1.53	25.14	1.49	0.00	104.71	2.37	0.00	8.06	2.06	0.00	25.62	6.49	2.89	6.91	0.44	2.24	4.36	23.91	1.11
cle15	2015	7.72	74.95	0.00	0.00	96.07	2.83	0.00	3.82	0.00	2.89	6.56	2.75	3.05	4.48	0.37	3.46	1.79	0.00	2.15
ele15	2015	3.20	0.00	0.00	0.00	122.56	0.00	0.00	3.03	0.00	0.34	8.88	3.73	3.64	5.82	0.00	2.11	1.21	0.00	1.29
hon15	2015	2.62	0.00	1.14	0.00	143.73	0.00	0.00	4.26	0.00	0.00	13.70	7.24	2.60	11.17	0.00	2.05	1.04	5.58	0.93

sample	year	benzaldehyde	linalool	DMMF	u5	acetophenone	3-furanmethanol	HOO2-meBu	u6	u7	a-terpineol	et2-meOProp	phenmeOAc	u8	meOSal	HOOHex	u13	g-octalactone	methyleugenol	g-nonalacton	DMHF	octOAc	u15
dar13	2013	1.43	29.68	21.51	5.40	2.12	2.20	11.95	1.50	0.00	17.05	7.06	8.34	5.65	4.07	74.36	0.00	1.12	0.00	0.00	1.78	8.64	4.28
els13	2013	2.56	19.17	43.28	0.00	0.82	2.35	26.89	0.00	0.00	7.44	0.00	2.22	0.84	1.74	155.83	0.00	5.51	0.00	1.90	4.56	11.54	4.06
evi13	2013	1.57	41.94	9.47	0.00	1.35	3.29	0.81	0.00	0.00	43.70	0.00	3.90	0.77	4.43	8.81	0.00	0.21	0.00	0.15	1.32	2.56	5.22
hon13	2013	2.73	56.65	43.09	0.00	0.86	3.03	13.98	0.00	0.00	44.96	0.00	4.03	0.97	5.23	157.11	0.00	3.12	0.00	1.64	4.24	26.70	4.77
rum13	2013	1.03	70.37	6.05	0.00	2.83	1.99	4.55	0.00	0.00	39.35	0.00	1.89	0.50	3.57	19.32	0.00	1.05	0.00	0.75	1.98	2.81	3.55
eli14	2014	2.89	72.97	13.15	4.05	5.05	1.99	9.13	0.00	0.00	17.96	5.54	11.37	3.91	2.79	120.60	4.38	3.13	0.00	2.02	4.71	17.21	3.51
ms14	2014	2.34	3.87	0.63	1.44	1.37	1.85	2.41	0.00	0.00	1.38	1.32	7.40	0.00	3.12	57.95	1.58	5.84	0.00	0.86	0.00	12.71	2.95
p32614	2014	2.58	37.53	24.21	0.00	0.91	1.50	8.03	0.00	0.00	16.85	1.45	1.10	0.00	1.68	85.06	0.00	3.89	0.00	0.34	6.18	15.97	3.17
p56514	2014	0.72	15.81	9.75	0.36	1.42	2.05	8.20	0.00	0.00	4.48	3.14	3.71	3.64	2.48	58.11	1.10	2.54	0.00	0.36	1.76	13.57	3.73
p71314	2014	5.08	50.14	192.22	6.68	6.39	2.81	0.00	13.20	1.53	10.61	7.28	23.73	8.62	8.12	37.92	1.33	3.69	5.43	0.10	6.33	5.67	2.85
p72514	2014	7.39	144.93	15.87	0.92	3.27	1.95	5.28	0.00	0.00	39.20	6.43	7.83	1.76	2.04	33.18	1.58	3.21	0.00	1.53	6.56	11.81	3.06
son14	2014	3.57	53.24	52.54	8.40	7.65	1.92	32.64	0.00	2.26	15.87	18.99	1.37	8.26	2.23	208.46	23.02	5.46	0.00	2.18	5.86	40.19	3.34
p56515	2015	3.04	11.10	42.61	4.33	13.91	3.30	19.31	9.56	0.00	3.83	9.35	5.55	12.22	5.75	87.39	0.42	1.27	0.00	0.00	4.54	9.79	4.74
p62215	2015	6.09	107.38	18.61	11.35	9.23	3.63	7.05	0.00	0.00	28.67	9.12	9.77	7.25	5.16	46.58	1.51	4.28	0.68	2.33	1.67	5.35	9.26
p70915	2015	3.04	43.76	48.52	0.00	8.39	4.19	13.14	0.00	0.00	12.46	5.33	3.06	1.81	4.83	55.53	0.00	1.89	0.00	0.00	5.13	7.18	5.54
p72515	2015	7.47	109.70	29.03	0.00	3.36	3.78	10.13	0.00	0.00	42.02	5.87	10.46	0.97	4.27	24.77	0.36	2.81	1.52	1.26	3.60	4.82	8.47
cle15	2015	2.36	20.38	0.00	1.43	11.84	4.56	4.50	0.00	0.00	6.91	3.76	6.40	1.03	5.35	48.08	1.58	1.52	0.00	0.00	1.77	4.58	5.60
ele15	2015	4.74	24.14	12.84	0.00	5.09	4.72	17.22	0.00	0.00	9.83	0.00	0.46	0.00	5.79	146.26	0.00	1.41	0.00	1.50	1.73	13.66	7.15
hon15	2015	3.47	27.27	6.14	0.00	9.09	3.91	4.71	0.00	0.00	17.17	0.00	1.63	0.46	4.95	82.97	0.00	1.72	0.00	0.35	1.29	6.48	5.17

sample	year	a-bisabololoxideB	g-gecalactone	u17	eugenol	HOONona	u18	u19	d-decalactone	u20	u21	MA	HOODeca	g-dodecalacton	a-bisabololoxideA	sweet	sour	aromatic	untypical	SSC	TA	SSC/TA	acceptance
dar13	2013	5.92	7.11	0.00	0.00	2.39	1.04	0.00	0.81	6.75	4.55	0.00	1.81	8.39	13.37	3.35	1.68	2.97	1.05	7.00	0.72	9.68	4.23
els13	2013	2.87	452.36	0.00	0.00	1.11	9.86	1.20	2.69	20.47	4.54	0.00	0.00	6.32	9.00	2.69	2.79	2.45	1.14	9.20	0.89	10.37	3.66
evi13	2013	2.43	116.97	0.00	0.00	1.72	1.30	0.00	0.00	8.98	2.59	0.00	0.00	5.67	5.74	2.45	2.70	2.34	1.26	6.30	0.96	6.57	3.70
hon13	2013	6.39	629.26	0.00	0.00	2.74	33.09	10.65	5.03	12.39	1.93	0.00	0.98	12.72	10.48	2.52	3.03	3.02	1.14	8.20	1.15	7.12	3.73
rum13	2013	7.40	127.29	0.00	0.00	2.43	2.63	0.00	0.00	14.33	2.69	0.00	1.45	7.65	17.31	2.92	2.26	2.74	1.20	8.60	0.89	9.68	3.94
eli14	2014	3.12	479.30	9.30	0.37	2.49	12.15	4.40	4.57	22.49	2.67	0.00	1.88	19.09	3.83	3.02	2.17	3.23	1.42	8.20	0.86	9.60	3.95
