Characteristic volatile compounds of Monastrell wines

Compuestos volátiles característicos de vinos Monastrell

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ABSTRACT

Seventy-five percent of the red wines of the Protected Designation of Origin (PDO) Alicante are based on Monastrell grapes. The wine aroma is one of the most important characteristics linked to the quality and consumers’ preferences. Scopus database was used to gather information about the concentrations ranges of the main volatile compounds present in the Monastrell red wines, with their aromatic descriptions and their detection and/or recognition thresholds. Seventeen volatile compounds were identified as those having a significant contribution to this red wine aroma. However, it is important to indicate that there is a need to continue reviewing critically the threshold values (detection and/or recognition) of the main volatile compounds with a "potentially" significant contribution to the odor/aroma/flavor of the Monastrell wines. This information will be essential in preparing reference materials for trained sensory panels calibration for descriptive sensory evaluation of wines.

Keywords: detection threshold; recognition threshold; esters; alcohols; organic acids; terpenes; odor-active-compounds; PDO Alicante.
INTRODUCTION

The production area of the Protected Designation of Origin (PDO) Alicante in 2017 was extended on 14,256 hectares, with 50 registered wineries. Among red wines of the PDO Alicante, 75% are based on Monastrell grapes. Moreover, among red grapes around the world, Monastrell is the second most important variety of red grape, after Tempranillo.

Monastrell wine presents an intense spiced aroma and has versatile characteristics which allows oenologists to develop new wines of high quality. Their aromatic range is very wide, from aromas of raspberries and cherries to black fruits, plums, figs or raisins, and with blackberry notes. Some are fruity and fresh, while others possess a great structure, are persistent and tannic. In some cases, the volatile compounds do not come from the grapes but are produced during winemaking or storage.

Wine aroma is the most important attribute and is linked with quality and consumer preferences. The specific wine flavor depends both on the agronomic conditions of a grape variety and on the winemaking process. Most of the compounds responsible for wine aroma are volatile molecules and can be classified into chemical families, for instance alcohols, carbonyl compounds, acids and esters, sulfur and nitrogen compounds, terpenes, phenols, lactones and hydrocarbons. These compounds are easily released from the hydro-alcoholic matrix and can interact with the olfactory receptors. A low olfactory threshold and enough concentration of each compound are necessary to be perceived. The detection threshold is defined as the minimum amount of substance needed to be detected by an organism, stimulating the olfactory neurons. A molecule to be detected by an olfactory neuron, it must be volatile.

There is a difference between non-active and active aromas, according to the aromatic activity of a compound in a determined matrix; if the odor active value (OAV) of a compound is above 1, the compound will be an odor-active compound and will significantly contribute to the wine odor/aroma.

The aim of this study was to establish the “odor-active” compounds in Monastrell variety red wines. The specific objectives were: (i) accurate review the scientific literature to establish the occurrence of volatile compounds, their normal concentration range, and mean values in Monastrell red wines; (ii) evaluation of the detection and/or recognition thresholds: the concentration from which a scent is detectable or recognizable, respectively, of the odor-active compounds of these wines, and (iii) to develop a final list of odor-active compounds in Monastrell red wines to be used in the preparation of reference materials for training of sensory panels specialized in wine.

MATERIALS AND METHODS

Bibliography

The main studied volatile compounds found in the Monastrell red wines, with their respective aromatic descriptions and their detection and/or recognition thresholds were searched using the Scopus’ database, and 18 references were obtained and studied in detail.

The detection and/or recognition thresholds of the volatile compounds were obtained mainly from four literature sources: Pino and Mesa; Burdock; Pardo-Garcia et al. and Salinas et al.

Statistical analysis

The minimum, maximum, mean and median values were statistically calculated using Micro-
soft Excel 2010 (Microsoft Corporation; Redmond, Washington, USA). With these data, it has been estimated the compounds that have a real contribution to the aroma of these wines, according to the odor activity value (OAV) of a compound “x”, which was calculated according to the Equation 1.

\[ OAV = \frac{C_x}{A_x} \]

Where \( C_x \) is the concentration of compound “x” in the food, \( A_x \) is the olfactory threshold concentration of the compound “x” in the food.

**RESULTS AND DISCUSSION**

**Odor thresholds**

The first finding to be presented and discussed is that there were problems when studying the values of the thresholds. The compound, 1-hexanol, will be taken as a model to discuss this situation. Looking for the threshold of this compound, four references were selected, and the values were as follows: (i) 8000 µg L\(^{-1}\), (ii) 1100 µg L\(^{-1}\), (iii) 8000 µg L\(^{-1}\), and (iv) 500 µg L\(^{-1}\)

Thus, the threshold values ranged between 500 and 8000 µg L\(^{-1}\), a too wide range. Besides there were other two facts, complicating the discussion of the results: (i) it was not always clearly stated whether the reported value corresponded to the detection or recognition threshold and (ii) the matrix used to calculate the threshold was not always reported. Therefore, there is a real need of rigorous research on the determination of detection and especially recognition thresholds in wine matrixes, for example using artificial wine as a model matrix.

