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1 Flavor compounds in blackcurrant berries: multivariate analysis of

2 datasets obtained with natural variability and various experimental

3 parameters

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11 Abstract

Berries of blackcurrant are source of vitamin C, flavonoids, beta-carotene, lutein and phenolic acid, with deep inky blue color and strong flavor. Within the works reported on blackcurrant berries, some studies suggested that a given cultivar of blackcurrant could yield berries with a specific profile in volatile compounds. However, in these studies, berries of various cultivars were obtained from different growing areas throughout the world. Moreover, methods used to study flavor compounds were different, and only few authors attempted to compare their results to other ones already published.

The present review aims to highlight the most important parameters influencing the reported results concerning aroma compounds in blackcurrant berries. We conducted a complete bibliometric and metaanalysis. We collected data from published studies, taking into account parameters linked with natural variability and experimental parameters. We obtained a pool of 351 identified volatile compounds, among which about twenty molecules we considered as representative of the general volatile profile of blackcurrant berries.

Collected data were analyzed first using Multiple Factor Analysis and Hierarchical Clustering on Principal Components, and then using Nonmetric MultiDimensional Scaling. We obtained mainly four consolidated clusters characterized by their richness/poorness in given volatile compounds. None of these clusters was linked with specific cultivars. Therefore, further research still has to be done to establish clearly the typicality of given cultivars that are empirically known to give specific organoleptic properties to manufactured products. Nevertheless, this study allowed identifying the important molecules to target with appropriate method and the experimental conditions to control.

- 31
- 32 Keywords: blackcurrant berries, aroma compounds, GC-MS, meta-analysis, multivariate statistical analyses
- 33

34 1. Introduction

Blackcurrant berries (*Ribes nigrum L.*) are cultivated in different countries for diverse uses. The biggest
producing country of blackcurrant is Poland (Cortez and Gonzalez de Mejia, 2019), where berries are usually
used for juices and jam.

Blackcurrant berries and buds are also commonly used for the production of alcoholic beverages (wine,
liqueur and spirits) or for the production of essential oil, especially to make perfumes and food flavoring.
This last commercial sector represents a small volume of production, but an important economical part.
(Gerbaka, 2013)

42 The variety of blackcurrant is chosen according to its use. For juices and jams, variety must yield large and43 juicy berries, unlike variety used for liquors, which must have a powerful flavor.

44 Several works have been reported on aroma compounds of blackcurrant berries since many years 45 ((Andersson and von Sydow, 1964) (Marsol-Vall et al., 2019)). Studied berries were from different growing 46 areas in different parts of the world and from different cultivars ((Andersson and von Sydow, 1966b), (Jung, 47 2018)). Nevertheless, some studies suggested that a given cultivar of blackcurrant could yield berries with 48 typical flavor ((Anjou and von Sydow, 1966), (Jung, 2018)).

However, as methods used to study flavor compounds were very different, authors did not succeed to compare their results to other ones already published. Besides, it was hard to find studies dealing with the impact of the geographic growing area on the aroma profile of berries. Finally, none of the published studies clearly highlighted which parameter affected the most the flavor profile of blackcurrant berries.

53 In-depth analysis of published data could permit defining a pool of molecules characteristic of the odor of 54 blackcurrant berries and selecting molecules that would be more specific of a variety or of a geographic zone 55 for example. Such results could be useful to prove adulteration or to confirm origin of commercial products.

It is thus essential to perform a bibliometric analysis and a meta-analysis using statistical methods to combine data from multiple experiments, as an objective and quantitative approach for summarizing results of published studies. 59 Therefore, the present review aimed to highlight the parameters that influenced the more the aroma 60 compounds recovered from blackcurrant berries. In order to proceed to this study, we compared several 61 publications, based on:

62 - Natural variability: blackcurrant variety, geography and year of growth.

Experimental parameters: storage temperature of berries, extraction method for aroma compounds,
berries process (juice, whole fruit...).

65

66 2. Material and methods

67 The methodology we followed to conduct the present meta-analysis was summed up by the flowchart on
68 figure 1. Data collection comprised extensive search and data recovery steps. In some cases, it was possible
69 to complete missing information directly from the authors.

70 **2.1. Data collection**

We carried out the literature search in the Google scholar and Web of Science databases using the following search criteria: (blackcurrant) and (volatile compounds). The search included the period from 1950 to March 2020. We retained only studies published in English or in French, and studies retained in our search had to meet these two criteria: (1) the study concerned berries, and (2) the study reported qualitative and quantitative data in either the text, figures, tables, or appendices. All these studied reported instrumental analysis of volatile compounds. Some of them reported also olfactometry data such as (Jung, 2018), or sensory results such as (Varming et al., 2004a).

As many papers were focused on blackcurrant buds or healthy compounds extract from berries and not on berries, only 22 papers were found eligible and their references were reported in table 1 in a chronological order. Studies ranged from 1964 to 2019. The reference Varming et al. (2004) was reported several times in table 1 because the authors reported different extraction methods for volatile compounds.

82 For each study case, we compiled the following information:

• cultivar of blackcurrant (for example, Ben Lemond),

- place and year of growth as indicated in the study or deduced from the country of the authors and the
 year of publication,
- degree of maturity of the berries if indicated in the paper,
- storage temperature of berries before analysis (for example, frozen),
- process undergone by fruits before the extraction of volatile compounds (for example, whole fruit of
 juice),
- extraction method for volatile compounds (for example, solvent extraction or Solid phase micro
 extraction (SPME)), extraction parameters such as temperature and duration
- type of chromatography column used for the analysis of volatile compounds by gas chromatography
 (GC)
- main volatile compounds identified and reported with their amount (quantities or area).

95 As it can be seen in table 1, reported studies embraced a wide variety of cultivars more or less specific of the geographical origin of the authors. For example, German authors studied the Titania cultivar, used for 96 97 nectars and jams, and French authors studied the Noir de Bourgogne cultivar, used in liquors. Methods used 98 to extract the volatile fraction were evolving with technological improvements along years: solvent 99 extraction was used mainly in the oldest studies and SPME was dominating for the newest ones. The 100 resulting main aroma compounds reported in studies were thus quite different but consistent. Giving the fact 101 that different extraction methods could give complementary information, we decided to keep data from all the different methods. 102

A mind-map was presented on figure 2 to give an overview of differences in the study parameters of the selected studies. Some of these parameters were missing in the various studies and could not be included in the multivariate study.

106 As a result, an in-depth analysis of these data was then necessary to be able to draw main conclusions.

107 **2.2. Data curation**

108 The 22 selected studies counted for 36 different types of samples. They gave a pool of 351 identified volatile
109 compounds, among which 22 molecules were the most frequently cited found in significant amount for at

least 10 samples among the 36 ones. We considered that these 22 molecules, most frequently cited, wererepresentative of the general volatile profile of blackcurrant berries (table 2).

The most cited compounds were 3-carene, eucalyptol, terpinen-4-ol, *g*-terpinene, *p*-cymene, terpinolene, *b*caryophyllene, and limonene. It is noticeable that esters, typical of fruity notes, appeared less frequently.

Table 2 compiled the odor descriptors of each compound. In order to facilitate further data analysis, we regrouped odor descriptors in larger categories, based on definitions from literature and personal knowledge: for example, citrus, orange, lemon, petit-grain, lime, peel, and rind gave a single category named citrus (Appendix Table A1).

Finally, in order to be able to compare data, we expressed data for one given compound as a percentage ofthe total chromatographic area.

120 **2.3. Data description**

We described data, considering parameters likely to explain variations one by one: blackcurrant cultivar, country of the study, storage of berries before analysis, sample preparation, extraction method for volatile compounds, GC column. We studied the evolution of the quality and quantity of volatile compounds as a function of each of these parameters.

For this in-depth analysis, we retained all the reported compounds in case of studies reporting less than 15 compounds, and we retained the 15 most important compounds (based of the relative chromatographic area) for the other studies. For direct comparison between studies, parameter by parameter, we took into account the molecules reported in at least 50 % of the samples. This selection of compounds was comforted by published data on the odor activity of these compounds, found in references indicated in table 1 by an asterisk (^a). This was done for each publication. Table 2 compiled all these selected compounds.

131 **2.3.1.** Cultivars

As previously seen, the studied cultivars were numerous. Nevertheless, only two cultivars were found at least twice in the different studies and could be used for comparison. The Brödtorp cultivar was reported in three studies ((Andersson and von Sydow, 1966); (Liu et al., 2018); (Andersson and von Sydow, 1964)) and the Ben Lemond cultivar was reported in four studies ((Mikkelsen and Poll, 2002); (Iversen et al., 1998);
(Marriott, 1986); (Bagger-Jørgensen et al., 2004)).

137 **2.3.2.** Countries

Nine different countries were represented among the 23 selected studies. Four countries were found in
several studies, and could be used for comparison: Finland ((Marsol-Vall et al., 2018), (Leino and Kallio,
140 1993), Titinen et al. 2004); Denmark ((Varming et al., 2004), (Mikkelsen and Poll, 2002), (Iversen et al.,
141 1998), (Bagger-Jørgensen et al., 2004)); Germany ((Hempfling et al., 2013), (Jung et al., 2017), (Harb et al.,
142 2008)); Great Britain ((Ruiz del Castillo and Dobson, 2002), (Marriott, 1986), (Nursten and Williams,
143 1969)).

144 **2.3.3.** Storage of berries

Sometimes, berries were frozen before analysis. As this step could result in aroma loss or modification, it was important to evaluate this parameter. Data were regrouped in three categories: without freezing, freezing (-20°C and above), and deep-freezing (below -20°C).

Category "without freezing" regrouped samples from (Orav et al., 2002) and (Marriott, 1986) who analyzed
fresh samples, (Nursten and Williams, 1969) who analyzed samples stored at 0°C, and (Jung et al., 2017) and
(Hempfling et al., 2013) who analyzed samples stored at 4°C.

