

# Flavor compounds in blackcurrant berries: Multivariate analysis of datasets obtained with natural variability and various experimental parameters

Sandy Pagès-Hélary Pagès-Hélary, Laurence Dujourdy, Nathalie Cayot

## ▶ To cite this version:

Sandy Pagès-Hélary Pagès-Hélary, Laurence Dujourdy, Nathalie Cayot. Flavor compounds in blackcurrant berries: Multivariate analysis of datasets obtained with natural variability and various experimental parameters. LWT - Food Science and Technology, 2022, 153, pp.112425. 10.1016/j.lwt.2021.112425 . hal-03394363

# HAL Id: hal-03394363

https://institut-agro-dijon.hal.science/hal-03394363v1

Submitted on 16 Oct 2023

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



- 1 Flavor compounds in blackcurrant berries: multivariate analysis of
- 2 datasets obtained with natural variability and various experimental
- **parameters**

9

- 4 Sandy Pagès-Hélary<sup>a</sup>, Laurence Dujourdy<sup>b</sup>, Nathalie Cayot<sup>a\*</sup>
- 5 a Univ. Bourgogne Franche-Comté, AgroSup Dijon, PAM UMR A 02.102, F-21000 Dijon, France
- 6 <sup>b</sup> Agrosup Dijon, Service d'Appui à la recherche, F-21000 Dijon, France
- 7 \* Corresponding author: AgroSup Dijon, PAM UMR A 02.102, 1 esplanade Erasme, F-21000 Dijon,
- 8 France, nathalie.cayot@agrosupdijon.fr

## 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 meta-analysis. 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.

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.

**Keywords**: blackcurrant berries, aroma compounds, GC-MS, meta-analysis, multivariate statistical analyses

## 1. Introduction

- 35 Blackcurrant berries (*Ribes nigrum L.*) are cultivated in different countries for diverse uses. The biggest
- 36 producing country of blackcurrant is Poland (Cortez and Gonzalez de Mejia, 2019), where berries are usually
- 37 used for juices and jam.
- 38 Blackcurrant berries and buds are also commonly used for the production of alcoholic beverages (wine,
- 39 liqueur and spirits) or for the production of essential oil, especially to make perfumes and food flavoring.
- 40 This last commercial sector represents a small volume of production, but an important economical part.
- 41 (Gerbaka, 2013)
- 42 The variety of blackcurrant is chosen according to its use. For juices and jams, variety must yield large and
- 43 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
- 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)).
- 49 However, as methods used to study flavor compounds were very different, authors did not succeed to
- 50 compare their results to other ones already published. Besides, it was hard to find studies dealing with the
- 51 impact of the geographic growing area on the aroma profile of berries. Finally, none of the published studies
- 52 clearly highlighted which parameter affected the most the flavor profile of blackcurrant berries.
- 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.
- 56 It is thus essential to perform a bibliometric analysis and a meta-analysis using statistical methods to
- 57 combine data from multiple experiments, as an objective and quantitative approach for summarizing results
- of published studies.

- Therefore, the present review aimed to highlight the parameters that influenced the more the aroma compounds recovered from blackcurrant berries. In order to proceed to this study, we compared several publications, based on:
  - 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

70

83

62

#### 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.

## 2.1. Data collection

- 71 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
- 73 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
- 75 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
- 81 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
   iuice),
- 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).

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 nectars and jams, and French authors studied the Noir de Bourgogne cultivar, used in liquors. Methods used to extract the volatile fraction were evolving with technological improvements along years: solvent extraction was used mainly in the oldest studies and SPME was dominating for the newest ones. The resulting main aroma compounds reported in studies were thus quite different but consistent. Giving the fact that different extraction methods could give complementary information, we decided to keep data from all the different methods.

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.

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

## 2.2. Data curation

94

95

96

97

98

99

100

101

102

107

108

109

The 22 selected studies counted for 36 different types of samples. They gave a pool of 351 identified volatile 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, were representative 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).