ms14	2014	0.00	4.53	0.00	0.00	1.61	0.00	0.00	4.37	4.38	1.50	1.06	8.05	1.57	0.00	3.36	1.78	3.28	1.82	9.30	0.95	9.80	3.82
p32614	2014	8.10	7.94	1.24	1.53	2.65	0.00	0.00	1.73	8.04	2.57	0.00	7.56	9.55	6.51	3.58	1.70	3.24	1.21	8.90	0.82	10.80	4.23
p56514	2014	1.06	9.58	0.00	0.00	3.63	0.00	0.00	1.29	3.76	2.32	0.00	6.03	13.27	1.61	2.90	1.81	2.78	1.33	7.50	0.67	11.30	3.76
p71314	2014	9.22	7.33	36.94	3.58	2.53	0.00	0.00	3.79	14.92	3.38	0.00	1.30	4.54	7.31	3.02	1.47	2.39	2.11	9.60	0.73	13.20	2.78
p72514	2014	7.91	725.49	10.70	1.65	3.94	25.29	10.98	4.30	6.60	4.05	0.00	7.98	24.27	4.69	3.74	2.23	3.84	1.40	10.50	1.02	10.30	4.73
son14	2014	6.07	504.11	3.71	0.98	2.46	10.42	4.05	6.65	3.44	2.45	0.00	0.86	12.37	4.85	3.23	2.37	3.37	1.20	10.70	0.73	14.70	4.22
p56515	2015	0.36	7.26	0.00	0.00	7.37	0.00	0.00	0.00	5.20	3.44	0.00	4.71	11.77	2.17	2.73	1.99	2.86	1.17	6.30	0.65	9.63	3.69
p62215	2015	6.59	979.27	22.49	1.26	7.58	27.00	10.94	4.99	27.35	4.85	0.00	2.41	17.58	14.66	3.58	2.17	3.14	0.75	7.30	0.83	8.84	4.45
p70915	2015	1.69	187.84	0.48	0.41	6.15	2.88	2.54	1.46	20.23	7.85	0.00	5.25	6.71	7.64	3.50	1.94	3.10	0.69	7.10	0.78	9.10	4.32
p72515	2015	6.26	653.69	9.32	0.44	5.91	18.70	7.71	2.38	10.03	4.07	0.00	1.41	17.41	12.93	3.25	2.65	3.32	0.85	7.70	0.99	7.79	4.20
cle15	2015	2.12	8.24	1.96	1.46	2.34	0.00	0.92	1.44	11.28	4.17	0.00	2.00	3.86	8.42	2.87	1.94	2.53	0.87	7.00	0.70	10.00	3.47
ele15	2015	1.35	361.71	0.44	0.00	3.15	9.20	4.44	1.76	4.99	5.95	0.00	2.27	3.83	3.73	2.21	2.39	2.04	0.97	7.30	0.78	9.38	3.31
hon15	2015	3.88	199.31	0.00	0.00	3.39	6.58	3.18	1.58	7.65	4.36	0.00	0.60	5.39	7.17	2.77	3.07	2.87	1.20	6.70	1.02	6.58	4.04

Table S4: Correlation analysis

Compound	CAS	MeOAc 79-20-9	EtOAc 141-78-6	1-MeetOAc 108-21-4	EtOH 64-17-5	2-Pentanone 107-87-9	MeOBu 623-42-7	Meisobuketone 108-10-1	Me2-meOBu 868-57-5	Me3-meOBu 659-70-1	EtOBu 105-54-4	1-MeetOBu 638-11-9	MethioOAc 16630-66-3	Et2-meOBu 7452-79-1	Et3-meOBu 108-64-5	BuOAc 123-86-2	Hexanal 66-25-1	MeOPent 624-24-8
MeOAc	79-20-9	1.00																
EtOAc	141-78-6	-0.39	1.00															
1-MeetOAc	108-21-4	0.07	-0.11	1.00														
EtOH	64-17-5	0.22	0.16	-0.28	1.00													
2-Pentanone	107-87-9	0.03	-0.20	-0.27	0.26	1.00												
MeOBu	623-42-7	0.33	0.15	-0.12	-0.17	-0.20	1.00											
Meisobuketone	108-10-1	-0.37	0.24	-0.27	0.15	0.74*	-0.31	1.00										
Me2-meOBu	868-57-5	0.31	0.14	0.30	-0.36	-0.40	0.62*	-0.38	1.00									
Me3-meOBu	659-70-1	0.01	0.54*	-0.04	0.03	-0.20	0.25	0.11	0.20	1.00								
EtOBu	105-54-4	-0.37	0.79*	-0.18	0.07	-0.08	0.37	0.19	0.10	0.31	1.00							
1-MeetOBu	638-11-9	0.29	-0.13	0.08	-0.39	0.00	0.61*	-0.19	0.70*	0.12	-0.04	1.00						
MethioOAc	16630-66-3	-0.19	0.49*	-0.02	0.02	-0.15	0.14	0.12	0.15	0.62*	0.34	0.07	1.00					
Et2-meOBu	7452-79-1	-0.27	0.76*	-0.08	0.25	0.12	-0.02	0.53*	-0.02	0.57*	0.59*	-0.09	0.73*	1.00				
Et3-meOBu	108-64-5	-0.26	0.85*	-0.07	0.26	0.06	-0.01	0.49*	-0.01	0.59*	0.68*	-0.12	0.60*	0.96*	1.00			
BuOAc	123-86-2	-0.13	0.79*	-0.06	0.28	0.12	0.07	0.49*	0.10	0.57*	0.64*	0.02	0.52*	0.93*	0.96*	1.00		
Hexanal	66-25-1	-0.06	-0.07	-0.05	0.43	-0.06	-0.43	-0.13	-0.26	0.10	-0.16	-0.39	-0.31	-0.28	-0.18	-0.21	1.00	
MeOPent	624-24-8	0.08	0.07	-0.14	-0.03	-0.07	0.70*	-0.20	0.29	-0.05	0.50*	0.23	-0.29	-0.24	-0.12	-0.09	-0.01	1.00
3-Me-1-ButylOAc	123-92-2	-0.18	0.76*	-0.05	0.32	-0.24	0.17	0.07	0.30	0.50*	0.40	0.08	0.26	0.53*	0.60*	0.65*	0.13	0.01
EtOPent	539-82-2	-0.21	0.57*	-0.01	0.14	0.01	0.22	0.24	0.15	0.26	0.78*	-0.07	0.18	0.40	0.54*	0.48*	0.10	0.58*
BuOProp	590-01-2	0.01	0.69*	0.08	0.13	-0.03	0.05	0.32	0.33	0.49*	0.51*	0.14	0.41	0.73*	0.78*	0.86*	-0.16	-0.11
PentOAc	628-63-7	-0.34	0.61*	-0.14	0.25	0.30	-0.20	0.75*	-0.19	0.42	0.47*	-0.19	0.48*	0.91*	0.88*	0.88*	-0.19	-0.27
2-Heptanone	110-43-0	-0.22	0.22	-0.22	0.12	0.54*	0.18	0.57*	-0.17	-0.15	0.39	-0.09	-0.18	0.09	0.14	0.11	-0.08	0.45