151 Category "freezing" regrouped samples stored at -15°C (Mikkelsen and Poll, 2002), at -18°C (Varming et
152 al., 2004), (Ohlsson, 2009), (Leino and Kallio, 1993), and at -20°C ((Marsol-Vall et al., 2018), (Latrasse et
153 al., 1982), (Liu et al., 2018), (Jung et al., 2017), (Bagger-Jørgensen et al., 2004), (Ruiz del Castillo and
154 Dobson, 2002), (Tiitinen et al., 2004)).

Category « deep freezing » regrouped samples stored at -26°C (Iversen et al., 1998), -30°C (Harb et al.,
2008), and -40°C ((Andersson and von Sydow, 1966a), (Andersson and von Sydow, 1966b), (Andersson and
von Sydow, 1964)).

158 **2.3.4.** Sample preparation

Blackcurrant berries were often processed before analysis. ((Ruiz del Castillo and Dobson, 2002) is the onlystudy using whole berries.

In case of "crushed berries", we found berries as such ((Marriott, 1986) (Ruiz del Castillo and Dobson, 2002)), but also berries mixed with water ((Latrasse et al., 1982), (Hempfling et al., 2013), (Jung et al., 2017), (Tiitinen et al., 2004)), or berries mixed with water and salts ((Andersson and von Sydow, 1964), (Andersson and von Sydow, 1966a), (Andersson and von Sydow, 1966b), (Marsol-Vall et al., 2018), (Harb et al., 2008).

Juices could be pure pasteurized juices ((Varming et al., 2004), (Mikkelsen and Poll, 2002), (BaggerJørgensen et al., 2004), (Ohlsson, 2009)), or pasteurized juices plus NaCl (Liu et al., 2018).

Finally, (Leino and Kallio, 1993) and (Nursten and Williams, 1969) studied concentrated juices, and (Iversen
et al., 1998) studied nectar with sucrose.

170 **2.3.5.** Extraction method for volatile compounds

We considered four categories of extraction methods that were reported in table 1: solvent extraction (SE),
vacuum-headspace extraction (VE), dynamic headspace extraction (DHS), and solid-phase micro-extraction
of the headspace (HS-SPME).

174 **2.3.6.** GC-column

- 175 GC-column used in the different studies were classified into three categories of polarity:
- Low polarity: SE-52 ((Latrasse et al., 1982), DB-5MS (Marsol-Vall et al., 2018), HP-5 (Ruiz del
 Castillo and Dobson, 2002), SPB-1 (Orav et al., 2002), VF5-MS (Ohlsson, 2009), RH-5 (Tiitinen et al., 2004), ApezonN/MS-550 (Nursten and Williams, 1969), OV-101 (Marriott, 1986)
- Intermediate polarity: Tween-80 (Andersson and von Sydow, 1966), DB-1701 (Leino and Kallio, 1993)
- High polarity: DB-WAX ((Varming et al., 2004), (Hempfling et al., 2013), (Jung et al., 2017),
 (Mikkelsen and Poll, 2002), (Bagger-Jørgensen et al., 2004)), HP-INNOWAX ((Liu et al., 2018)
 (Iversen et al., 1998), ZB-WAX (Harb et al., 2008).

185 **2.4. Multivariate data analyses**

186 In order to explore more in depth the dataset and reveal the existence of some specific groups, we used187 factorial analysis and hierarchical clustering.

188 Multiple factor analysis (MFA) is a multivariate data analysis method for summarizing and visualizing a complex data table, in which observations are described by several sets of variables (quantitative and /or 189 qualitative) structured into groups. MFA seeks the common structures present in all or some of these sets. It 190 is performed in 2 steps: (1) a Principal Component Analysis (PCA) is performed on each data set, which is 191 then "normalized" by dividing all its elements by the square root of the first eigenvalue obtained from of its 192 PCA and (2), the normalized data sets are merged to form a unique matrix and a global PCA is performed on 193 194 this matrix. The observation datasets are then projected onto the global analysis to explore communalities 195 and discrepancies. The basis of MFA can be viewed as a weighted PCA applied to the multiple table. (Pagès, 196 2002, Husson, 2017, Abdi and Valentin, 2007)

197 Clustering can be performed from the principal coordinates without any loss of information by computing 198 the classical Euclidean distance from the principal coordinates. The HCPC (Hierarchical Clustering on 199 Principal Components) function allows performing a clustering on individuals. This function combines 200 principal components methods, hierarchical clustering and partitioning to better visualize and highlight the 201 similarities between individuals. The simultaneous analysis of a principal component map and a hierarchical 202 clustering mainly means representing the partition issue from the dendrogram on the map (Bécue-Bertaut, 203 2008, Husson, 2010).

Multidimensional scaling (MDS) is a multivariate statistical technique used to create a map in which the distances between all pairs of items match the distances in the original distance matrix as closely as possible. The input to an MDS analysis is the same as the input to hierarchical cluster analysis—a distance matrix. Conversely, when the distances are converted into rank distances, a nonmetric multidimensional scaling (NMDS) is used. A benefit of NMDS is that it allows responses that are less precise. Therefore, easier response tasks can be used to obtain this type of similarity data.

The results produced by the MDS methods and clustering techniques are used to describe the interrelations between observations but cluster analysis is a tool for classifying objects into groups and is not concerned with the geometric representation of the objects in a low-dimensional space. To explore the dimensionality
of the space, the use of multidimensional scaling is preferred. MDS and cluster analysis are not mutually
exclusive both approaches can complement each other (Roskos-Ewoldsen, 2007, Timm, 2002).

In the resent study, calculations were done using RStudio Version 1.2.5042 (RStudio_Team, 2020) with R4.0.0 (R_Core_Team, 2020) and RStudio 1.2.5042 (RStudio_Team, 2020) with packages: "FactoMineR" (Lê

et al., 2008), "factoextra" (Kassambara and Mundt, 2020), "ggplot2" (Wickham, 2016), "Hmisc" (Harrell

and others, 2020), "magritt" (Bache and Wickham, 2014), "dplyr" (Hadley Wickham, 2020), "ggpubr "

219 (Kassambara, 2020), "MASS" (Venables and Ripley, 2002), "vegan" (Oksanen et al., 2010).

220

221 **3. Results - Discussion**

In a first step, we undertook a descriptive analysis focused on the impact of each studied parameter on the volatile profile. Then, we performed multivariate data analyses, using the whole dataset, to highlight the possible existence of more specific groups.

We calculated the mean values of normalized abundance percentages (relative chromatographic area reported in the different studies) for the different volatile compounds. Figure 3 reported the 21 most abundant compounds, which we considered for the present meta-analysis as representative of the global volatile profile for blackcurrant berries. The vast majority of compounds represented in figure 3 (most abundant) were included in the list of most frequently cited compounds (light grey and dark grey cells in table 2). It is noticeable that standard deviations were huge and did not allow an easy interpretation of data.

231

3.1. Differences in study parameters and their impact on data

Table 2 regrouped details (CAS n°, odor descriptors) on the volatile molecules discussed in the following
paragraphs. For other molecules (not reported in table 2), details were given in the text.

In the following development, we abbreviated molecules names in this way: "*a*" for alpha; "*b*" for beta; "*d*" for delta; "*g*" for gamma; "*p*" for para. Additionally, we did not make any difference between 3-carene and d-3-carene, because these molecules had the same organoleptic properties and chemical structure. We stated the impact of the different parameters by comparison with the list of molecules representative of the global profile in volatile compounds based on most abundant compounds (figure 3). We checked that the list of molecules was consistent with highest odorant impacts reported in publications with olfactometry measurements.

242

243

3.1.1. Impact of cultivars

The volatile profile of the cultivar Brödtorp was mainly characterized by ethyl acetate, terpinen-4-ol, *p*cymen-8-ol, 3-methyl-1-butanol, *cis*-3-hexen-1-ol. Among these five molecules, ethyl acetate (CAS n° 141-78-6, odor description: ethereal, fruity, sweet, green, rummy) and 3-methyl-1-butanol (CAS n° 123-51-3, odor description: alcoholic, fusel, banana, molasses, ethereal) did not appear in the global profile of volatile compounds for blackcurrant berries.

The volatile profile of the cultivar Ben Lomond was mainly characterized by methyl butanoate, ethyl butanoate, ethyl hexanoate, terpinolene, 3-carene, *b*-caryophyllene, ethyl acetate, *cis-b*-ocimene, terpinen-4ol, *trans-b*-ocimene, limonene, *b*-phellandrene, myrcene, *a*-terpinene ((Iversen et al., 1998), (Mikkelsen and Poll, 2002), (Varming et al., 2004b), (Bagger-Jørgensen et al., 2004), (Marriott, 1986)). Among these 14 molecules, ethyl hexanoate and ethyl acetate did not appear in the global profile of volatile compounds for blackcurrant berries.

255 **3.1.2.** Impact of countries

In studies reported for Germany, the following compounds seemed to be specific (found only for this country): 3-carene, 2-methyl-3-buten-2-ol, *cis-b*-ocimene, *trans*-2-hexenal, *b*-phellandrene, *trans*-2-hexen-1ol, *trans-b*-ocimene ((Harb et al., 2008), (Hempfling et al., 2013), (Jung et al., 2017), (Jung, 2018)).

In studies reported for Great Britain, the following 10 compounds were specific: a-terpinene, *b*caryophyllene, *p*-cymene, sabinene, *g*-terpinene, *a*-pinene, *a*-phellandrene, *a*-humulene (CAS n°6753-98-6, odor descriptor: sweet, spicy, WOODY), *b*-pinene, ocimene (CAS n°13877-91-3, odor descriptor: sweet, herbal) ((Nursten and Williams, 1969), (Marriott, 1986)). Ethyl hexanoate was specific for Denmark ((Iversen et al., 1998), (Mikkelsen and Poll, 2002), (Varming et al., 2004b), (Bagger-Jørgensen et al., 2004), (Christensen and Pedersen, 2006)), and bornyl acetate was
specific for Finland ((Leino and Kallio, 1993), (Tiitinen et al., 2004), (Marsol-Vall et al., 2018)).