In this study, threshold values from a single reference source were used to avoid mixing different matrixes and procedures,\(^6\) besides, it was checked that he reported threshold values in this manuscript agreed well with those also published in trustable wine references.\(^6,7\)

**Concentration of volatile compounds**

The method used to estimate whether a compound was odor-active will be illustrated in two examples:

- For example, a detected volatile compound in Monastrell red wine was 2-methyl-1-butanol, which smells as “onion”. Its concentration range was wide, 19220-231000 µg L\(^{-1}\), with a mean of 130040 µg L\(^{-1}\), a median of 134970 µg L\(^{-1}\) and a threshold value of 300 µg L\(^{-1}\). As the threshold value was much lower than the found concentration, considering the median as the valid value (because it is less sensitive to the found extreme values), its OAV was 450, and thus, 2-methyl-1-butanol can be considered as an odor-active compound in this type of wines.

- The same protocol was used for instance with benzyl alcohol, which has cherry, grapefruit, walnut, slightly spicy notes as odor descriptors. Its concentration range was also wide 40-421 µg L\(^{-1}\), and the mean and median values were 209 and 116 µg L\(^{-1}\), respectively, with a threshold value of 20000 µg L\(^{-1}\). As the threshold value was much higher than the concentration found, the OAV was below 1 and thus the benzyl alcohol is a non-active compound in this type of wines.

As it can be easily guessed from the previous discussion, there were two main factors contributing to the fact that a particular volatile compound was considered as an active-odor-compound, they were that (i) its detection/recognition thresholds are low (low concentration is needed for this compound to be perceived), and (ii) its con-
Concentration is high in the particular wine, whether because it was already present in the grape or because it was generated during winemaking or storage.

Based on the literature survey and the detailed study of the references describing the composition of Monastrell red wines, it was established that 21 compounds should be considered as non-odor-active compounds (Table 1). This meant that these compounds, based on the found data, have no significant contribution to the Monastrell red wines aroma. These volatile compounds were:

(i) alcohols (n = 9): cis-3-hexen-7-ol, 1-butanol, 1-decanol, 1-heptanol, 1-octanol, 1-pentanol, 3-metil-1-pentanol, 4-ethylfenol, and benzyl alcohol; (ii) terpenes (n = 1): nerol; (iii) esters (n = 7): ethyl heptanoate, hexyl acetate, ethyl decanoate, ethyl dodecanoate, ethyl lactate, isobutyl acetate, and methyl acetate; and, (iv) organic acids (n = 4): hexanoic acid, octanoic acid, nonanoic acid, and decanoic acid.

Reviewing the scientific literature on volatile compounds, a total of 17 compounds were found that can have a significant contribution to the Monastrell red wines aroma, and can be nominated as odor-active compounds (Table 2). These compounds can be grouped into 6 chemical families: (i) alcohols (n = 8): 1-hexanol, 1-octen-3-ol (defect), 1-propanol, 2-methyl-1-butanol, 2-phenyl-ethanol, isoamyl alcohol, isobutanol, and methanol (defect); (ii) phenolic compounds (n = 1): 4-ethylguaiačol; (iii) terpenes (n = 3): geraniol, linalool, and nerolidol; (iv) ethyl esters (n = 2): ethyl hexanoate, and ethyl octanoate; (v) Acetates (esters), (n = 2): ethyl acetate, and isoamyl acetate; and (vi) organic acids (n = 1): isobutyric acid.

The median values were selected in this study to calculate the OAV because they are less sensitive to extreme values, and in some cases, wide ranges of concentrations were found. This big fluctuation in the concentrations was expected because of the differences in the Monastrell red wines, due to the diversity of characteristics as affected by farming practices, the age of the wine, or the type of oak barrels used, among other factors.