MeOHex	106-70-7	-0.09	0.32	0.04	-0.15	-0.24	0.62*	-0.21	0.23	0.01	0.53*	0.12	0.04	-0.08	0.02	-0.06	-0.22	0.67*
S-Me Butanthioate	23747-45-7	-0.07	0.57*	-0.19	0.19	0.02	0.42	0.12	0.24	0.44	0.52*	0.35	0.55*	0.68*	0.65*	0.69*	-0.34	0.07
3-Mebutanol+	123-51-3	-0.49*	0.85*	-0.21	0.33	-0.09	-0.04	0.29	0.04	0.26	0.57*	-0.19	0.30	0.64*	0.71*	0.65*	0.06	0.00
E-2-Hexenal+	6728-26-3	0.07	0.03	0.29	-0.01	-0.08	-0.47*	-0.11	-0.22	0.35	-0.17	-0.20	-0.03	-0.04	0.07	0.01	0.56*	-0.37
EtOHex	123-66-0	-0.47*	0.61*	-0.16	0.06	-0.10	0.25	0.12	-0.03	0.06	0.87*	-0.18	0.08	0.26	0.40	0.30	0.04	0.62*
3-MebutylOBu	106-27-4	-0.14	0.62*	-0.11	0.13	0.24	0.25	0.49*	0.16	0.55*	0.56*	0.30	0.62*	0.89*	0.85*	0.88*	-0.39	-0.06
HexOAc	142-92-7	-0.30	0.69*	0.00	0.05	-0.06	-0.14	0.40	0.20	0.22	0.42	0.03	0.25	0.61*	0.67*	0.72*	-0.16	-0.21
Z-3-HexenylOAc	3681-71-8	-0.22	0.32	0.24	-0.39	-0.41	-0.07	-0.11	0.35	0.04	0.16	0.15	0.08	0.04	0.11	0.12	-0.09	-0.11
2-Heptanol	543-49-7	0.30	0.45	0.03	0.31	-0.01	0.31	0.13	0.21	0.21	0.36	-0.02	0.05	0.26	0.38	0.37	-0.05	0.29
E-2-HexenylOAc	2497-18-9	0.20	-0.09	0.25	-0.38	-0.13	-0.08	-0.07	0.38	-0.12	-0.23	0.34	-0.13	-0.16	-0.13	-0.02	-0.22	-0.22
1-Hexanol	111-27-3	-0.06	-0.49*	0.19	-0.04	0.19	-0.55*	0.29	-0.32	-0.27	-0.48*	-0.24	-0.11	-0.06	-0.15	-0.16	0.02	-0.40
Nonanal	124-19-6	0.49*	-0.14	-0.10	0.45	0.01	0.31	-0.31	0.30	0.00	-0.21	0.39	-0.12	-0.13	-0.14	0.03	0.08	0.11
E-2-Hexenol	928-95-0	0.06	-0.57*	0.40	-0.08	0.22	-0.52*	0.21	-0.26	-0.26	-0.59*	-0.14	-0.05	-0.08	-0.20	-0.20	-0.06	-0.49*
EtmethioOAc	4455-13-4	0.20	0.60*	-0.03	0.09	0.02	0.39	0.25	0.43	0.55*	0.51*	0.38	0.40	0.73*	0.77*	0.87*	-0.39	0.08
HOOAc	64-19-7	0.60*	-0.30	0.39	0.02	0.09	0.14	0.00	0.18	0.39	-0.42	0.17	0.17	0.01	-0.08	0.00	-0.06	-0.22
Furfural	98-01-1	0.63*	-0.17	0.09	-0.17	-0.15	0.30	-0.28	0.48*	0.00	-0.24	0.25	-0.06	-0.16	-0.15	-0.02	-0.32	0.00
Z-Linalooloxid	5989-33-3	-0.11	-0.11	-0.01	-0.02	-0.32	-0.11	-0.18	0.09	-0.07	-0.12	-0.08	0.07	-0.08	-0.12	-0.07	0.10	-0.10
u2S	u2S	0.57*	0.39	-0.15	0.56*	0.03	0.31	0.04	0.31	0.28	0.28	0.12	0.14	0.45	0.50*	0.63*	-0.11	0.10
Benzaldehyde	100-52-7	0.24	0.20	-0.01	0.39	0.03	0.01	-0.04	0.25	-0.01	0.11	0.02	-0.02	0.12	0.18	0.30	0.15	0.07
Linalool	78-70-6	-0.12	0.09	-0.11	0.21	-0.22	-0.10	-0.04	0.14	-0.01	0.06	-0.14	-0.04	-0.01	-0.01	0.09	0.30	0.05
Methoxyfuraneol	4077-47-8	-0.22	0.72*	0.05	0.17	0.12	0.08	0.49*	0.12	0.51*	0.67*	-0.03	0.52*	0.90*	0.92*	0.91*	-0.25	0.03
u5	u5	0.00	0.45	0.06	-0.09	-0.11	0.46*	0.04	0.52*	0.29	0.62*	0.45	0.31	0.32	0.37	0.44	-0.19	0.43
Acetophenone	98-86-2	0.70*	-0.05	-0.17	0.26	0.05	0.60*	-0.15	0.36	0.07	0.19	0.48*	-0.15	0.00	0.06	0.21	-0.18	0.50*
3-Furanmethanol	4412-91-3	0.89*	-0.33	-0.04	0.36	0.30	0.11	-0.06	0.02	0.14	-0.33	0.06	-0.11	-0.07	-0.07	0.05	0.03	-0.06
2-MeBuOOAc	116-53-0	0.00	-0.31	0.40	-0.18	0.20	0.21	-0.09	0.16	-0.35	0.14	0.16	-0.22	-0.28	-0.26	-0.27	-0.07	0.56*
u6	u6	-0.04	0.59*	-0.10	0.10	0.12	0.36	0.30	0.26	0.52*	0.55*	0.42	0.49*	0.77*	0.78*	0.83*	-0.38	0.06
u7	u7	-0.28	0.61*	-0.07	0.20	0.04	0.19	0.28	0.02	0.28	0.81*	-0.17	0.25	0.48*	0.61*	0.51*	0.08	0.54*
a-Terpineole	98-55-5	-0.18	-0.20	-0.14	0.06	0.02	-0.37	0.19	-0.14	0.16	-0.29	-0.23	0.01	-0.08	-0.14	-0.10	0.49*	-0.23
Et2-meOProp	97-62-1	-0.01	0.36	-0.09	-0.02	-0.17	0.68*	-0.11	0.48*	0.18	0.69*	0.32	0.16	0.12	0.21	0.22	-0.13	0.82*
PhenmeOAc	140-11-4	-0.12	0.76*	-0.05	0.11	-0.14	0.20	0.23	0.20	0.52*	0.57*	0.07	0.60*	0.77*	0.77*	0.82*	-0.34	-0.15
u8	u8	0.00	0.40	-0.05	-0.14	-0.01	0.71*	0.03	0.53*	0.36	0.68*	0.66*	0.32	0.37	0.40	0.49*	-0.34	0.58*
MeOSal	119-36-8	0.47*	0.20	-0.24	0.32	0.42	0.15	0.42	0.02	0.52*	0.12	0.21	0.38	0.59*	0.55*	0.66*	-0.23	-0.18
HexOOAc	142-62-1	-0.16	-0.20	0.23	0.00	0.48*	-0.10	0.23	-0.17	-0.45	0.19	-0.06	-0.25	-0.15	-0.14	-0.17	0.03	0.34
u13	u13	-0.22	0.23	-0.06	0.05	-0.03	0.26	0.01	0.02	-0.06	0.60*	-0.13	-0.12	-0.07	0.07	-0.02	0.20	0.77*
g-Octalactone	104-50-7	-0.38	0.37	0.43	-0.20	-0.03	-0.11	0.17	0.15	-0.29	0.34	-0.10	-0.20	0.06	0.18	0.14	-0.12	0.18