266

3.1.3. Impact of storage of berries

Among the main volatile compounds, some molecules were only present in samples without freezing: caryophyllene, *b*-phellandrene, *a*-terpineol, *b*-caryophyllene, sabinene, *trans*-2-hexenal, *a*-terpinene. Nevertheless, the other volatile compounds found in the frozen samples could drive the corresponding odor descriptors.

3.1.4. Impact of sample preparation

272 The identified volatile compounds reported for the different ways of sample preparation were clearly273 different.

274 Compounds with odor descriptors such as terpenic, citrus, and woody characterized whole berries. 2-methyl-

3-buten-2-ol, myrcene, *cis-b*-ocimene, *trans-b*-ocimene were found only in the case of crushed berries. These
compounds had odor descriptors such as herbal, and green.

For more processed samples (juices and nectars), fruity, aldehydic and fatty notes, given by ethyl acetate,
butyric acid, benzyl alcohol, hexanoic acid, *trans*-2-octen-1-olmethyl hexanoate, methyl octanoate, and
hexanal, could be enhanced.

280 **3.1.5.** Impact of the extraction method for volatile compounds

It seemed that extraction methods using solvents (SE) allowed extracting higher quantities of terpenes and terpenoids related to sweet and fruity notes, such as *b*-caryophyllene and limonene.

Vacuum-headspace extraction (VE) methods gave a higher proportion of alcohols, related with green leaf
and herbal notes, such as 2-methyl-3-buten-2-ol and *trans*-2-hexen-1-ol.

285 Dynamic headspace extraction (DHS) favored esters (fruity notes), such as ethyl hexanoate and methyl286 acetate.

Finally, solid-phase micro-extraction of the headspace (HS-SPME) was linked with higher amounts of carboxylic acids, such as butyric acid, acetic acid, and hexanoic acid. These compounds were related with cheesy, acid, fermented and fatty notes.

290 **3.1.6. Impact of GC-column**

Molecules identified using low polarity columns were molecules with quite high molecular weights (above
10 carbons), and were mainly terpenes and terpenoids.

High polarity columns allowed identifying esters and alcohols together with terpenes and terpenoids.

For medium polarity columns, there was no specific molecule or chemical function highlighted.

295

3.2. Multivariate analysis and clusters of individuals

Dataset was composed of several categorical variables such as variety of studied blackcurrant berries or country, and numerical data such as percentages of specific compounds. Due to the variety of data, we applied a Multiple Factor Analysis (MFA) to the dataset. This analysis had two objectives: first, we searched to obtain a typology of the various studies and second we wished to know if there were correlated variables.

301 The complete data consisted in three datasets. Each study was an I x J[k] rectangular data matrix denoted 302 Y[k], where I was the number of observations and J[k] the number of variables of the k-th study.

The complete dataset was composed of I = 46 observations corresponding to the studies (in terms of articles) with 45 variables including descriptive characters, J[1]= 7: berry variety used, country of the study, storage type, nature of samples, publications, extraction method, GC column and 18 quantitative data: volatile molecules (J[2] = 18 variables), and 30 frequency data with chemical family (J[3] = 7 variables), and odor descriptors (J[4] = 13 variables). These three last groups were named active groups and the group of qualitative variables (J[1]) was named supplementary group.

- 309 Codes used for factors and observations were given in tables 3 and 4.
- 310 Cumulative variance of three dimensions counted for more than 53 % of the total variance.
- 311 The graph in figure 4a revealed the common structure of the observation space (dimension 1 x dimension 2).

Squared cosines reflected the representation quality of a variable on a factorial axis. A squared cosine of 1 meant that the observation was on the factorial axis (i.e. the angle is zero) and was perfectly represented, whereas a squared cosine of 0 indicated that the observation is on an orthogonal direction to the axis. We considered that observations with a sum of squared cosines on dimension 1 and dimension 2 above 0.6 meant that observation was correctly represented in the plan. We identified four groups of observations: 15-22-23-41 (named g1) in the down-right quarter, 26-27-28-38 (g2) in the up-right quarter, 12-31-36 (g3) in the left side dimension 1-axis, and 29-30 (g4) in the upper side along dimension 2-axis.

Figure 4b showed the dimension 1 x dimension 3 plan for observations. We considered that observations with sum of cos² above 0.6 were correctly represented in the plan. We also obtained four clusters of observations: 28-38 was confirmed in the up-right quarter; 8-9-39 in the down-left quarter, 31-32-34-35 in the up-left quarter, and 36 on the left along the dimension 3 axis.

As in standard PCA, the variable loadings were the correlation between the original variables and the global factor scores. These loadings were plotted along with the "circles of correlation" on the left in Figures 5a and 5b. They showed correlation between quantitative variables (group named Mole with "volatile molecules") and dimensions.

The relationships between the groups and the dimensions were plotted on the right in Figure 5. It meant that observations, which were along dimension 1 such as g1, were influenced by the chemical family group and odor descriptors. Terpene molecules and herbal (mint) odor mainly characterized them. At the opposite side, there was g3, which was mainly characterized by ester molecules and floral odor. On dimension 2, g4 was mainly characterized by chemical molecules especially M.t4o; on the contrary, g1 was mainly characterized by M.phi and M.3ca.

On figure 5a, the coordinates of the three active groups of frequencies (named Famy and Odor) on the first dimension were almost identical. This meant that they contributed similarly to the first dimension. Concerning the second dimension, the two groups - Mole and Quali - had the highest coordinates indicating a highest contribution to the second dimension.

From figure 5b, it could be observed that the variable "Chemical family - Famy" mainly contributed todimensions 1 and 3. The variable "odor description - Odor" contributed to dimension 1 mainly and the

variable "volatile molecules - Mole" contributed mostly to dimensions 1 and 2. Contribution of the
supplementary group "Quali" was the same along the three dimensions. From "correlation circles", it could
be observed that variables were rather widespread meaning that they were not correlated between them but in
1x2 plan. Two groups of variables were close: M. bca and M.atp and M.3ca, M. cib and M. trb. It was
confirmed by their correlation coefficients (Appendix. Figure A2).

344 The same type of analysis was done in 2x3 plan.

345

To complete the presence of clusters, a hierarchical clustering on principal components (HCPC) was applied and dendrograms were generated. Finally five clusters were obtained and they were synthetized as a, b, c, d and e in table 5.

349 Cluster a and cluster b regrouped observations from different studies with different experimental conditions.

350 Cluster c regrouped observations for which samples were all frozen.

351 Cluster d regroups observations for which samples were mainly crushed berries, with freezing as storage, and352 from northern countries (Sweden, Denmark, Germany, and Finland).

353 Finally, cluster e regrouped observations from northern countries (Scotland, Germany and mainly Denmark).

354

355 4. Conclusions

From the pool of 351 identified volatile compounds collected in the present study, our methodology resulted in the selection of about twenty molecules we considered as representative of the volatile profile of blackcurrant berries. The most cited compounds were terpinen-4-ol (citation frequency: 61%, mean value of normalized abundance: 8±13), terpinolene (53%, 9±11), limonene (50%, 4±3), 3-carene (47%, 15±13), eucalyptol (44%, 4±6), *g*-terpinene (28%, 4±6), *b*-caryophyllene (36%, 8±8), and *p*-cymene (33%, 4±4).

We considered parameters one by one (blackcurrant cultivar, country of the study, storage of berries before analysis, sample preparation, extraction method for volatile compounds, GC column) to make an in-depth description of data. 364 Indications for volatile compounds typical of some cultivars could be given. They concerned volatile 365 compounds that were representative of a cultivar but that did not appear in the list of the main volatile 366 compounds given for blackcurrant berries:

367 - ethyl acetate and 3-methyl-1-butanol for the cultivar Brödtorp

- ethyl hexanoate and ethyl acetate for the cultivar Ben Lomond.

369 Other parameters clearly had an impact on the detected volatile compounds but no clear tendency could be370 drawn from data description.

Linear multivariate analysis was firstly done, but, as representativeness of observations might seem quite
low, we decided to comfort the linear multivariate analysis with another method: non-Metric
Multidimensional Scaling (NMDS).

374 Even though there are similarities in the type of research questions to which MFA+HCPC and NDMS can be applied, Multidimensional Scaling and Factor Analysis are fundamentally different methods. Factor analysis 375 376 requires that the underlying data are distributed as multivariate normal, and that the relationships are linear. 377 Multidimensional Scaling (MDS) imposes no such restrictions. As long as the rank-ordering of distances (or similarities) in the matrix is meaningful, MDS can be used. In terms of resultant differences, factor analysis 378 379 tends to extract more factors (dimensions) than MDS; as a result, MDS often yields more readily, interpretable solutions. Most importantly, however, MDS can be applied to any kind of distances or 380 similarities, while factor analysis requires us to first compute a correlation matrix. MDS can be based on 381 382 subjects' direct assessment of similarities between stimuli, while factor analysis requires subjects to rate 383 those stimuli on some list of attributes (for which the factor analysis is performed) (TIBCO, 2020).

- In the present study, NMDS gave new clusters, reported as α , β , χ , δ , ϵ , and ϕ in table 5.
- 385 Observations belonging to a same cluster whatever the multivariate analysis were in color other than black.
- 386 From that, we obtained mainly four consolidated clusters, which were the following ones, characterized by
- 387 their richness/poorness in given volatile compounds:

- 25-26-27-28-38. Observations were characterized by a profile of volatile molecules rich in *a*-terpinene, *g*-terpene, *p*-cymene, *a*-terpinolene (*b*-caryophyllene)/ poor in methyl and ethylbutanoate.
 The profile was poor in aldehydes.
- 4-10-14: Observations were characterized by a profile of volatile molecules rich in *a*-pinene,
 limonene, terpinene, and myrcene. The profile was rich in terpenes. Associated odor descriptors
 were poor in alcoholic, fermented, and dairy notes.
- 1-31-32-33-34-35: Observations were characterized by a profile of volatile molecules poor in 3 carene, *cis* and *trans-b*-ocimene, phellandrene. The profile was rich in acids, terpenoids and
 alcohols. Associated odor descriptors were rich in nuts and fermented notes.
- 15-23-41-44: Observations were characterized by a profile of volatile molecules rich in sabinene, 3 carene, phellandrene, *cis* and *trans-b*-ocimene, methyl and ethyl butanoate. The profile was rich in
 aldehydes.