112

113

114

115

116

117

118

119

120

125

126

127

128

129

130

131

132

133

134

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

## 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.

## 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)).

## 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.,
- 2008)); Great Britain ((Ruiz del Castillo and Dobson, 2002), (Marriott, 1986), (Nursten and Williams,
- 143 1969)).

144

136

137

# 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
- 147 (-20°C and above), and deep-freezing (below -20°C).
- 148 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
- 150 (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
- 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)).
- 155 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
- 157 von Sydow, 1964)).

158

## 2.3.4. Sample preparation

- Blackcurrant berries were often processed before analysis. ((Ruiz del Castillo and Dobson, 2002) is the only
- study using whole berries.
- In case of "crushed berries", we found berries as such ((Marriott, 1986) (Ruiz del Castillo and Dobson,
- 162 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),
- 164 (Andersson and von Sydow, 1966a), (Andersson and von Sydow, 1966b), (Marsol-Vall et al., 2018), (Harb
- 165 et al., 2008).

170

174

- Juices could be pure pasteurized juices ((Varming et al., 2004), (Mikkelsen and Poll, 2002), (Bagger-
- Jørgensen 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.

## 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).

## 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
- 177 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,
- 180 1993)
- High polarity: DB-WAX ((Varming et al., 2004), (Hempfling et al., 2013), (Jung et al., 2017),
- 182 (Mikkelsen and Poll, 2002), (Bagger-Jørgensen et al., 2004)), HP-INNOWAX ((Liu et al., 2018)
- 183 (Iversen et al., 1998), ZB-WAX (Harb et al., 2008).

# 2.4. Multivariate data analyses

186	In order to explore more in depth the dataset and reveal the existence of some specific groups, we used
187	factorial analysis and hierarchical clustering.
188	Multiple factor analysis (MFA) is a multivariate data analysis method for summarizing and visualizing a
189	complex data table, in which observations are described by several sets of variables (quantitative and /or
190	qualitative) structured into groups. MFA seeks the common structures present in all or some of these sets. It
191	is performed in 2 steps: (1) a Principal Component Analysis (PCA) is performed on each data set, which is
192	then "normalized" by dividing all its elements by the square root of the first eigenvalue obtained from of its
193	PCA and (2), the normalized data sets are merged to form a unique matrix and a global PCA is performed on
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).
204	Multidimensional scaling (MDS) is a multivariate statistical technique used to create a map in which the
205	distances between all pairs of items match the distances in the original distance matrix as closely as possible.
206	The input to an MDS analysis is the same as the input to hierarchical cluster analysis—a distance matrix.
207	Conversely, when the distances are converted into rank distances, a nonmetric multidimensional scaling
208	(NMDS) is used. A benefit of NMDS is that it allows responses that are less precise. Therefore, easier
209	response tasks can be used to obtain this type of similarity data.
210	The results produced by the MDS methods and clustering techniques are used to describe the interrelations
211	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 R-4.0.0 (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 " (Kassambara 2020), "MASS" (Venables and Ripley 2002), "yegan" (Oksanen et al., 2010)

 $\textbf{219} \qquad \textbf{(Kassambara, 2020)} \text{ , "MASS" (Venables and Ripley, 2002), "vegan" (Oksanen et al., 2010).}\\$ 

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.

## 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.

The volatile profile of the cultivar Brödtorp was mainly characterized by ethyl acetate, terpinen-4-ol, p-

# 3.1.1. Impact of cultivars

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-4-ol, *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

## 3.1.2. Impact of countries

blackcurrant berries.

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-1-ol, *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)).

# 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

# 3.1.4. Impact of sample preparation

- The identified volatile compounds reported for the different ways of sample preparation were clearly
- 273 different.

descriptors.

266

270

271

280

- 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.

# 3.1.5. Impact of the extraction method for volatile compounds

- 281 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.
- Dynamic headspace extraction (DHS) favored esters (fruity notes), such as ethyl hexanoate and methyl
- 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.