Methyleugenol	93-15-12	-0.11	0.79*	-0.03	0.21	-0.01	0.02	0.37	0.12	0.54*	0.60*	-0.09	0.58*	0.91*	0.94*	0.94*	-0.23	-0.17
g-Nonalactone	104-61-0	-0.20	-0.12	0.33	-0.02	0.14	-0.28	0.06	-0.06	-0.44	0.10	-0.15	-0.38	-0.26	-0.20	-0.14	0.24	0.17
Furaneol+	3658-77-3	-0.33	0.34	0.01	0.14	-0.05	0.10	0.17	0.20	-0.01	0.45	-0.06	0.02	0.29	0.32	0.34	0.04	0.33
OctOAc	124-07-2	-0.43	0.04	-0.08	-0.03	0.41	0.02	0.34	-0.17	-0.34	0.39	-0.15	-0.25	-0.13	-0.08	-0.14	0.13	0.54*
u15	u15	0.74*	-0.38	0.13	-0.04	0.09	0.09	-0.23	0.34	0.03	-0.37	0.22	-0.13	-0.27	-0.28	-0.13	0.03	-0.06
a-Bisabololoxid	26181-88-3	-0.38	0.38	-0.09	0.20	-0.10	-0.25	0.32	0.17	0.12	0.26	-0.19	0.38	0.47*	0.41	0.41	0.17	-0.15
g-Decalactone	706-14-9	0.05	-0.18	0.24	0.10	0.11	-0.17	0.02	0.11	-0.26	-0.05	-0.07	-0.31	-0.24	-0.22	-0.08	0.28	0.13
u17	u17	-0.07	0.77*	-0.01	0.24	-0.12	0.07	0.24	0.27	0.43	0.61*	0.01	0.40	0.73*	0.78*	0.86*	-0.09	-0.05
Eugenol	97-53-0	-0.08	0.81*	-0.10	0.43	-0.17	0.11	0.23	0.30	0.38	0.57*	-0.11	0.32	0.68*	0.75*	0.77*	0.05	0.06
NonaOOH	112-05-0	0.50*	-0.18	-0.17	-0.16	0.01	0.53*	-0.19	0.56*	0.01	-0.03	0.59*	-0.18	-0.17	-0.16	0.04	-0.28	0.35
u18	u18	-0.04	-0.20	0.10	0.15	0.35	-0.23	0.28	-0.01	-0.26	-0.13	-0.08	-0.26	-0.15	-0.19	-0.05	0.24	0.00
u19	u19	0.08	-0.17	-0.04	0.26	0.31	-0.14	0.20	0.02	-0.25	-0.11	-0.07	-0.28	-0.18	-0.20	-0.04	0.25	0.08
d-Decalactone	705-86-2	-0.32	0.36	0.08	0.12	0.22	-0.09	0.38	-0.05	-0.18	0.46*	-0.21	-0.15	0.12	0.22	0.23	0.07	0.29
u20	u20	0.14	-0.03	0.42	-0.19	-0.25	-0.16	0.01	0.20	0.02	-0.03	0.00	-0.06	0.10	0.09	0.22	-0.16	-0.20
u21	u21	0.63*	-0.29	0.15	0.26	-0.09	0.12	-0.32	0.18	-0.01	-0.26	0.04	0.05	-0.07	-0.11	-0.03	-0.14	0.00
MA	134-20-5	-0.19	0.14	-0.01	-0.25	0.05	-0.10	0.14	-0.19	-0.08	-0.10	0.02	-0.10	-0.08	0.01	-0.09	-0.26	-0.17
DecaOOH	334-48-5	-0.20	0.14	-0.33	-0.09	-0.11	0.20	-0.10	0.15	-0.24	-0.05	0.17	-0.26	-0.21	-0.17	-0.17	-0.17	0.12
g-Dodecalactone	2305-05-7	-0.20	0.00	-0.12	-0.04	-0.15	0.21	-0.17	0.26	-0.21	0.18	0.12	-0.18	-0.22	-0.24	-0.11	0.14	0.33
a-Bisabololoxide	22567-36-8	0.13	-0.23	0.21	-0.11	-0.15	-0.17	0.07	0.24	0.06	-0.27	-0.01	0.30	0.12	-0.01	0.03	-0.10	-0.31
sweet		-0.18	0.31	-0.10	-0.16	-0.52*	0.27	-0.21	0.47*	-0.05	0.17	0.10	0.10	-0.01	0.01	0.00	-0.20	0.21
sour		0.15	-0.58*	0.26	0.13	0.32	-0.48*	0.06	-0.37	-0.25	-0.44	-0.26	-0.40	-0.39	-0.39	-0.35	0.49*	-0.13
aromatic		-0.29	0.03	-0.23	-0.16	-0.21	0.19	-0.07	0.20	-0.31	0.09	0.06	-0.19	-0.28	-0.26	-0.25	-0.05	0.35
untypical		-0.64*	0.73*	-0.15	0.12	0.03	-0.19	0.38	-0.33	0.25	0.53*	-0.17	0.30	0.60*	0.67*	0.57*	-0.04	-0.17
SSC		-0.65*	0.48*	0.11	0.18	-0.06	-0.23	0.27	-0.13	-0.21	0.44	-0.38	-0.04	0.24	0.33	0.23	0.12	0.19
TA		-0.21	-0.29	0.04	0.11	0.25	-0.68*	0.32	-0.45	-0.18	-0.48*	-0.38	-0.23	-0.17	-0.20	-0.19	0.38	-0.48*
SSC/TA		-0.37	0.62*	0.03	0.08	-0.17	0.33	0.05	0.20	0.01	0.77*	-0.05	0.16	0.37	0.46*	0.37	-0.17	0.54*
acceptance		-0.06	-0.34	-0.07	-0.19	-0.36	0.10	-0.39	0.26	-0.33	-0.26	0.09	-0.25	-0.57*	-0.59*	-0.57*	0.15	0.26

Compound	CAS	3-Me-1-ButylOAc 123-92-2	EtOPent 539-82-2	BuOProp 590-01-2	PentOAc 628-63-7	2-Heptanone 110-43-0	MeOHex 106-70-7	S-Me Butanthioate 23747-45-7	3-Mebutanol+ 123-51-3	E-2-Hexenal+ 6728-26-3	EtOHex 123-66-0	3-MebutylOBu 106-27-4	HexOAc 142-92-7	Z-3-HexenylOAc 3681-71-8	2-Heptanol 543-49-7	E-2-HexenylOAc 2497-18-9	1-Hexanol 111-27-3	Nonanal 124-19-6	E-2-Hexenol 928-95-0	EtmethioOAc 4455-13-4	HOOAc 64-19-7	Furfural 98-01-1	Z-Linalooloxid 5989-33-3	u2S u2S	Benzaldehyde 100-52-7	Linalool 78-70-6	Methoxyfuraneol 4077-47-8	u5 u5	Acetophenone 98-86-2	3-Furanmethanol 4412-91-3	2-MeBuOOAc 116-53-0
3-Me-1-ButylOAc	123-92-2	1.00																													
EtOPent	539-82-2	0.24	1.00																												
BuOProp	590-01-2	0.57*	0.47*	1.00																											
PentOAc	628-63-7	0.43	0.35	0.66*	1.00																										
2-Heptanone	110-43-0	-0.02	0.50*	-0.04	0.18	1.00																									