400 Unfortunately, none of the clusters of individuals was linked with specific cultivars, which was not obvious401 considering raw data.

The present bibliometric and meta-analysis study failed to draw main conclusions concerning typicality of blackcurrant cultivars. Moreover, the different parameters taken into account in the multivariate statistical analysis did not allow explaining the overall variability within data set. We showed that most of the variables were not correlated between them. This observation should be considered with caution due to the limits of the database used to retrieve the studied articles.

407 Nevertheless, this confirms that further research still has to be done to establish clearly the typically of given 408 cultivars that are empirically known to give specific organoleptic properties to manufactured products. It also 409 permitted us identifying the important molecules to target, the experimental conditions to control, and 410 selecting appropriate method for future works.

412	Credit authorship contribution statement
413	Sandy Pagès-Hélary: data collection and curation, data analysis and interpretation, writing. Laurence
414	Dujourdy: statistical analysis, data interpretation, writing. Nathalie Cayot: methodology, project
415	administration, writing,
416	
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418	The authors declare that they have no known competing financial interests or personal relationships that
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420	
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431 **References**

- 432 Dictionary of Flavors.
- ABDI, H. & VALENTIN, D. (2007). Multiple factor analysis (MFA). In N.J. Salkind (ed.) Encyclopedia of
 measurement and statistics (pp 657-663). Thousand Oaks.
- ANDERSSON, J. & VON SYDOW, E. 1964. The Aroma of Black Currants. I. Higher Boiling Compounds.
 Acta Chemica Scandinavica, 18, 1105-1114.
- ANDERSSON, J. & VON SYDOW, E. 1966a. The Aroma of Black Currants. II. Lower Boiling Compounds.
 Acta Chemica Scandinavica, 522-528.
- ANDERSSON, J. & VON SYDOW, E. 1966b. The Aroma of Black Currants. III. Chemical Characterization
 of Different Varieties and Stages of Ripeness by Gas Chromatography. *Acta Chemica Scandinavica*, 20, 529-535.
- ANJOU, K. & VON SYDOW, E. 1966. Variation in the composition of fruit juices : a study of the
 literature. *SIK Rapport.*
- 444 BACHE, S. M. & WICKHAM, H. 2014. magrittr: A Forward-Pipe Operator for R. R package version 1.5. .
- BAGGER-JØRGENSEN, R., MEYER, A. S., VARMING, C. & JONSSON, G. 2004. Recovery of volatile aroma
 compounds from black currant juice by vacuum membrane distillation. *Journal of Food Engineering*, 64, 23-31.
- 448 BÉCUE-BERTAUT, M., PAGÈS, J. 2008. Multiple factor analysis and clustering of a mixture of
 449 quantitative, categorical and frequency data *Computational Statistics & Data Analysis*, 52,
 450 3255-3268.
- CHRISTENSEN, L. P. & PEDERSEN, H. L. (2006). Varietal differences in the aroma compound profile of
 blackcurrant berries. In W. L. P. BREDIE, & M. A. PETERSEN (eds.), Developments in Food
 Science (pp. 257-260). Elsevier.
- 454 CORTEZ, R. E. & GONZALEZ DE MEJIA, E. 2019. Blackcurrants (*Ribes nigrum*): A Review on Chemistry,
 455 Processing, and Health Benefits. *Journal of Food Science*, 84, 2387-2401.
- 456 DE ROVIRA, D. A. (1999). The Dictionary of Flavors: And General Guide for Those Training in the Art
 457 and Science of Flavor Chemistry. Wiley.
- 458 GERBAKA, S. 2013. Le cassis (Ribes nigrum L.) : études botanique, chimique et effets thérapeutiques.
 459 Sciences pharmaceutiques. dumas-00844030
- 460 HADLEY WICKHAM, R. F., LIONEL HENRY AND KIRILL MÜLLER 2020. dplyr: A Grammar of Data
 461 Manipulation. *R package version 0.8.5.*
- HARB, J., BISHARAT, R. & STREIF, J. 2008. Changes in volatile constituents of blackcurrants (*Ribes nigrum L. cv. 'Titania'*) following controlled atmosphere storage. *Postharvest Biology and Technology*, 47, 271-279.
- HARRELL, F. E. J. & OTHERS, W. C. F. C. D. A. M. 2020. *Hmisc: Harrell Miscellaneous. R package version 4.4-0.* [Online]. Available: https://CRAN.R-project.org/package=Hmisc [Accessed].
- HEMPFLING, K., FASTOWSKI, O., CELIK, J. & ENGEL, K. H. 2013. Analysis and Sensory Evaluation of
 Jostaberry (*Ribes x nidigrolaria Bauer*) Volatiles. *Journal of Agricultural and Food Chemistry*,
 61, 9067-9075.
- HUSSON, F., JOSSE, J., PAGÈS, J. 2010. Principal component methods hierarchical clustering partitional clustering: why would we need to choose for visualizing data ? : Agrocampus
 Applied Mathematics Department.
- 473 HUSSON, F., LÊ S., PAGÈS J. (2017). Exploratory Multivariate Analysis by Example Using R. Chapman;
 474 Hall/CRC.
- IVERSEN, C. K., JAKOBSEN, H. B. & OLSEN, C. E. 1998. Aroma changes during black currant (*Ribes nigrum L.*) nectar processing. *Journal of Agricultural and Food Chemistry*, 46, 1132-1136.
- JUNG, K. 2018. Analysis and sensory evaluation of volatile constituents of blackcurrant (Ribes nigrum
 L) and redcurrant (Ribes rubrum L.) fruits. PhD, Technical University Munich.

- JUNG, K., FASTOWSKI, O., POPLACEAN, J. & ENGEL, K.-H. 2017. Analysis and Sensory Evaluation of
 Volatile Constituents of Fresh Blackcurrant (*Ribes nigrum L.*) Fruits. *Journal of Agricultural* and Food Chemistry, 65, 9475-9487.
- 482 KASSAMBARA, A. 2020. ggpubr: 'ggplot2' Based Publication Ready Plots. . *R package version 0.3.0*.
- KASSAMBARA, A. & MUNDT, F. 2020. Factoextra: Extract and Visualize the Results of Multivariate
 Data Analyses. . [Online]. Available: https://CRAN.R-project.org/package=factoextra
 [Accessed].
- LATRASSE, A., RIGAUD, J. & SARRIS, J. 1982. L'arôme du cassis (*Ribes nigrum L.*) odeur principale et
 notes secondaires. *Sciences des Aliments*, 2, 145–162.
- 488 LÊ, S., JOSSE, J. & HUSSON, F. 2008. FactoMineR: An R package for multivariate analysis. *Journal of* 489 *Statistical Software*, 25, 1-18.
- 490 LEINO, M. & KALLIO, H. 1993. Volatile compounds of blackcurrant juice and wine. *Zeitschrift für* 491 *Lebensmittel-Untersuchung und Forschung*, 196, 410-414.
- LIU, Y., WANG, S., REN, J., YUAN, G., LI, Y., ZHANG, B. & ZHU, B. 2018. Characterization of free and
 bound volatile compounds in six Ribes nigrum L. blackcurrant cultivars. *Food Research International*, 103, 301-315.
- MARRIOTT, R. J. (1986). Biogenesis of Blackcurrant (*Ribes nigrum*) Aroma. In T.H. Parliament , & R.
 Croteau (Eds.), Biogeneration of Aromas (pp. 184-192). American Chemical Society.
- MARSOL-VALL, A., KORTESNIEMI, M., KARHU, S. T., KALLIO, H. & YANG, B. 2018. Profiles of Volatile
 Compounds in Blackcurrant (*Ribes nigrum*) Cultivars with a Special Focus on the Influence of
 Growth Latitude and Weather Conditions. *Journal of Agricultural and Food Chemistry*, 66,
 7485-7495.
- MARSOL-VALL, A., LAAKSONEN, O. & YANG, B. 2019. Effects of processing and storage conditions on
 volatile composition and odor characteristics of blackcurrant (*Ribes nigrum*) juices. *Food Chemistry*, 293, 151-160.
- MIKKELSEN, B. B. & POLL, L. 2002. Decomposition and transformation of aroma compounds and
 anthocyanins during black currant (*Ribes nigrum L.*) juice processing. *Journal of Food Science*,
 67, 3447-3455.
- 507 NURSTEN, H. E. & WILLIAMS, A. A. 1969. Volatile constituents of the black currant, *RIBES NIGRUM L*.:
 508 II.—The fresh fruit. *Journal of the Science of Food and Agriculture*, 20, 613-619.
- 509 OHLSSON, A. 2009. Comparison of flavour compounds in juices from different blackcurrant varieties.
 510 PhD, University of Kalmar, School of Pure and Applied Natural Sciences.
- 511 OKSANEN, J., BLANCHET, F. G., KINDT, R., LEGENDRE, P., O'HARA, B., SIMPSON, G., SOLYMOS, P.,
 512 STEVENS, H. & WAGNER, H. 2010. Vegan: Community Ecology Package.
- ORAV, A., KAILAS, T. & MUURISEPP, M. 2002. Composition of blackcurrant aroma isolated from
 leaves, buds, and berries of *Ribes nigrum L. Proceedings of the Estonian Academy Sciences. Chemistry*, 51, 225-234.
- PAGÈS, J. 2002. Analyse Factorielle Multiple Appliquée Aux Variables Qualitatives et Aux Données
 Mixtes. *Revue Statistique Appliquée*, 50, 5-37.
- 518 R_CORE_TEAM 2020. *R: A language and environment for statistical computing. ,* Vienna, Austria, R
 519 Foundation for Statistical Computing.
- ROSKOS-EWOLDSEN, D. R., ROSKOS-EWOLDSEN, B. (2007). Scaling and Cluster Analysis. In A. F.
 HAYES, M. D. SLATER, & L. B. SNYDER (Eds.), *The SAGE Sourcebook of Advanced Data Analysis Methods for Communication Research*. SAGE Publications, Inc.
- 523 RSTUDIO_TEAM. 2020. RStudio: Integrated Development for R. , Available from:
 524 http://www.rstudio.com/.
- RUIZ DEL CASTILLO, M. L. & DOBSON, G. 2002. Varietal differences in terpene composition of
 blackcurrant (Ribes nigrum L) berries by solid phase microextraction/gas chromatography.
 Journal of the Science of Food and Agriculture, 82, 1510-1515.
- TIBCO (2020). Multidimensional Scaling Introductory Overview MDS and Factor Analysis. In INC., T.
 S. (Ed.), Data Science Textbook. TIBCO Software Inc.