# 3.1.6. Impact of GC-column

- Molecules identified using low polarity columns were molecules with quite high molecular weights (above
- 292 10 carbons), and were mainly terpenes and terpenoids.
- 293 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

296

287

288

289

290

# 3.2. Multivariate analysis and clusters of individuals

- 297 Dataset was composed of several categorical variables such as variety of studied blackcurrant berries or
- 298 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
- 300 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
- 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
- 305 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.
- 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).

312 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, 313 314 whereas a squared cosine of 0 indicated that the observation is on an orthogonal direction to the axis. We 315 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: 15-22-23-316 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 317 side dimension 1-axis, and 29-30 (g4) in the upper side along dimension 2-axis. 318 319 Figure 4b showed the dimension 1 x dimension 3 plan for observations. We considered that observations with sum of cos<sup>2</sup> above 0.6 were correctly represented in the plan. We also obtained four clusters of 320 321 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. 322 As in standard PCA, the variable loadings were the correlation between the original variables and the global 323 324 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") 325 and dimensions. 326 327 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 328 329 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 330 mainly characterized by chemical molecules especially M.t4o; on the contrary, g1 was mainly characterized 331 by M.phi and M.3ca. 332 On figure 5a, the coordinates of the three active groups of frequencies (named Famy and Odor) on the first 333 dimension were almost identical. This meant that they contributed similarly to the first dimension. 334 Concerning the second dimension, the two groups - Mole and Quali - had the highest coordinates indicating 335 336 a highest contribution to the second dimension. From figure 5b, it could be observed that the variable "Chemical family - Famy" mainly contributed to 337

dimensions 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).

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

345

346

347

348

339

340

341

342

343

344

- 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.
- 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, and
- from northern countries (Sweden, Denmark, Germany, and Finland).
- 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.

Indications for volatile compounds typical of some cultivars could be given. They concerned volatile compounds that were representative of a cultivar but that did not appear in the list of the main volatile compounds given for blackcurrant berries:

- ethyl acetate and 3-methyl-1-butanol for the cultivar Brödtorp
- ethyl hexanoate and ethyl acetate for the cultivar Ben Lomond.
- Other parameters clearly had an impact on the detected volatile compounds but no clear tendency could be drawn from data description.
- 371 Linear multivariate analysis was firstly done, but, as representativeness of observations might seem quite
- 372 low, we decided to comfort the linear multivariate analysis with another method: non-Metric
- 373 Multidimensional Scaling (NMDS).

367

- 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
- 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
- tends to extract more factors (dimensions) than MDS; as a result, MDS often yields more readily,
- 380 interpretable solutions. Most importantly, however, MDS can be applied to any kind of distances or
- similarities, while factor analysis requires us to first compute a correlation matrix. MDS can be based on
- 382 subjects' direct assessment of similarities between stimuli, while factor analysis requires subjects to rate
- 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  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\delta$ ,  $\epsilon$ , and  $\phi$  in table 5.
- Observations belonging to a same cluster whatever the multivariate analysis were in color other than black.
- From that, we obtained mainly four consolidated clusters, which were the following ones, characterized by
- 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.
- Nevertheless, this confirms that further research still has to be done to establish clearly the typically of given cultivars that are empirically known to give specific organoleptic properties to manufactured products. It also permitted us identifying the important molecules to target, the experimental conditions to control, and selecting appropriate method for future works.

**Credit authorship contribution statement** 412 413 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 **Declaration of Competing Interest** 417 The authors declare that they have no known competing financial interests or personal relationships that 418 419 could have appeared to influence the work reported in this paper. 420 Acknowledgement 421 422 We want to acknowledge Geoff Langford (brand manager at Bayer New Zealand Limited, New Zealand) for 423 additional information on publication (Ohlsson, 2009), and Stefanie Sharma (general manager at 424 International blackcurrant association, France) and Dorota Jarret (fruit breeder and researcher at James 425 Hutton Limited, Scotland) for details on blackcurrant cultivation. 426 **Funding** 427 428 This work was supported by the Regional Council of Bourgogne – Franche Comté and the "Fond Européen agricole pour le développement rural" (FEADER) for the project "Pérennité de la filière cassis en 429 430 Bourgogne".