MeOHex	106-70-7	0.03	0.50*	-0.09	-0.24	0.57*	1.00																								
S-Me Butanthioate	23747-45-7	0.63*	0.19	0.47*	0.53*	-0.07	0.00	1.00																							
3-Mebutanol+	123-51-3	0.82*	0.41	0.49*	0.56*	0.19	0.08	0.55*	1.00																						
E-2-Hexenal+	6728-26-3	-0.02	0.00	0.10	-0.05	-0.26	-0.26	-0.23	-0.13	1.00																					
EtOHex	123-66-0	0.23	0.83*	0.20	0.18	0.58*	0.71*	0.16	0.49*	-0.15	1.00																				
3-MebutylOBu	106-27-4	0.52*	0.33	0.63*	0.80*	0.13	-0.04	0.84*	0.52*	-0.14	0.20	1.00																			
HexOAc	142-92-7	0.66*	0.36	0.81*	0.63*	0.09	-0.05	0.37	0.65*	-0.04	0.27	0.49*	1.00																		
Z-3-HexenylOAc	3681-71-8	0.25	0.21	0.46*	-0.02	-0.09	0.19	-0.12	0.15	0.11	0.21	-0.10	0.68*	1.00																	
2-Heptanol	543-49-7	0.26	0.54*	0.41	0.21	0.53*	0.57*	0.00	0.23	-0.01	0.39	0.17	0.33	0.20	1.00																
E-2-HexenylOAc	2497-18-9	0.00	-0.08	0.40	-0.12	-0.19	-0.12	-0.21	-0.20	0.10	-0.25	-0.19	0.51*	0.81*	0.10	1.00															
1-Hexanol	111-27-3	-0.41	-0.22	-0.16	0.22	-0.19	-0.55*	-0.27	-0.35	0.04	-0.45	-0.15	-0.04	-0.10	-0.29	0.15	1.00														
Nonanal	124-19-6	0.40	-0.25	0.05	-0.22	-0.29	-0.19	0.34	0.06	-0.27	-0.30	0.07	0.00	-0.12	-0.07	0.06	-0.26	1.00													
E-2-Hexenol	928-95-0	-0.48*	-0.34	-0.20	0.12	-0.25	-0.56*	-0.27	-0.46*	0.14	-0.59*	-0.14	-0.18	-0.20	-0.32	0.13	0.93*	-0.23	1.00												
EtmethioOAc	4455-13-4	0.59*	0.36	0.80*	0.65*	-0.02	-0.02	0.74*	0.43	-0.12	0.12	0.84*	0.60*	0.11	0.35	0.12	-0.23	0.26	-0.25	1.00											
HOOAc	64-19-7	-0.18	-0.24	0.06	-0.01	-0.14	-0.14	-0.14	-0.53*	0.23	-0.57*	0.04	-0.27	-0.22	0.23	0.09	0.20	0.09	0.39	0.13	1.00										
Furfural	98-01-1	0.02	-0.18	0.21	-0.19	-0.31	-0.13	0.04	-0.29	-0.14	-0.39	-0.12	0.16	0.31	0.08	0.62*	0.04	0.37	0.03	0.30	0.31	1.00									
Z-Linalooloxid	5989-33-3	0.15	-0.11	0.03	0.01	-0.40	-0.26	0.08	-0.04	-0.20	-0.14	-0.16	0.27	0.38	-0.34	0.34	0.42	0.23	0.22	-0.05	-0.14	0.43	1.00								
u2S	u2S	0.51*	0.25	0.61*	0.36	-0.02	-0.03	0.46*	0.33	-0.16	0.02	0.46*	0.40	-0.03	0.55*	0.07	-0.28	0.55*	-0.30	0.75*	0.20	0.43	-0.03	1.00							
Benzaldehyde	100-52-7	0.48*	0.21	0.38	0.08	-0.08	-0.15	0.27	0.30	-0.12	0.07	0.10	0.48*	0.32	0.10	0.34	-0.13	0.62*	-0.23	0.35	-0.15	0.54*	0.51*	0.58*	1.00						
Linalool	78-70-6	0.37	0.11	0.24	0.06	-0.18	-0.18	0.03	0.19	-0.22	0.08	-0.13	0.43	0.44	-0.12	0.33	0.13	0.37	-0.10	0.05	-0.21	0.35	0.84*	0.20	0.72*	1.00					
Methoxyfuraneol	4077-47-8	0.53*	0.56*	0.70*	0.83*	0.15	-0.02	0.66*	0.63*	-0.08	0.38	0.86*	0.56*	-0.02	0.23	-0.19	-0.12	-0.06	-0.14	0.80*	-0.05	-0.09	-0.11	0.49*	0.25	0.02	1.00				
u5	u5	0.24	0.69*	0.65*	0.17	0.24	0.47+	0.25	0.17	-0.12	0.53*	0.36	0.47*	0.54*	0.48*	0.38	-0.38	0.02	-0.42	0.48*	-0.04	0.10	-0.01	0.33	0.25	0.21	0.36	1.00			
Acetophenone	98-86-2	0.04	0.24	0.23	-0.06	0.11	0.23	0.26	-0.16	-0.22	0.06	0.23	-0.04	-0.18	0.45	0.05	-0.25	0.47*	-0.24	0.51*	0.23	0.31	-0.18	0.68*	0.21	-0.07	0.12	0.42	1.00		
3-Furanmethanol	4412-91-3	-0.18	-0.17	0.09	-0.07	-0.17	-0.31	-0.04	-0.43	0.17	-0.49*	0.00	-0.25	-0.35	0.20	0.07	0.04	0.42	0.15	0.25	0.64*	0.55*	-0.13	0.59*	0.27	-0.08	-0.03	-0.10	0.56*	1.00	
2-MeBuOOAc	116-53-0	-0.42	0.37	-0.30	-0.28	0.30	0.33	-0.18	-0.29	-0.21	0.31	-0.13	-0.41	-0.21	-0.06	-0.21	0.03	-0.06	0.11	-0.19	-0.04	-0.13	-0.17	-0.23	-0.01	-0.17	0.03	0.17	0.11	-0.05	1.00
u6	u6	0.55*	0.31	0.59*	0.67*	0.04	0.01	0.87*	0.50*	-0.13	0.20	0.96*	0.44	-0.09	0.18	-0.17	-0.23	0.19	-0.22	0.89*	-0.02	-0.06	-0.17	0.52*	0.13	-0.16	0.80*	0.36	0.38	0.02	-0.09
u7	u7	0.25	0.97*	0.38	0.43	0.53*	0.49*	0.27	0.48*	-0.02	0.85*	0.41	0.30	0.06	0.50*	-0.28	-0.21	-0.29	-0.33	0.35	-0.29	-0.29	-0.16	0.23	0.14	0.02	0.63*	0.54*	0.18	-0.21	0.36
a-Terpineole	98-55-5	0.06	-0.10	-0.04	0.11	-0.19	-0.46*	-0.18	-0.12	0.13	-0.24	-0.19	0.12	0.16	-0.33	0.16	0.49*	0.04	0.30	-0.20	0.10	0.14	0.73*	-0.18	0.30	0.72*	-0.14	-0.14	-0.34	-0.01	-0.23
Et2-meOProp	97-62-1	0.22	0.77*	0.26	-0.02	0.38	0.68*	0.29	0.20	-0.38	0.72*	0.22	0.17	0.23	0.39	0.00	-0.46	0.13	-0.56*	0.34	-0.22	0.10	0.08	0.27	0.32	0.27	0.31	0.77*	0.47*	-0.14	0.44