- TIITINEN, K., HAKALA, M., POHJANHEIMO, T., TAHVONEN, R. & KALLIO, H. 2004. Flavour profile of
 frozen black currant: Extraction by SPME and analysis by GC sniffing. *In:* HOFMANN, T.,
 ROTHE, M. & SCHIEBERLE, P. (eds.) *State-of-the-art in flavour chemistry and biology.*
- 533 Garching: Deutsche Forschungsanstalt für Lebensmittelchemie.
- TIMM, N. H. (2002). Cluster Analysis and Multidimensional Scaling. In N. H. Timm (Ed.), Applied
 Multivariate Analysis. Springer Texts in Statistics. Springer.
- VARMING, C., ANDERSEN, M. L. & POLL, L. 2004a. Influence of thermal treatment on black currant
 (*Ribes nigrum L.*) juice aroma. *Journal of Agricultural and Food Chemistry*, 52, 7628-7636.
- VARMING, C., PETERSEN, M. A. & POLL, L. 2004b. Comparison of isolation methods for the
 determination of important aroma compounds in black currant (*Ribes nigrum L.*) juice, using
 nasal impact frequency profiling. *Journal of Agricultural and Food Chemistry*, 52, 1647-1652.
- 541 VENABLES, W. N. & RIPLEY, B. D. (2002). Modern Applied Statistics with S. Springer.
- 542 WICKHAM, H. (2016). ggplot2: Elegant Graphics for Data Analysis. Springer-Verlag.
- 543 ZARZO, M. 2013. What is a Fresh Scent in Perfumery? Perceptual Freshness is Correlated with 544 Substantivity. *Sensors*, 13, 463-483.

547 Table 1. List of the different publications included in the meta-analysis with their specificities and main volatile compounds reported

References		Growth area of berries	f Variety of berries	Extraction methods used for volatile compounds analysis	Main aroma compounds reported	
(Andersson and Sydow, 1964)	von	Sweden	Brödtorp	SE + distillation of the extract	myrcene, <i>cis-b</i> -ocimene, <i>trans-b</i> -ocimene, limonene, <i>b</i> -phallandrene, terpinolene, <i>a</i> -pinene, 3-carene, citronellol, terpinen-4-ol, <i>p</i> -cymene, citronellyl acetate, caryophyllene	
(Andersson and Sydow, 1966a)	von	Sweden	Brödtorp	VE: 48°C + distillation of the extract	acetone, methyl acetate, ethyl acetate, propanol, 2-methyl- 3-buten-2-ol, isobutanol, terpinen-4-ol	
(Andersson and Sydow, 1966b)			Brödtorp, Wellington XXX, Silvergieters Zwarte, Cotswold Cross, and two crossing (WellingtonXXX x Brôdtorp, Cotswold Cross x Brödtorp)	SE + distillation of the extract	3-carene, <i>g</i> -terpinene, terpinolene, terpinen-4-ol, citronellyl acetate, caryophyllene	
(Nursten Williams, 1969)	and	UK	NI (English blackcurrant varieties mix)		<i>a</i> -terpinene, <i>b</i> -phellandrene, <i>g</i> -terpinene, <i>p</i> -methyliso- propenylbenzene, eucalyptol, 2-hexenal, methanol, ethanol, <i>n</i> -propanol, <i>n</i> -butanol, isobutanol, isopentanol, 2- methylbut-3-en-2-ol, <i>n</i> -hexanol, <i>cis-</i> & <i>trans-</i> 2-hexen-1-ol, terpinen-4-ol, ethyl butanoate, methyl <i>n</i> -hexanoate, and methyl benzoate.	

(Latrasse et al., 1982)	France	Noir de Bourgogne and Royal de Naples	SE	diacetyle, ethyl butanoate, methyl butyrate, eucalyptol, linalool, limonene-4-ol, <i>a</i> -terpineol, terpinen-4-ol
(Marriott, 1986)	UK	Ben Lemond and WellingtonXXX	SE	sabinene, 3-carene, limonene, linalool, <i>a</i> -terpineol, <i>b</i> -caryophyllene, caryophyllene oxide
1993) ^b fused		DHS: 40°C - deactivated fused silica capillary tubing	Butanoic acid, hexanoic acid, ethyl octanoate, octanoic acid, bornyl acetate, methyl decanoate, ethyl decanoate, ethyl dodecanoate, 2,6-bis(1,1-dimethylethyl)-4-methyl phenol	
(Iversen et al., 1998) ^a	Denmark	Ben Lemond	DHS: 18°C – 60 min – Poropak trap	Methyl butanoate, ethyl butanoate, 3-carene, methyl hexanoate, limonene, ethyl hexanoate
(Ruiz del Castillo and Dobson, 2002)	Scottland		HS-SPME: 55°C – 20 min – PDMS-DVB fiber	<i>a</i> -pinene, myrcene, limonene, eucalyptol, <i>a</i> -phellandrene
(Orav et al., 2002)	Estonia	N.I. (Saxifragacae, wild black currant, from north America)	SE (with simultaneous distillation)	3-carene, <i>cis-b</i> -ocimene, limonene, <i>b</i> -phellandrene, terpinolene, <i>p</i> -cymene, <i>trans-b</i> -caryophyllene
(Mikkelsen and Poll, 2002) ^a	Denmark	Ben Lemond	DHS: 30°C – 60 min – Tenax trap	3-carene, <i>cis</i> -ocimene, <i>a</i> -terpinolene, <i>b</i> -caryophyllene, ethyl acetate, methyl butanoate, ethyl butanoate
(Varming et al., 2004a)	Denmark	Ben Lemond	DHS: 30°C – 45 min – Tenax trap	2-methyl-1-propanol, 2-and 3-methyl-1-butanol, methyl butanoate, ethyl butanoate, 4-terpineol
Varming et al.2004 ^b	Denmark	Ben Lemond	HS: 30°C – 60 min – Tenax trap	ethyl butanoate, 2,3-butanedione, methyl 2- methylbutanoate, 2-methylpropyl acetate, methyl acetate, ethyl hexanoate
Varming et al.2004 ^b	Denmark	Ben Lemond	DHS: 30°C – 15 et 60 min – Tenax trap	ethyl butanoate, methyl butanoate, 2,3-butanedione, 2- methyl-3-furanthiol, cineole, 2-methyl-1-butanol, 3-methyl- 1-butanol
Varming et al.2004 ^b	Denmark	Ben Lemond	SE	ethyl butanoate, 2-methyl-3-furanthiol, methional, butanoic acid
(Bagger-Jørgensen et al., 2004)	Denmark	Ben Lemond	trap	methyl butanoate, ethyl butanoate, furfural, ethyl hexanoate, eucalyptol, <i>cis</i> -3-hexen-1-ol, <i>b</i> -damascenone
(Tiitinen et al., 2004)	Finland	NI	HS-SPME: 25°C – 30 min – triphasic fiber	<i>a</i> -pinene, <i>b</i> -pinene, sabinene, 3-carene, <i>b</i> -phellandrene, terpinolene, myrcene, limonene, <i>cis</i> -ocimene, <i>trans</i> - ocimene, <i>g</i> -terpinene, linalool, <i>a</i> -terpineol, citronellol
(Christensen and	Denmark	NI (13 different	DHS: 25°C – 90 min –	methyl butanoate, ethyl butanoate, methyl hexanoate, ethyl

Pedersen, 2006)		organic varieties)	Porapak trap	hexanoate, sabinene, 3-carene, <i>g</i> -terpinene, terpinolene, <i>cis</i> - <i>b</i> -ocimene, eucalyptol
(Harb et al., 2008)	Germany	Titania	HS-SPME: 30°C – 60 min – PDMS fiber	terpinen-4-ol, 3-carene, <i>a</i> -pinene, 4-carene, hexanal, <i>b</i> -pinene, limonene, 1-hexanol
(Ohlsson, 2009)	New Zealand	Ben Hope, Magnus	HS-SPME: 55°C – 20 min – PDMS fiber	2-methyl-3-buten-2-ol, methyl butanoate, ethyl butanoate, thujol, linalool, terpinene, <i>a</i> -terpineol, <i>p</i> -cymen-8-ol, eucalyptol, damascenone, <i>a</i> -cadinol
(Hempfling et al., 2013) ^a	Germany	N.I.	VE: 35°C – 2h at 1-10 mbar	<i>trans</i> -2-hexenal, <i>trans</i> -2-hexen-1-ol, <i>cis</i> -3-hexen-1-ol, methyl butanoate, ethyl butanoate, 2-methylbut-3-en-2-ol, eucalyptol
(Jung et al., 2017)	Germany Deutenkofen	Titania, 8 Bona, Ben Sarek, Rosenthals, Silvergieters, Supernova, Tsema, Ometa	VE: 35°C – 2h at 1-10 mbar	4-methoxy-2-methyl-2-butanethiol, <i>cis</i> -3-hexanal, ethyl butanoate, eucalyptol, oct-1-en-3-one, alkyl-substituted 3-methoxypyrazines
(Marsol-Vall et al., 2018)	Finland	Mortti, Ola, Melahati and other crossing cultivar		undecane, eucalyptol, <i>cis</i> -rose-oxide, terpinolene, terpinen- 4-ol, <i>a</i> -terpineol
(Jung, 2018) ^a	Germany	Andega, 8 Bona, Ben Sarek, Rosenthals, Silvergieters, Supernova, Titania, Tsema, Ometa	VE: 35°C – 2h at 1-10 mbar	<i>trans</i> -2-hexenal, <i>cis</i> -3-hexenal, ethyl butanoate, methyl butanoate, 3-carene, <i>b</i> -phellandrene, sabinene, terpinen-4-ol, 2-methylbut-3-en-2-ol
(Liu et al., 2018)	China	Risagar, Fertodi, Brodtorp, Sofya, Yadrionaya, Liangye	HS-SPME: 40°C – 30 min – triphasic fiber	butyric acid, hexanal, nonanal, <i>trans</i> -octenal, decanal, methyl 4-hydroxybenzoate, guaiacol, 4-vinylguaiacol, isoamyl acetate, hexyl acetate, <i>cis</i> -3-hexanol acetate, ethyl butanoate, ethyl hexanoate, methyl butanoate, heptanol, <i>trans-b</i> -damascenone, lilac alcohol D