The information generated in this study will be very useful for groups training sensory panels on wine, such as the group “Food Quality and Safe-

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### Table 1. List of theoretically "non odor-active" volatile compounds (21) found in the literature dealing with Monastrell red wines

<table>
<thead>
<tr>
<th>Compound</th>
<th>Mean</th>
<th>Median</th>
<th>Range</th>
<th>Threshold*</th>
<th>Odor descriptors</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>ALCOHOLS (n=9)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>cis-3-Hexen-1-ol</td>
<td>92</td>
<td>40</td>
<td>3-410</td>
<td>70</td>
<td>Intense green, herbaceous</td>
<td>11,12,13,14,8,15,16,17</td>
</tr>
<tr>
<td>1-Butanol</td>
<td>1258</td>
<td>170</td>
<td>22-3930</td>
<td>500</td>
<td>Fruity, whiskey, vinous</td>
<td>11,18,19,12,14,20</td>
</tr>
<tr>
<td>1-Decanol</td>
<td>339</td>
<td>260</td>
<td>3-780</td>
<td>2200-102000</td>
<td>Greasy, wax, rose</td>
<td>19,14</td>
</tr>
<tr>
<td>1-Heptanol</td>
<td>36</td>
<td>40</td>
<td>2-23</td>
<td>425</td>
<td>Apple, apricot, coconut, walnut</td>
<td>14,19,20,17</td>
</tr>
<tr>
<td>1-Octanol</td>
<td>20</td>
<td>19</td>
<td>3-45</td>
<td>150</td>
<td>Fatty, woody, fresh orange</td>
<td>12,14,10,20,17</td>
</tr>
<tr>
<td>1-Pentanol</td>
<td>66</td>
<td>60</td>
<td>10-170</td>
<td>4000</td>
<td>Sweet, vanilla, fufle</td>
<td>11,21,14,16,20,17</td>
</tr>
<tr>
<td>3-Metil-1-pentanol</td>
<td>56</td>
<td>10</td>
<td>10-301</td>
<td>610</td>
<td>Chocolate, green, vinous, fruity</td>
<td>21,12,14,20,17</td>
</tr>
<tr>
<td>4-Ethylfenol</td>
<td>273</td>
<td>260</td>
<td>100-300</td>
<td>440</td>
<td>Woody, phenolic, medicinal,</td>
<td>21,17</td>
</tr>
<tr>
<td>Benzyl alcohol</td>
<td>209</td>
<td>116</td>
<td>40-421</td>
<td>20000</td>
<td>Cherry, grapefruit, walnut</td>
<td>12,19,20,17</td>
</tr>
</tbody>
</table>

**ESTERS (n=7)** | | | | | | |
| Ethyl heptanoate | 3 | 1 | 1-3 | 2 | Berry, melon, peach, pineapple | 12,14,16 |
| Hexyl acetate | 1145 | 30 | 7-15810 | 2000 | Apple, banana, cherry, floral, pear | 11,19,12,13,14,15,16,20 |
| Ethyl dodecanoate | 215 | 200 | 1-759 | 6300 | Grape, oily, pear, vinous | 11,12,22,14,15,16,20 |
| Ethyl decanoate | 363 | 98 | 16-1972 | 5900 | Green, floral, fruity | 12,22,14,16,20 |
| Ethyl lactate | 59376 | 6420 | 130-923000 | 50000-250000 | Light smell of butter | 11,18,19,21,14,15,20,17 |
| Isobutyl acetate | 94 | 50 | 30-250 | 65-899 | Apple, banana, pineapple, rose | 11,18,15 |
| Methyl acetate | 12813 | 11050 | 7430-21440 | 1500-47000 | Sweet, fruity | 11,19 |

**ACIDS (n=4)** | | | | | | |
| Hexanoic acid | 778 | 260 | 7-4120 | 3000 | Cheese, fatty, rancid, sour, spacy | 19,21,13,14,15,16,20,17 |
| Octanoic acid | 1354 | 1115 | 9.5690 | 3000 | Cheese, oily, fruity-acid | 19,21,12,22,13,14,15,16,20,17 |
| Nonanoic acid | 21 | 10 | 10-48 | 3000 | Wax, bat, cheese, fatty | 21,20,17 |
| Decanoic acid | 483 | 300 | 19-1990 | 10000 | Fatty, sour, unpleasant rancid | 19,21,12,22,13,14,15,20,17 |

* references 6,8
ty” of the Miguel Hernández University of Elche, who is training the certified panel of the PDO Alicante wines (http://www.vinosalicantedop.org/). In particular, the collected information (concentration ranges, mean and median) will serve as a key information for the preparation of the reference materials to be used to describe the main sensory attributes of the Monastrell wines.

CONCLUSIONS

The main reached conclusions in this study were: (i) there is a need of further studies dealing with the threshold determination in wine matrices, and (ii) 17 compounds were considered as odor-active volatile compounds in Monastrell red wines, including 9 alcohols, 3 terpenes, 4 esters, and 1 organic acid.

REFERENCES


7. Burdock GA. *Fenaroli’s Handbook of Flavor Ingre-