## References

431

445

446

447

448

449

450

451

452

453

454

455

456

457

458

459

460

461

462

463

464

465

466

467

468

469

470

471

- 432 Dictionary of Flavors.
- 433 ABDI, H. & VALENTIN, D. (2007). Multiple factor analysis (MFA). In N.J. Salkind (ed.) Encyclopedia of measurement and statistics (pp 657-663). Thousand Oaks.
- 435 ANDERSSON, J. & VON SYDOW, E. 1964. The Aroma of Black Currants. I. Higher Boiling Compounds. 436 *Acta Chemica Scandinavica*, 18, 1105-1114.
- 437 ANDERSSON, J. & VON SYDOW, E. 1966a. The Aroma of Black Currants. II. Lower Boiling Compounds. 438 *Acta Chemica Scandinavica*, 522-528.
- 439 ANDERSSON, J. & VON SYDOW, E. 1966b. The Aroma of Black Currants. III. Chemical Characterization 440 of Different Varieties and Stages of Ripeness by Gas Chromatography. *Acta Chemica* 441 *Scandinavica*, 20, 529-535.
- 442 ANJOU, K. & VON SYDOW, E. 1966. Variation in the composition of fruit juices: a study of the literature. *SIK Rapport*.
- 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.
  - BÉCUE-BERTAUT, M., PAGÈS, J. 2008. Multiple factor analysis and clustering of a mixture of quantitative, categorical and frequency data *Computational Statistics & Data Analysis*, 52, 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.
  - CORTEZ, R. E. & GONZALEZ DE MEJIA, E. 2019. Blackcurrants (*Ribes nigrum*): A Review on Chemistry, Processing, and Health Benefits. *Journal of Food Science*, 84, 2387-2401.
  - DE ROVIRA, D. A. (1999). The Dictionary of Flavors: And General Guide for Those Training in the Art and Science of Flavor Chemistry. Wiley.
  - GERBAKA, S. 2013. Le cassis (Ribes nigrum L.) : études botanique, chimique et effets thérapeutiques. Sciences pharmaceutiques. dumas-00844030
  - HADLEY WICKHAM, R. F., LIONEL HENRY AND KIRILL MÜLLER 2020. dplyr: A Grammar of Data 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.
- HUSSON, F., LÊ S., PAGÈS J. (2017). Exploratory Multivariate Analysis by Example Using R. Chapman;
  Hall/CRC.
- 475 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.
- 483 KASSAMBARA, A. & MUNDT, F. 2020. Factoextra: Extract and Visualize the Results of Multivariate
  484 Data Analyses. . [Online]. Available: https://CRAN.R-project.org/package=factoextra
  485 [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.
- LÊ, S., JOSSE, J. & HUSSON, F. 2008. FactoMineR: An R package for multivariate analysis. *Journal of Statistical Software*, 25, 1-18.
  - LEINO, M. & KALLIO, H. 1993. Volatile compounds of blackcurrant juice and wine. *Zeitschrift für 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.
  - NURSTEN, H. E. & WILLIAMS, A. A. 1969. Volatile constituents of the black currant, *RIBES NIGRUM L*.: II.—The fresh fruit. *Journal of the Science of Food and Agriculture*, 20, 613-619.
  - OHLSSON, A. 2009. *Comparison of flavour compounds in juices from different blackcurrant varieties.*PhD, University of Kalmar, School of Pure and Applied Natural Sciences.
  - OKSANEN, J., BLANCHET, F. G., KINDT, R., LEGENDRE, P., O'HARA, B., SIMPSON, G., SOLYMOS, P., 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.
  - R\_CORE\_TEAM 2020. *R: A language and environment for statistical computing. ,* Vienna, Austria, R 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.
- RSTUDIO\_TEAM. 2020. RStudio: Integrated Development for R. , Available from: 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.