- 550 SE: solvent extraction, VE: vacuum-headspace extraction, DHS: dynamic headspace extraction, HS-SPME: solid-phase micro extraction of the headspace, 551 N.I.: not indicated
- ³ ^a reference with GC-O or GC-sniffing results, ^b reference with sensory results

Table 2. Citation frequencies and descriptors of the main volatile compounds reported in the studied publications

Aroma compounds are in white cells when reported between 10 and 20 times, in light grey cells when reported between 20 and 30 times, and in dark grey cells when reported more than 30 times.

Descriptors were taken from www.thegoodscentscompany.com, unless otherwise specified. Descriptors in normal letters are for odor, in italic for flavor, and in capital letters for both odor and flavor.

Compounds	CAS	Sensory descriptor
3-carene	13466-78-9	CITRUS, TERPENIC, PINE, HERBAL, RESINOUS, phenolic, medicinal, spicy
eucalyptol	470-82-6	Balsamic * / EUCALYPTUS, CAMPHREOUS, MEDICINAL, herbal, cooling
terpinen-4-ol	562-74-3	WOODY, EARTHY, CITRUS, SPICY, musty, sweet, mentholic, cooling, clove
g-terpinene	99-85-4	TERPENIC, LIME, OILY, TROPICAL, CITRUS, herbal, woody, fruity
<i>p</i> -cymene	99-87-6	TERPENIC, CITRUS, WOODY, SPICY, ORIGANO, fresh, cilantro, rancid
terpinolene	586-62-9	WOODY, CITRUS, fresh, pine, sweet, terpenic, herbal
<i>b</i> -caryophyllene	87-44-5	SPICY, WOODY, CLOVE, dry, nutty, powdery, peppery, skin
limonene	138-86-3	root * / citrus, herbal, terpenic, camphorated
ethyl butanoate	105-54-4	Fruity * / FRUITY, TUTTI FRUTTI, SWEET, juicy, pineapple, cognac, fresh, apple
myrcene	123-35-3	WOODY, spicy, peppery, terpenic, balsamic, herbal, rose, vegetable, tropical, minty
<i>a</i> -pinene	80-56-8	WOODY, PINE, CAMPHOREOUS, HERBAL, TERPENIC, earthy, tropical
methyl butanoate	623-42-7	FRUITY, FUSEL, DAIRY, ESTERY, sweet, fermented, pungent, tropical, acidic
<i>a</i> -phellandrene	99-83-2	TERPENIC, CITRUS, GREEN, woody, black pepper, fresh
<i>a</i> -terpinene	99-86-5	WOODY, TERPENIC, CITRUS, SPICY, herbal, medicinal, camphorated, pine, minty
hexanal	66-25-1	GREEN, GRASSY, FRESH, VEGETABLE, leafy, fruity, citrus, apple
trans-2-hexen-1-ol	928-95-0	FRUITY, GREEN, FRESH, LEAFY, vegetable, banana, fatty, juicy
cis-3-hexen-1-ol	928-96-1	GREEN, FRESH, PUNGENT, grassy, vegetable, melon, rind, fruity
sabinene	3387-41-5	WOODY, SPICY, CAMPHOREOUS, terpenic, citrus, pine, green, oily
<i>b</i> -pinene	127-91-3	PINE, WOODY, RESINOUS, SPICY, MINTY, CAMPHOREOUS, TERPENIC, hay
<i>b</i> -phellandrene	555-10-2	minty, terpenic
trans-2-hexenal	6728-26-3	apple ** /GREEN, FRUITY, LEAFY, FRESH, cheesy, spicy, aldehydic, vegetable
a-terpineol	98-55-5	CITRUS, FLORAL, WOODY, terpenic, lilac, pine, cooling, soapy
nonanal	124-19-6	ALDEHYDIC, CITRUS, FATTY, CUCUMBER, waxy, fresh, rose, iris, nutty, potato
hexanol	111-27-3	GREEN, FRUITY, OILY, ethereal, sweet, alcoholic, herbal, fruity, apple
p-cymen-8-ol	1197-01-9	FRUITY, CHERRY, SWEET, camphorated, floral, coumarinic, hay, cereal, bready
methyl hexanoate	106-70-7	FRUITY, PINEAPPLE, ethereal, fatty, apple, apricot
trans-b-ocimene	3779-61-1	herbal, sweet
bornyl acetate	76-49-3	WOODY, CAMPHROREOUS, MENTHOLIC, cedar, spicy, berry, seedy, soapy
linalool	78-70-6	Floral * / FLORAL, CITRUS, WOODY, WAXY, blueberry, terpenic, aldehydic
methyl benzoate	93-58-3	PHENOLIC, CHERRY, CAMPHOREOUS, almond, floral, cananga
decanal	112-31-2	citrus ***/ WAXY, CITRUS, ORANGE, PEEL, sweet, aldehydic, floral, green, melon
2-methyl-3-buten-2-ol	115-18-4	herbal, earthy, oily
citronellyl acetate	150-84-5	FLORAL, GREEN, FRUITY, WAXY, citrus, woody, aldehydic, pear, apple
ethyl benzoate	93-89-0	SWEET, WINTERGREEN, FRUITY, dry, musty, medicinal, cherry, minty, green
methyl octanoate	111-11-5	GREEN, WAXY, CITRUS, ALDEHYDIC, vegetal, herbal, fatty, fruity
ethyl octanoate	106-32-1	WAXY, FRUITY, SWEET, PINEAPPLE, CREAMY, banana, musty, brandy, <i>fatty</i> , <i>mushroom</i> , <i>cognac</i>

ethyl hexanoate	123-66-0	SWEET, FRUITY, PINEAPPLE, WAXY, GREEN, BANANA, ESTERY, fatty
pentanol	71-41-0	FUSEL, FERMENTED, BREADY, oily, balsamic, winey, solvent, fruity, cereal
a-caryophyllene	6753-98-6	woody, spicy
benzaldehyde	100-52-7	ALMOND, CHERRY, SWEET, NUTTY, bitter, powdery, maraschino, oily, woody
heptanol	111-70-6	GREEN, musty, leafy, fruity, peony, banana, fermented, aldehydic, oily, nutty
cis-b-ocimene	3338-55-13	FLORAL, warm, herbal, sweet, green, tropical, spicy, woody
sabinene hydrate	546-79-2	MINTY, GREEN, COOLING, terpenic, eucalyptus, spicy, camphorated, oily, woody

*(Latrasse et al., 1982), ** (Hempfling et al., 2013), ***(Jung et al., 2017)

Table 3. Codes of factors used for figure 4 and table 4

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Factors	Whole name (code)
Cultivars	Brödtorp (Bro), BC-group (BCg), BenLoyal (Bly), BenNevis (BNe), Cie5-32 (C32), Cie5-63 (C63), Kristin (Kri), Pasille-group (PaG), Sunniva (Sun), Tenah (Teh), Wellington XXX (Wel), Silvergieters Zwarte (Sil), Cotswold Cross (Cos), WellingtonXXX x Brôdtorp (WxB), Cotswold Cross x Brödtorp (CxB), English blackcurrant varieties mix (NiE), Noir de Bourgogne (NB), Royal de Naples (RN), Ben Lomond (BLo), Öjeby (Obj), Géant de Boskoop (GBo), Malvern Cross (MCr), Davison's eight (Da8), Golubka (Gol), Ben Tirran (BTi), Ben Dorian (BDo), Hedda (Hdd), Ben Avon (BAv), black currant, from north America (NiA), NI (NI), Titania (Tit), Ben Hope (BHo), Magnus (Mag), Mortti (Mor), Ola (Ola), Melahati (Mel), Andega (And), 8 Bona (8Bo), Ben Sarek (BSa), Rosenthals (Ros), Supernova (Sup), Tsema (Tse), Ometa (Ome), Risagar (Ris), Fertodi (Fer), Sofya (Sof), Yadrionaya (Yad), Liangye (Lia)
Countries	Sweden (Swe), UK (UK), France (Fra), Finland (Fin), Denmark (Den), Scottland (Sco), Estonia (Est), Germany (Ger), New Zealand (NZ), China (Chi)
Storage	Frozed (Fro), Unfrozed (UFr)
Samples type	Whole (Who), Crushed (Cru), Juice (Jui), Concentrated juice (Con)
Publications	Andersson and von Sydow 1964 (A64), Andersson and von Sydow 1966a (A66a), Andersson and von Sydow 1966b (A66b), Nursten and Williams 1969 (N69), Latrasse et al. 1982 (L82), Marriott 1986 (M87), Leino and Kallio 1993 (L93), Iversen et al. 1998 (I98) Ruiz del Castillo and Dobson 2002 (C02), Orav et al. 2002 (O02), Mikkelsen and Poll 2002 (M02), Varming et al. 2004a (V04), Varming et al.2004 (V04b), Bagger-Jørgensen et al. 2004 (B04), Tiitinen et al. 2004 (T04), Christensen and Pedersen 2006 (C06), Harb et al. 2008 (H08), Ohlsson 2009 (O09), Hempfling et al. 2013 (H13), Jung et al. 2017 (J17), Marsol-Vall et al. 2018 (M18), Jung 2018 (J18), Liu et al. 2018 (L18)
Methods	Solvent extraction (SE), Vacuum extraction (VE), Purge and trap extraction (PT), SPME extraction (SP)
Columns	Low polarity (LPo), Medium polarity (MPo), High polarity (HPo)