PhenmeOAc	140-11-4	0.65*	0.26	0.74*	0.63*	0.00	0.13	0.65*	0.53*	-0.11	0.27	0.71*	0.74*	0.41	0.32	0.18	-0.30	0.11	-0.36	0.75*	0.00	0.21	0.21	0.55*	0.40	0.30	0.67*	0.47*	0.11	-0.04	-0.43
u8	u8	0.29	0.56*	0.48*	0.23	0.20	0.42	0.62*	0.19	-0.28	0.47*	0.62*	0.25	0.12	0.23	0.02	-0.41	0.17	-0.43	0.65*	-0.07	0.02	-0.09	0.32	0.12	0.00	0.50*	0.79*	0.55*	-0.09	0.29
MeOSal	119-36-8	0.17	0.10	0.56*	0.57+	-0.01	-0.29	0.47*	0.02	0.08	-0.23	0.66*	0.25	-0.20	0.30	0.05	0.01	0.24	0.04	0.72*	0.47*	0.29	-0.16	0.68*	0.20	-0.11	0.51*	0.23	0.51*	0.68*	-0.29
HexOOAc	142-62-1	-0.46+	0.37	-0.24	-0.11	0.55*	0.28	-0.28	-0.17	-0.08	0.41	-0.09	-0.29	-0.22	0.03	-0.26	-0.01	-0.25	0.07	-0.28	-0.15	-0.41	-0.40	-0.26	-0.10	-0.27	0.05	0.14	0.00	-0.11	0.83*
u13	u13	-0.07	0.84*	-0.04	-0.09	0.61*	0.71*	-0.14	0.12	-0.09	0.86*	-0.10	-0.02	0.11	0.42	-0.20	-0.24	-0.28	-0.38	-0.10	-0.34	-0.28	-0.10	-0.07	0.06	0.08	0.12	0.50*	0.19	-0.28	0.56*
g-Octalactone	104-50-7	0.20	0.46*	0.24	0.06	0.46*	0.41	-0.13	0.38	-0.04	0.53*	-0.03	0.49*	0.54*	0.30	0.33	-0.15	-0.26	-0.16	0.02	-0.38	-0.06	-0.09	-0.09	0.24	0.09	0.23	0.32	-0.21	-0.47*	0.32
Methyleugenol	93-15-12	0.62*	0.44	0.81*	0.83*	-0.01	-0.09	0.68*	0.64*	0.04	0.26	0.80*	0.72*	0.19	0.31	0.03	-0.11	-0.03	-0.17	0.83*	-0.04	0.14	0.09	0.61*	0.39	0.16	0.89*	0.33	0.09	0.06	-0.30
g-Nonalactone	104-61-0	-0.14	0.30	0.07	-0.15	0.24	0.12	-0.40	-0.12	0.02	0.31	-0.34	0.22	0.48*	0.02	0.40	0.13	-0.04	0.04	-0.26	-0.24	0.05	0.32	-0.15	0.42	0.49*	-0.12	0.31	-0.16	-0.17	0.45
Furaneol+	3658-77-3	0.42	0.38	0.15	0.30	0.16	0.05	0.32	0.53*	-0.43	0.44	0.35	0.23	-0.12	-0.09	-0.36	-0.15	0.19	-0.25	0.30	-0.37	-0.20	0.13	0.22	0.36	0.36	0.57*	0.13	0.05	-0.29	0.34
OctOAc	124-07-2	-0.22	0.54*	-0.23	-0.06	0.77+	0.47*	-0.23	0.10	-0.21	0.68*	-0.10	-0.12	-0.09	0.10	-0.29	-0.16	-0.33	-0.22	-0.31	-0.40	-0.46*	-0.26	-0.33	-0.05	-0.04	0.05	0.21	-0.12	-0.38	0.66*
u15	u15	-0.23	-0.15	0.17	-0.28	-0.31	-0.29	-0.20	-0.54*	0.18	-0.48*	-0.24	-0.06	0.17	0.04	0.55*	0.09	0.33	0.14	0.11	0.50*	0.82*	0.25	0.34	0.45	0.26	-0.23	0.14	0.31	0.75*	0.02
a-Bisabololoxid	26181-88-3	0.39	0.38	0.45	0.51*	-0.01	-0.22	0.22	0.5*	-0.19	0.21	0.28	0.58*	0.30	0.02	0.10	0.27	-0.07	0.09	0.21	-0.24	-0.04	0.53*	0.16	0.40	0.64*	0.42	0.29	-0.21	-0.32	-0.15
g-Decalactone	706-14-9	0.01	0.17	0.16	-0.14	0.04	-0.11	-0.26	-0.15	-0.04	0.05	-0.30	0.24	0.42	-0.07	0.48*	0.15	0.27	0.07	-0.11	-0.02	0.36	0.55*	0.07	0.68*	0.76*	-0.10	0.29	-0.02	0.10	0.26
u17	u17	0.69*	0.48*	0.92*	0.65*	-0.02	-0.01	0.53*	0.61*	-0.02	0.33	0.61*	0.85*	0.48*	0.37	0.30	-0.23	0.16	-0.34	0.77*	-0.11	0.23	0.24	0.66*	0.58*	0.47*	0.72*	0.60*	0.19	0.01	-0.31
Eugenol	97-53-0	0.78*	0.52*	0.73*	0.59*	0.15	0.10	0.47*	0.80*	-0.15	0.41	0.55*	0.71*	0.22	0.54	-0.04	-0.33	0.17	-0.43	0.66*	-0.16	0.01	0.02	0.71*	0.46*	0.33	0.70*	0.42	0.21	-0.06	-0.28
NonaOOH	112-05-0	0.10	-0.04	0.23	-0.18	-0.22	-0.14	0.26	-0.18	-0.34	-0.21	0.07	0.09	0.12	-0.12	0.43	-0.15	0.58*	-0.19	0.42	0.06	0.73*	0.29	0.42	0.48*	0.35	0.01	0.31	0.57*	0.41	0.05
u18	u18	0.03	0.04	0.11	0.00	0.18	-0.22	-0.19	-0.11	-0.12	-0.05	-0.19	0.24	0.26	-0.13	0.38	0.24	0.25	0.16	-0.13	0.03	0.26	0.51*	0.02	0.60*	0.71*	-0.08	0.15	-0.11	0.08	0.16
u19	u19	0.09	0.06	0.14	-0.06	0.15	-0.19	-0.16	-0.06	-0.17	-0.03	-0.21	0.25	0.26	-0.06	0.39	0.11	0.40	0.01	-0.08	-0.01	0.37	0.51*	0.17	0.71*	0.77*	-0.10	0.18	0.02	0.18	0.09
d-Decalactone	705-86-2	0.19	0.59*	0.31	0.16	0.64*	0.40	-0.13	0.31	-0.12	0.64*	0.00	0.49*	0.46*	0.37	0.25	-0.19	-0.12	-0.29	0.03	-0.32	-0.07	0.06	0.08	0.44	0.39	0.24	0.49*	-0.05	-0.27	0.26
u20	u20	-0.03	-0.04	0.45	0.16	-0.31	-0.22	-0.22	-0.20	0.00	-0.17	0.00	0.34	0.41	0.03	0.49*	0.22	-0.02	0.22	0.26	0.29	0.31	0.24	0.22	0.15	0.33	0.17	0.28	0.12	0.15	-0.07
u21	u21	-0.14	-0.15	0.08	-0.20	-0.47*	-0.28	-0.03	-0.25	-0.17	-0.38	-0.09	-0.24	-0.22	-0.07	0.05	-0.01	0.53*	0.12	0.16	0.35	0.47*	0.02	0.46*	0.32	0.08	0.04	-0.02	0.39	0.65*	0.16