530 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., 531 ROTHE, M. & SCHIEBERLE, P. (eds.) State-of-the-art in flavour chemistry and biology. 532 533 Garching: Deutsche Forschungsanstalt für Lebensmittelchemie. 534 TIMM, N. H. (2002). Cluster Analysis and Multidimensional Scaling. In N. H. Timm (Ed.), Applied Multivariate Analysis. Springer Texts in Statistics. Springer. 535 536 VARMING, C., ANDERSEN, M. L. & POLL, L. 2004a. Influence of thermal treatment on black currant 537 (Ribes nigrum L.) juice aroma. Journal of Agricultural and Food Chemistry, 52, 7628-7636. 538 VARMING, C., PETERSEN, M. A. & POLL, L. 2004b. Comparison of isolation methods for the 539 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. 540 541 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. ZARZO, M. 2013. What is a Fresh Scent in Perfumery? Perceptual Freshness is Correlated with 543 544 Substantivity. Sensors, 13, 463-483.

References		Growth area of Variety of berries berries		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)	1		acetone, methyl acetate, ethyl acetate, propanol, 2-methyl-3-buten-2-ol, isobutanol, terpinen-4-ol				
(Andersson and Sydow, 1966b)	von	Sweden		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 warieties mix)	SE + distillation of the extract	<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
(Leino and Kallio, 1993) <sup>b</sup>	Finland	Öjeby	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) <sup>a</sup>	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	a-pinene, myrcene, limonene, eucalyptol, a-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) <sup>a</sup>	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 <sup>b</sup>	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 <sup>b</sup>	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 <sup>b</sup>	Denmark	Ben Lemond	SE	ethyl butanoate, 2-methyl-3-furanthiol, methional, butanoic acid
(Bagger-Jørgensen et al., 2004)	Denmark	Ben Lemond	DHS: 30°C – 60 min – Tenax 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- 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	1	
(Hempfling et al. 2013) <sup>a</sup>	, Germany	N.I.	VE: 35°C – 2h at 1-10 mbar	trans-2-hexenal, trans-2-hexen-1-ol, cis-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	HS-SPME: 45°C – 30 min – triphasic fiber	undecane, eucalyptol, <i>cis</i> -rose-oxide, terpinolene, terpinen-4-ol, <i>a</i> -terpineol	
(Jung, 2018) <sup>a</sup>	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	

SE: solvent extraction, VE: vacuum-headspace extraction, DHS: dynamic headspace extraction, HS-SPME: solid-phase micro extraction of the headspace,

N.I.: not indicated

549

<sup>&</sup>lt;sup>a</sup> reference with GC-O or GC-sniffing results, <sup>b</sup> 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		
a-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		
a-phellandrene	99-83-2	TERPENIC, CITRUS, GREEN, woody, black pepper, fresh		
a-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, fatty, mushroom, cognac		

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

<sup>\*(</sup>Latrasse et al., 1982), \*\* (Hempfling et al., 2013), \*\*\*(Jung et al., 2017)

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

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)