Individuals	Varieties	Countries	Storage	Sample type	Publications	Methods	Columns
1	Bro	Swe	Fro	Cru	A64	SE	HPo
2	Bro	Swe	Fro	Cru	A66a	VE	MPo
3	BTi	Sco	Fro	Cru	C02	SP	LPo
4	BDo	Sco	Fro	Cru	C02	SP	LPo
5	Hdd	Sco	Fro	Cru	C02	SP	LPo
6	BAv	Sco	Fro	Cru	C02	SP	LPo
7	Hdd	Sco	Fro	Who	C02	SP	LPo
8	BLy	Den	Fro	Cru	C06	РТ	HPo
9	BNe	Den	Fro	Cru	C06	РТ	HPo
10	C32	Den	Fro	Cru	C06	РТ	HPo
11	C63	Den	Fro	Cru	C06	РТ	HPo
12	Kri	Den	Fro	Cru	C06	PT	HPo
13	Sun	Den	Fro	Cru	C06	PT	HPo
14	Tse	Den	Fro	Cru	C06	PT	HPo
15	Tit	Ger	Fro	Cru	H08	SP	HPo
16	BLo	Den	Fro	Con	198	PT	HPo
17	Ros	Ger	Fro	Cru	J17	VE	HPo
18	Tit	Ger	Fro	Cru	J18	VE	HPo
19	Sup	Ger	Fro	Cru	J18	VE	HPo
20	Sup	Ger	UFr	Cru	J18	VE	HPo
21	Teh	Ger	UFr	Cru	J18	VE	HPo
22	Teh	Ger	Fro	Cru	J18	VE	HPo
23	8Bo	Ger	Fro	Cru	J18	VE	HPo
24	BSa	Ger	Fro	Cru	J18	VE	HPo
25	Ome	Ger	Fro	Cru	J18	VE	HPo
26	Obj	Fin	Fro	Jui	L93	PT	MPo
27	Bro	Chi	Fro	Jui	L18	SP	HPo
28	Sof	Chi	Fro	Jui	L18	SP	HPo
29	Yad	Chi	Fro	Jui	L18	SP	HPo
30	Lia	Chi	Fro	Jui	L18	SP	HPo
31	Ris	Chi	Fro	Jui	L18	SP	HPo
32	Fer	Chi	Fro	Jui	L18	SP	HPo
33	BLo	UK	UFr	Cru	M87	SE	LPo
34	Wel	UK	UFr	Cru	M87	SE	LPo
35	Mor	Fin	Fro	Cru	M18	SP	LPo
36	BLo	Den	Fro	Jui	M02	РТ	HPo
37	NiE	UK	UFr	Con	N69	SE	LPo
38	BCg	NZ	Fro	Jui	O09	SP	LPo
39	PaG	NZ	Fro	Jui	O09	SP	LPo
40	NI	Est	UFr	Cru	002	SE	LPo
41	NI	Fin	Fro	Cru	T04	SP	LPo
42	BLo	Den	Fro	Jui	V04b	РТ	HPo

Table 4. Correspondence between individuals and factors used for figure 4 and table 5 $\,$

43	BLo	Den	Fro	Jui	V04b	PT	HPo
44	BLo	Den	Fro	Jui	V04b	PT	HPo
45	BLo	Den	Fro	Jui	V04b	SE	HPo
46	BLo	Den	Fro	Jui	V04a	PT	HPo

Table 5. Comparison and interpretation of NMDS and MFA+HCPC data analyses

Individuals in color are regrouped in the same cluster whatever the multivariate analysis

Multivariate analysis	Cluster	Individuals	Characteristics of the cluster
	a		Molecules: rich in ethyl butanoate, phellandrene, terpinen-4-ol/ poor in <i>a</i> -terpinene, myrcene, limonene, <i>b</i> -caryophyllene Varieties concerned: Ojeby, Fertodi, Yadrionaya, Sofya,
	b	3-5-7-8-9-11-29- 30-37-39	Risagar, Liangye Molecules: rich in ethyl butanoate, phellandrene, terpinen-4-ol/ poor in <i>a</i> -terpinene, myrcene, limonene, <i>b</i> -caryophyllene Varieties concerned: Liangye, Ben Lomond
MFA + HCPC	с	13-25-26-27-28- 38	
	d		Molecules: rich in <i>cis-b</i> -ocimene, <i>trans-b</i> -ocimene, 3- carene, terpinolene/ poor in eucalyptol, <i>b</i> - caryophyllene, <i>a</i> -terpineol, terpinolen-4-ol Varieties concerned: Tenah, Ben Nevis, Wellington, Kristin
	e	6-16-17-18-19- 20-21-24-40-42- 43-45-46	Poor graphical representation, it is not possible to draw conclusion
	α	25-26-27-28-38	Molecules: rich in <i>a</i> -terpinene, <i>g</i> -terpene, <i>p</i> -cymene, <i>a</i> -terpinolene (<i>b</i> -caryophyllene)/ poor in methyl and ethylbutanoate Chemical family: poor in aldehydes
	β	4-10-14	Molecules: rich in <i>a</i> -pinene, limonene, terpinene, myrcene Chemical family : rich in terpene Odor: poor in alcoholic, fermented, and dairy notes
NMDS	χ	(1-5)-31-32-33- 34-35	Molecules: poor in 3-carene, <i>cis</i> and <i>trans-b</i> -ocimene, phellandrene Chemical family : rich in acids, terpenoids and alcohold Odor: rich in nuts and fermented notes
	δ	39	Molecules: poor in <i>a</i> -pinene, limonene, terpinene, myrcene Chemical family : rich in ketones
	ε	15- (22)-23-40- 41-44-45	Molecules: rich in sabinene, 3-carene, phellandrene, <i>cis</i> and <i>trans-b</i> -ocimene, methyl and ethyl butanoate Chemical family : rich in aldehydes

	Molecules: poor in <i>a</i> -pinene, limonene, terpinene,
9.0.10	, myrcene
ф 8-9-12-:	Chemical family : rich in esters
	Odor : rich in fermented, alcoholic, oily, fruity, and
	dairy notes

Figure captions

Figure 1: Flowchart for the methodology of the meta-analysis

Figure 2: Mind-map overview of differences in study parameters of the reviewed studies.

Figure 3: Main flavor compounds reported for Blackcurrant berries

(Among the 351 molecules reported in the different publications, these 21 compounds were reported with the highest contents for at least 10 varieties upon 36). Error bars correspond to standard deviation.

Figure 4: MFA: graphs of individuals. 4a: dimensions 1 x 2 - 4b: dimensions 1 x 3

Figure 5: MFA graphs of variables and plots of the groups of variables

5a: dimensions 1 x 2 - 5b: dimensions 1 x 3

Correspondence of codes for correlation circles

M.t4o = terpinen-4-ol, M.ebu = ethyl butanoate, M.lim = limonene, M.eca = eucalyptol, M.ter = terpinolene, M.3ca = 3-carene, M.mbu = methyl butanoate, M.myr = myrcene, M.cib = *cis*-b-ocimene, M.ato = *a*-terpineol, M.gtp = *g*-terpinene, M.sab = sabinene, M.api = *a*-pinene, M.trb = *trans-b*-ocimene, M.phl = *b*-phellandrene, M.atp = *a*-terpinene, M.pcy = *p*-cymene, M.bca = *b*-caryophyllene.

Correspondence of codes for groups' representation

Quali = qualitative variables (supplementary variable), Famy = chemical family, Mole = volatile molecules, Odor = odor description.

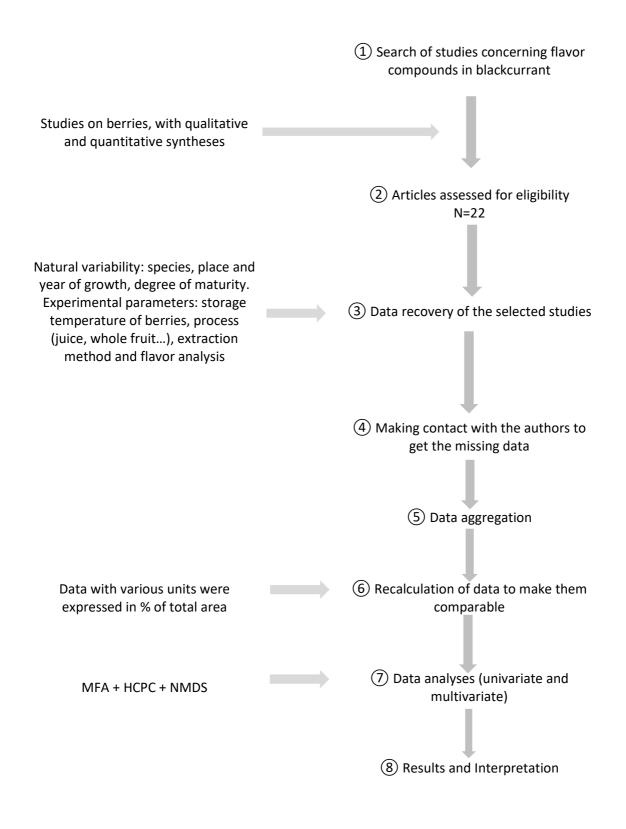


Figure 1.

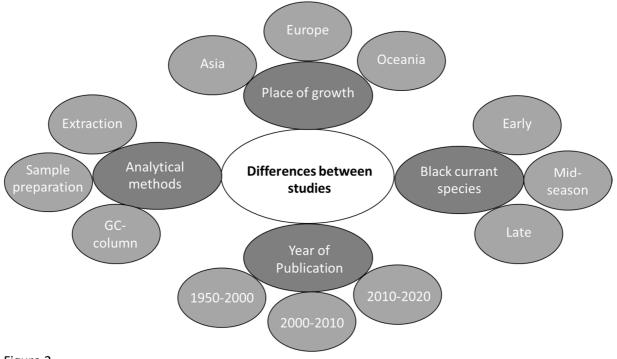


Figure 2.