MA	134-20-5	0.05	-0.09	-0.08	-0.09	0.31	0.30	-0.15	0.12	0.11	0.09	-0.10	0.25	0.40	0.22	0.34	-0.14	-0.19	-0.13	-0.12	-0.18	-0.03	-0.25	-0.23	-0.13	-0.29	-0.17	-0.06	-0.22	-0.25	-0.23
DecaOOH	334-48-5	0.35	-0.25	-0.15	-0.25	0.08	0.13	0.09	0.42	-0.42	0.04	-0.12	0.13	0.11	-0.09	0.05	-0.43	0.31	-0.47*	-0.07	-0.50*	0.01	-0.11	-0.04	0.06	0.02	-0.19	-0.16	-0.10	-0.34	-0.22
g-Dodecalactone	2305-05-7	0.24	0.04	0.01	-0.19	-0.02	0.07	0.10	0.08	-0.39	0.21	-0.16	0.18	0.30	-0.28	0.19	-0.14	0.36	-0.30	-0.07	-0.36	0.22	0.66*	-0.02	0.51*	0.79*	-0.13	0.25	-0.03	-0.27	0.09
a-Bisabololoxide	22567-36-8	-0.20	-0.03	0.23	0.21	-0.34	-0.36	-0.14	-0.29	-0.11	-0.37	-0.03	0.18	0.24	-0.04	0.40	0.67*	-0.13	0.61*	0.05	0.40	0.38	0.57*	0.04	0.10	0.41	0.02	0.14	-0.06	0.13	-0.08
sweet		0.38	0.17	0.19	-0.14	-0.02	0.29	0.06	0.40	-0.47*	0.26	-0.11	0.42	0.55*	0.10	0.35	-0.29	0.17	-0.39	0.08	-0.37	0.27	0.34	0.11	0.34	0.49*	0.02	0.34	0.00	-0.39	-0.15
sour		-0.41	-0.13	-0.33	-0.19	-0.04	-0.39	-0.38	-0.51*	0.44	-0.29	-0.38	-0.32	-0.20	-0.32	0.04	0.55*	-0.03	0.58*	-0.42	0.24	0.03	0.26	-0.28	0.14	0.17	-0.29	-0.33	-0.11	0.28	0.26
aromatic		0.17	0.10	-0.16	-0.28	0.24	0.31	-0.05	0.20	-0.49*	0.32	-0.27	0.21	0.39	-0.11	0.24	-0.16	0.16	-0.32	-0.21	-0.49*	0.14	0.45	-0.16	0.36	0.57*	-0.20	0.17	-0.06	-0.46*	0.03
untypical		0.54*	0.26	0.32	0.57*	0.26	0.16	0.48*	0.73*	0.14	0.47*	0.54*	0.54*	0.17	0.13	-0.20	-0.21	-0.25	-0.28	0.29	-0.48*	-0.54*	-0.17	-0.02	-0.08	-0.14	0.49*	0.08	-0.27	-0.54*	-0.33
SSC		0.39	0.53*	0.14	0.29	0.42	0.31	0.03	0.65*	-0.24	0.66*	0.07	0.49*	0.32	0.21	-0.08	0.01	-0.17	-0.15	-0.04	-0.59*	-0.36	0.16	-0.07	0.27	0.33	0.33	0.16	-0.34	-0.64*	0.21
TA		-0.05	-0.30	-0.19	0.04	-0.01	-0.49*	-0.31	-0.10	0.28	-0.31	-0.29	0.13	0.12	-0.36	0.22	0.51*	-0.03	0.45	-0.38	0.01	0.01	0.44	-0.31	0.26	0.41	-0.22	-0.42	-0.45	-0.04	-0.23
SSC/TA		0.33	0.72*	0.28	0.26	0.42	0.62*	0.28	0.60*	-0.36	0.80*	0.31	0.28	0.11	0.46*	-0.28	-0.37	-0.18	-0.45	0.27	-0.46	-0.32	-0.23	0.17	0.00	-0.07	0.48*	0.45	0.08	-0.46*	0.36
acceptance		-0.10	-0.09	-0.31	-0.59*	-0.15	0.07	-0.33	-0.17	-0.30	-0.01	-0.59*	-0.11	0.31	-0.31	0.31	0.00	0.23	-0.08	-0.45	-0.25	0.24	0.50*	-0.29	0.25	0.56*	-0.50*	0.08	-0.07	-0.25	0.10

Compound	CAS	u6 u6	u7 u7	a-Terpineole 98-55-5	Et2-meOProp 97-62-1	PhenmeOAc 140-11-4	u8 u8	MeOSal 119-36-8	HexOOAc 142-62-1	u13 u13	g-Octalactone 104-50-7	Methyleugenol 93-15-12	g-Nonalactone 104-61-0	Furaneol+ 3658-77-3	OctOAc 124-07-2	u15 u15	a-Bisabololoxid 26181-88-3	g-Decalacton 706-14-9	u17 u17	Eugenol 97-53-0	NonaOOH 112-05-0	u18 u18	u19 u19	d-Decalactone 705-86-2	u20 u20	u21 u21	MA 134-20-5	DecaOOH 334-48-5	g-Dodecalactone 2305-05-7	a-Bisabolol oxide 22567-36-8	sweet	sour	aromatic	untypical	SSC	TA	SSC/TA	acceptance
u6	u6	1.00																																				
u7	u7	0.38	1.00																																			
a-Terpineole	98-55-5	-0.29	-0.15	1.00																																		
Et2-meOProp	97-62-1	0.28	0.70*	-0.13	1.00																																	
PhenmeOAc	140-11-4	0.65*	0.28	-0.01	0.27	1.00																																
u8	u8	0.70*	0.51*	-0.27	0.77*	0.43	1.00																															
MeOSal	119-36-8	0.62*	0.10	-0.03	-0.01	0.48*	0.32	1.00																														
HexOOAc	142-62-1	-0.13	0.38	-0.27	0.25	-0.37	0.13	-0.23	1.00																													
u13	u13	-0.07	0.82*	-0.10	0.77*	-0.10	0.38	-0.28	0.55*	1.00																												
g-Octalactone	104-50-7	-0.06	0.40	-0.24	0.29	0.15	0.08	-0.40	0.42	0.44	1.00																											
Methyleugenol	93-15-12	0.74+	0.48*	-0.03	0.19	0.84*	0.36	0.59*	-0.26	-0.05	0.15	1.00																										
g-Nonalactone	104-61-0	-0.38	0.18	0.27	0.24	-0.07	-0.01	-0.35	0.53	0.43	0.59*	-0.15	1.00																									
Furaneol+	3658-77-3	0.35	0.44	0.07	0.42	0.23	0.31	-0.14	0.28	0.30	0.31	0.31	0.17	1.00																								
OctOAc	124-07-2	-0.17	0.56*	-0.08	0.45	-0.27	0.18	-0.38	0.83*	0.76*	0.51*	-0.23	0.51*	0.39	1.00																							