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

Individuals	Varieties	Countries	Storage	Sample type	Publications	Methods	Columns
1	Bro	Swe	Fro	Cru	A64	SE	НРо
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	PT	НРо
9	BNe	Den	Fro	Cru	C06	PT	НРо
10	C32	Den	Fro	Cru	C06	PT	НРо
11	C63	Den	Fro	Cru	C06	PT	НРо
12	Kri	Den	Fro	Cru	C06	PT	НРо
13	Sun	Den	Fro	Cru	C06	PT	НРо
14	Tse	Den	Fro	Cru	C06	PT	НРо
15	Tit	Ger	Fro	Cru	H08	SP	НРо
16	BLo	Den	Fro	Con	198	PT	НРо
17	Ros	Ger	Fro	Cru	J17	VE	НРо
18	Tit	Ger	Fro	Cru	J18	VE	НРо
19	Sup	Ger	Fro	Cru	J18	VE	НРо
20	Sup	Ger	UFr	Cru	J18	VE	НРо
21	Teh	Ger	UFr	Cru	J18	VE	НРо
22	Teh	Ger	Fro	Cru	J18	VE	НРо
23	8Bo	Ger	Fro	Cru	J18	VE	НРо
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	НРо
28	Sof	Chi	Fro	Jui	L18	SP	HPo
29	Yad	Chi	Fro	Jui	L18	SP	НРо
30	Lia	Chi	Fro	Jui	L18	SP	НРо
31	Ris	Chi	Fro	Jui	L18	SP	HPo
32	Fer	Chi	Fro	Jui	L18	SP	НРо
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	PT	НРо
37	NiE	UK	UFr	Con	N69	SE	LPo
38	BCg	NZ	Fro	Jui	009	SP	LPo
39	PaG	NZ	Fro	Jui	009	SP	LPo
40	NI	Est	UFr	Cru	002	SE	LPo
41	NI	Fin	Fro	Cru	T04	SP	LPo
42	BLo	Den	Fro	Jui	V04b	PT	НРо

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

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, Risagar, Liangye
	b	3-5-7-8-9-11-29- 30-37-39	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 α-pinene, limonene, terpinene, myrcene

β-9-12-36

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-bocimene, M.ato = a-terpineol, M.gtp = g-terpinene, M.sab = sabinene, M.api = a-pinene, M.trb = trans-bocimene, 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.

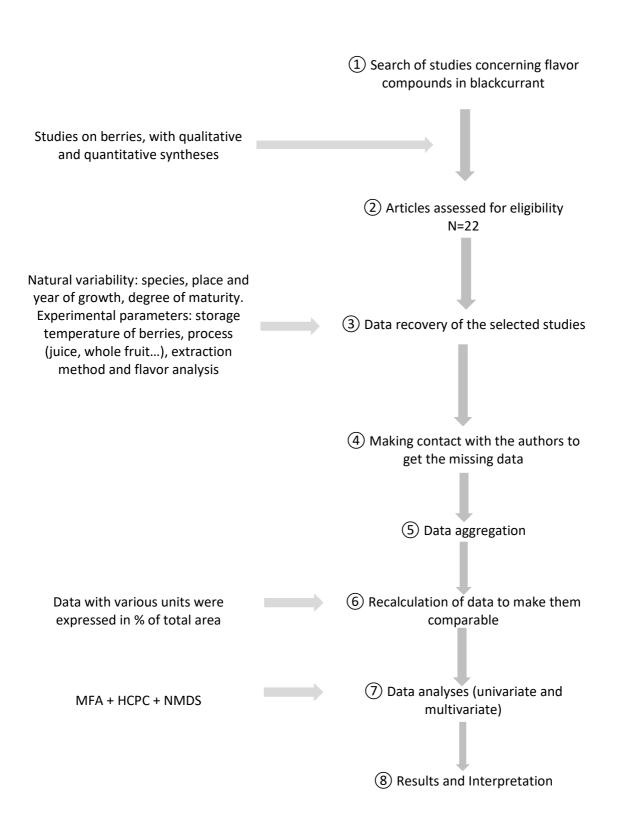


Figure 1.

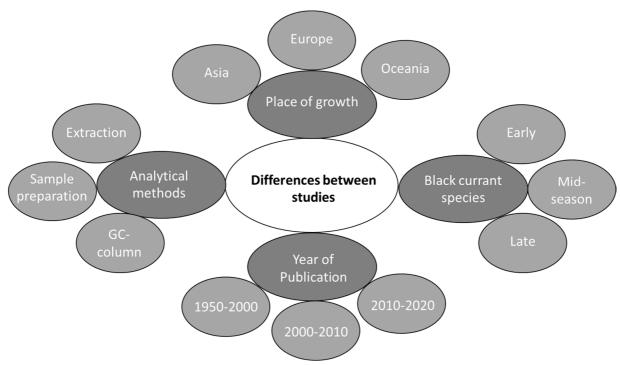


Figure 2.