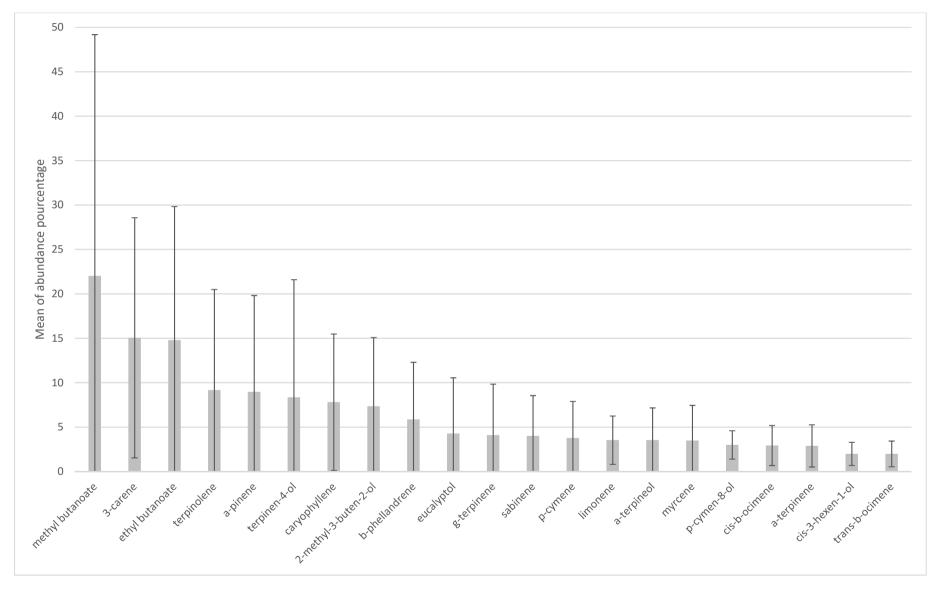


Figure 3.

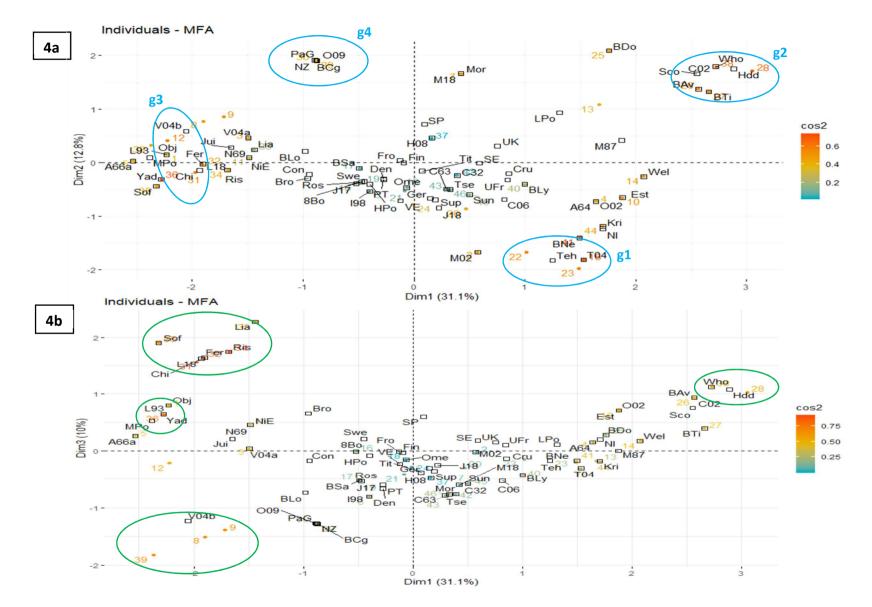


Figure 4.

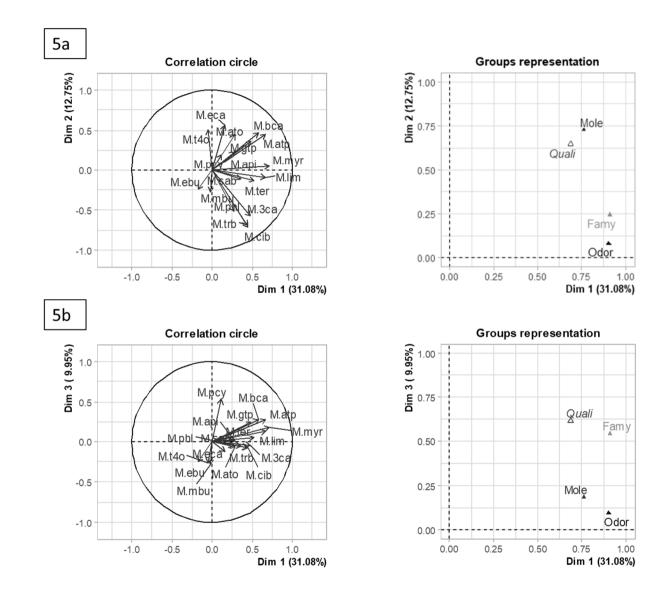


Figure 5.

Appendices

Table A.1.

Odor descriptors regrouped by categories on the basis of personal knowledge and definitions from (*) (Zarzo, 2013) and (**)(De Rovira, 1999)

Category	Descriptors
Citrus	Citrus, orange, lemon, petit-grain, lime, peel**, rind
Green	Green, herbal, leafy, grassy, cucumber
Spicy	Spicy, clove, thyme, pepper, cilantro, oregano, cumin, caraway, licorice
Woody	Woody, pine, cypress, cedar, resinous, balsamic*, powdery*
Dairy	Dairy, buttery, milky, cheesy, butyric, creamy
Floral	Floral, violet, lilac, rose, geranium, vanilla, soapy, iris, coumarin**, cananga**, honey
Minty	Minty, fresh, eucalyptus, camphorated, cooling, medicinal, wintergreen
Alcohol	Alcohol, winey, cognac, fusel*, maraschino
Fermented	Fermented, spoiled, bready, yeast
Nutty	Nutty, marzipan, almond, walnut, peanut, cereal**, seed**, cocoa
Cooked	Cooked, burnt, roasted, smoky, cooked meat, coffee, caramel
Fruity	Fruity, apple, berry, grape, plum, pear, apricot, juicy, tutti fruity, melon, cherry
Lipid	Lipid, fatty, gassy, rancid, oily, frying, waxy
Tropical	Tropical, pineapple, banana, mango, lychee, coconut
Vegetable	Vegetable, cabbage, onion, garlic, beany, cauliflower, tea, hay, horseradish, potato
Earthy	Earthy, moody, dirty, tobacco, root, beetroot, mushroom, musty
Chemical	Chemical, solvent, ethereal, aldehydic, estery, phenolic, vitamin, terpenic
Taste & trigeminal	Warm, acidic, sour, pungent, bitter, dry**, Sweet

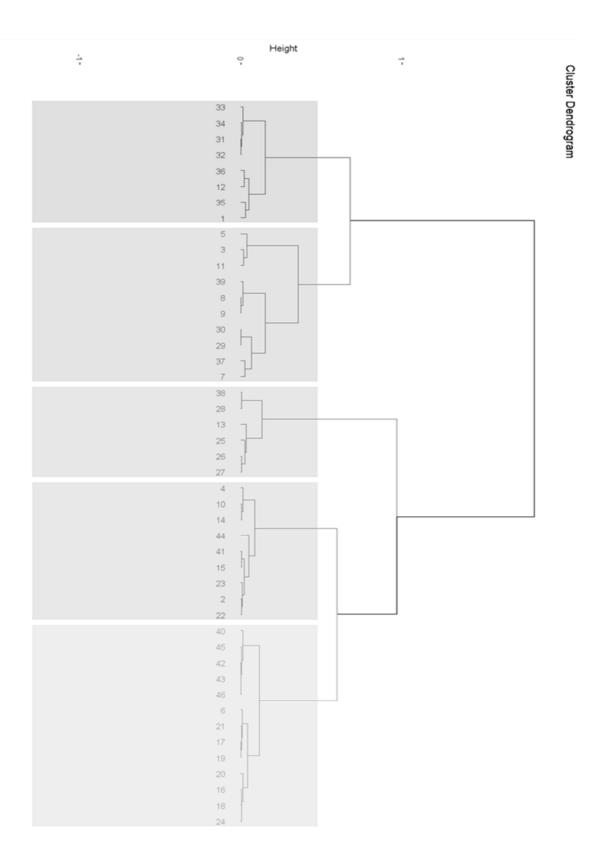


Figure A.1.

Dendrogramm generated by the hierarchical clustering on principal components (HCPC) showing the different groups of individuals

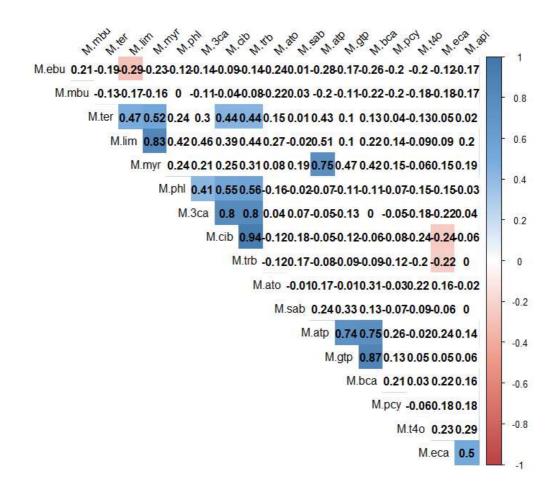


Figure A.2.

Matrix of correlations showing significant p-values

(M.bca/M.atp = 0 /0.75; M.cib/M.3ca = 0 / 0.8; M.3ca/M.trb = 0 / 0.8; M.cib/M.trb = 0 / 0.94).