u15	u15	-0.22	-0.30	0.26	0.00	-0.04	-0.04	0.38	-0.15	-0.22	-0.23	-0.04	0.21	-0.35	-0.33	1.00																						
a-Bisabololoxid	26181-88-3	0.15	0.35	0.55*	0.22	0.36	0.09	0.01	-0.10	0.13	0.17	0.46*	0.20	0.49*	0.08	-0.10	1.00																					
g-Decalactone	706-14-9	-0.34	0.02	0.53*	0.25	0.04	0.00	-0.14	0.24	0.21	0.35	-0.07	0.86*	0.21	0.25	0.49*	0.34	1.00																				
u17	u17	0.58*	0.43	0.07	0.36	0.87*	0.45	0.46*	-0.26	0.05	0.28	0.86*	0.17	0.35	-0.17	0.10	0.55*	0.28	1.00																			
Eugenol	97-53-0	0.53*	0.52*	-0.05	0.36	0.68*	0.31	0.30	-0.21	0.15	0.27	0.76*	-0.06	0.54*	-0.05	-0.16	0.60*	0.03	0.82*	1.00																		
NonaOOH	112-05-0	0.19	-0.17	0.07	0.37	0.10	0.44	0.31	-0.24	-0.13	-0.16	0.04	0.01	0.10	-0.22	0.61*	-0.04	0.34	0.22	0.02	1.00																	
u18	u18	-0.30	-0.07	0.61*	0.10	0.04	-0.07	-0.05	0.23	0.07	0.27	-0.07	0.75*	0.21	0.29	0.39	0.38	0.93*	0.22	0.01	0.28	1.00																
u19	u19	-0.30	-0.07	0.57*	0.18	0.07	-0.05	0.00	0.14	0.09	0.21	-0.06	0.68*	0.21	0.24	0.47*	0.36	0.92*	0.27	0.09	0.40	0.97*	1.00															
d-Decalactone	705-86-2	-0.09	0.51*	0.07	0.47*	0.28	0.17	-0.16	0.48*	0.59*	0.78*	0.18	0.75*	0.35	0.66*	-0.08	0.32	0.63*	0.42	0.35	-0.06	0.61*	0.60*	1.00														
u20	u20	-0.03	-0.16	0.15	-0.04	0.29	0.04	0.13	-0.08	-0.20	0.16	0.18	0.34	0.14	-0.27	0.31	0.18	0.44	0.42	0.17	0.23	0.32	0.28	0.20	1.00													
u21	u21	-0.05	-0.19	-0.15	0.03	-0.08	-0.04	0.29	-0.06	-0.24	-0.28	-0.01	-0.10	0.06	-0.36	0.51*	-0.13	0.16	0.04	0.01	0.44	0.03	0.14	-0.23	0.34	1.00												
MA	134-20-5	-0.09	-0.08	-0.30	-0.16	0.06	-0.21	-0.14	-0.09	-0.02	0.44	-0.08	-0.02	-0.40	0.03	-0.24	-0.36	-0.23	-0.13	-0.16	-0.23	-0.20	-0.19	0.22	-0.24	-0.34	1.00											
DecaOOH	334-48-5	-0.04	-0.25	-0.28	-0.01	-0.06	-0.07	-0.35	-0.25	-0.15	0.21	-0.19	-0.20	0.14	0.02	-0.31	-0.14	-0.20	-0.10	0.11	0.21	-0.14	-0.04	0.02	-0.30	-0.07	0.45	1.00										
g-Dodecalactone	2305-05-7	-0.15	-0.05	0.46*	0.40	0.16	0.24	-0.34	-0.01	0.18	0.14	-0.10	0.52*	0.42	0.22	0.13	0.37	0.69*	0.24	0.10	0.44	0.67*	0.70*	0.40	0.18	-0.09	-0.34	0.19	1.00									
a-Bisabololoxide	22567-36-8	-0.14	-0.12	0.55*	-0.05	0.07	-0.09	0.16	-0.24	-0.20	-0.19	0.12	0.10	-0.09	-0.33	0.41	0.58*	0.31	0.17	0.03	0.14	0.31	0.25	-0.12	0.48*	0.22	-0.39	-0.49*	0.09	1.00								
sweet		-0.09	0.09	0.03	0.44	0.25	0.13	-0.35	-0.30	0.16	0.40	0.06	[illegible]	0.32	0.00	-0.10	0.41	0.19	0.30	0.40	0.30	0.11	0.22	0.32	0.16	0.10	0.18	0.57*	0.43	0.14	1.00							
sour		-0.43	-0.15	0.52*	-0.29	-0.43	-0.38	-0.08	0.31	0.02	-0.07	-0.32	0.43	-0.13	0.14	0.33	-0.03	0.51*	-0.32	-0.47*	-0.07	0.54*	0.45	0.09	0.07	0.00	-0.23	-0.55*	0.11	0.20	-0.48*	1.00						
aromatic		-0.26	0.04	0.26	0.43	0.04	0.07	-0.51*	-0.02	0.31	0.40	-0.21	0.31	0.36	0.33	-0.15	0.32	0.41	0.04	0.08	0.28	0.42	0.48*	0.49*	-0.03	-0.17	0.20	0.51*	0.69*	-0.02	0.79*	-0.07	1.00					
untypical		0.51*	0.37	-0.20	-0.03	0.52*	0.15	0.04	-0.08	0.07	0.33	0.52*	-0.12	0.16	0.09	-0.72*	0.15	-0.35	0.39	0.40	-0.48*	-0.27	-0.31	0.24	-0.24	-0.59*	0.44	0.20	-0.16	-0.45	-0.01	-0.33	-0.01	1.00				
SSC		0.02	0.57*	0.03	0.31	0.17	0.00	-0.44	0.29	0.51*	0.74*	0.24	0.47*	0.55*	0.53*	-0.56*	0.50*	0.25	0.30	0.46*	-0.38	0.23	0.19	0.67*	-0.06	-0.34	0.22	0.23	0.24	-0.12	0.40	-0.13	0.44	0.51*	1.00			
TA		-0.40	-0.30	0.69*	-0.46*	-0.11	-0.58*	-0.14	-0.04	-0.23	0.11	-0.14	0.34	-0.05	0.02	0.08	0.25	0.47*	-0.11	-0.22	-0.17	0.62*	0.54*	0.25	0.09	-0.21	0.17	-0.11	0.20	0.20	-0.06	0.70*	0.29	0.04	0.15	1.00		
SSC/TA		0.34	0.75*	-0.47*	0.62*	0.23	0.47*	-0.19	0.31	0.64*	0.50*	0.33	0.11	0.48*	0.47*	-0.50*	0.23	-0.16	0.33	0.54*	-0.19	-0.27	-0.26	0.37	-0.15	-0.16	0.01	0.19	0.02	-0.25	0.30	-0.58*	0.10	0.39	0.67*	-0.62*	1.00	
acceptance		-0.56*	-0.21	0.37	0.27	-0.32	-0.10	-0.58*	-0.08	0.17	0.12	-0.52*	0.28	0.12	0.13	0.14	0.23	0.47*	-0.21	-0.20	0.36	0.40	0.47*	0.18	0.07	0.15	-0.05	0.34	0.61*	0.22	0.70*	0.12	0.81*	-0.45	0.12	0.27	-0.15	1.00

Abbreviations of compounds refer to Table S1