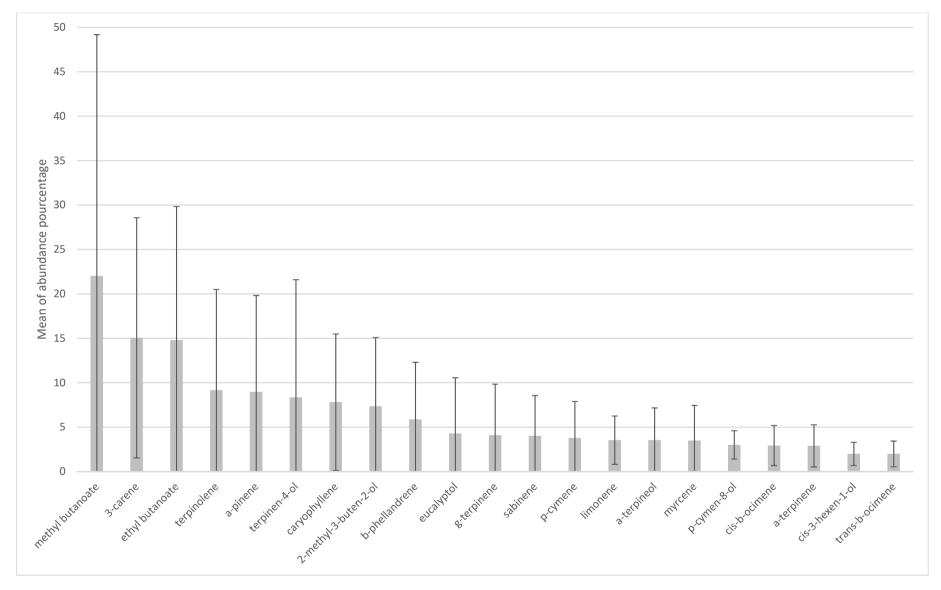


Figure 3.

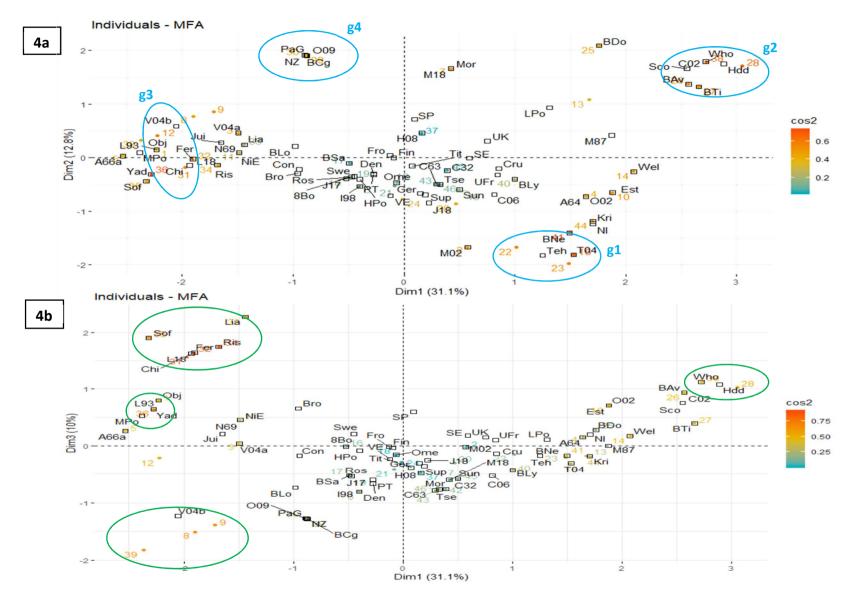


Figure 4.

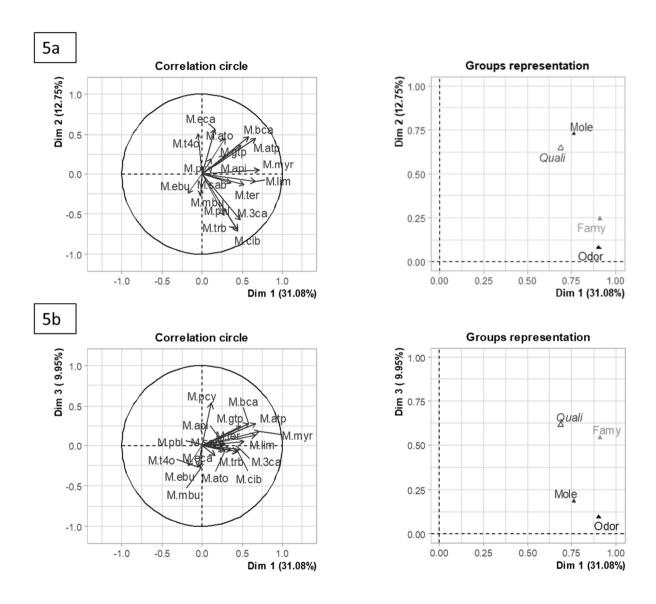


Figure 5.

# 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

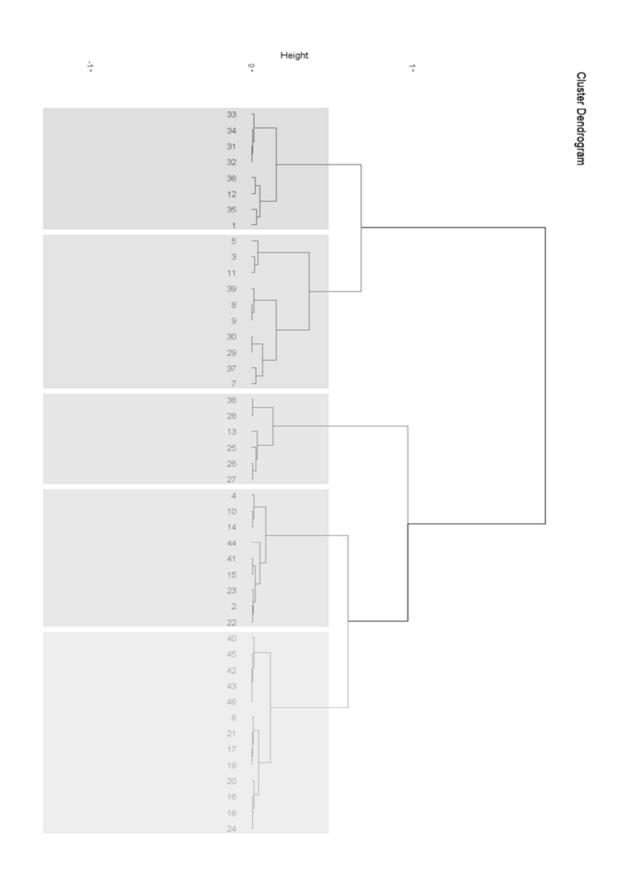


Figure A.1.

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

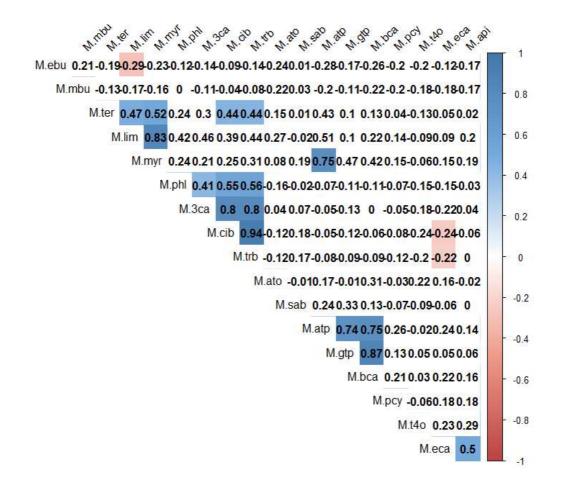


Figure A.2.

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).