

Characteristic volatile compounds
of Monastrell wines

Compuestos volátiles característicos
de vinos Monastrell

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Recibido/ Received:
27.01.2018

Aceptado/ Accepted:
08.03.2019

Cómo citar este trabajo | How to cite this paper

Rita Szikszai A, Issa Issa H, Cano-Lamadrid M and Carbonell-Barrachina AA. Characteristic volatile compounds of Monastrell wines. Revista Doctorado UMH 4(2): p3 (2018). [Online].

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.¹ Moreover, among red grapes around the world, *Monastrell* is the second most important variety of red grape, after Tempranillo.²

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.³

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.⁴ 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.⁵

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,⁶ Burdock,⁷ Pardo-Garcia *et al.*⁸ and Salinas *et al.*⁹

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 $\mu\text{g L}^{-1}$,⁸ (ii) 1100 $\mu\text{g L}^{-1}$,⁹ (iii) 8000 $\mu\text{g L}^{-1}$,¹⁰ and (iv) 500 $\mu\text{g L}^{-1}$.⁶ Thus, the threshold values ranged between 500 and 8000 $\mu\text{g L}^{-1}$, 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 $\mu\text{g L}^{-1}$, with a mean of 130040 $\mu\text{g L}^{-1}$, a median of 134970 $\mu\text{g L}^{-1}$ and a threshold value of 300 $\mu\text{g L}^{-1}$. 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 $\mu\text{g L}^{-1}$, and the mean and median values were 209 and 116 $\mu\text{g L}^{-1}$, respectively with a threshold value of 20000 $\mu\text{g L}^{-1}$. 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-

centration 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-etilfenol, 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 *Mo-*

nastrell 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-ethylguaiacol; (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-

Compound	Mean	Median	Range ($\mu\text{g L}^{-1}$)	Threshold†	Odor descriptors	References
ALCOHOLS (n=9)						
cis-3-Hexen-1-ol	92	40	3-410	70	Intense green, herbaceous	11,12,13,14,8,15,16,17
1-Butanol	1258	170	22-3930	500	Fruity, whiskey, vinous	11,18,19,12,14,20
1-Decanol	339	260	3-750	2200-102000	Greasy, wax, rose	19,14
1-Heptanol	36	40	2-63	425	Apple, apricot, coconut, walnut	14,16,20,17
1-Octanol	20	19	3-45	190	Fatty, woody, fresh orange	12,14,16,20,17
1-Pentanol	66	60	10-170	4000	Sweet, vanilla, fusel	11,21,14,16,20,17
3-Metil-1-pentanol	56	10	10-301	810	Chocolate, green, vinous, fruity	21,12,14,20,17
4-Etilfenol	273	260	160-390	440	Woody, phenolic, medicinal,	21,17
Benzyl alcohol	209	116	40-421	20000	Cherry, grapefruit, walnut	12,16,20,17
TERPENES (n=1)						
Nerol	9	6	3-18	300	Fresh and sweet rose	8,20,17
ESTERS (n=7)						
Ethyl heptanoate	3	1	1-8	2	Berry, melon, peach, pineapple	12,14,16
Hexyl acetate	1145	30	7-15510	2000	Apple, banana, cherry, floral, pear	11,19,12,13,14,15,16,20
Ethyl decanoate	215	200	1-759	6300	Grape, oily, pear, vinous	11,12,22,14,15,16,20
Ethyl dodecanoate	353	98	16-1672	5900	Green, floral, fruity	12,22,14,16,20
Ethyl lactate	59376	6420	130-923300	50000-250000	Light smell of butter	11,18,19,21,14,15,20,17
Isobutyl acetate	84	50	30-250	65-880	Apple, banana, pineapple, rose	11,18,15
Methyl acetate	12813	11690	7430-21440	1500-47000	Sweet, fruity	11,18
ACIDS (n=4)						
Hexanoic acid	778	260	7-4120	3000	Cheese, fatty, rancid, sour, spicy	19,21,13,14,15,16,20,17
Octanoic acid	1354	1115	9-5960	3000	Cheese, oily, fruity-acid	19,21,12,22,13,14,15,16,20,17
Nonanoic acid	21	10	10-46	3000	Wax, bait, 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 6-9

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

Compound	Mean	Median	Range ($\mu\text{g L}^{-1}$)	Threshold [†]	Odor descriptors	References
ALCOHOLS (n=9)						
1-Hexanol	846	709	8-3450	500	Green, herbaceous, woody, sweet	19,21,12,13,14,8,15,16,20,17
1-Octen-3-ol	6	5	4-8	1	Cheese, mushroom, herbaceous,	14,16,20
1-Propanol	18552	22500	60-34640	9000	Apple, musty, earthy, peanut	11,18,19,22,13,14,15
2-Methyl-1-butanol	130040	134970	19220-231000	300	Onion	22,14,15
2-Phenylethanol	26787	13700	112-89190	1100	Honey, rose	11,18,19,21,12,22,13,14,20,17
4-Ethylguaiaicol	39	40	20-60	25	Meaty, smoked	21,17
Isoamyl alcohol	84426	47010	33650-182220	30000	Oily, whiskey	19,21
Isobutanol	39731	46880	1640-106000	75000	Fruity, whiskey, wine-like	18,19,22,13,14,15
Methanol	157547	203105	34640-240180	100000	Fruity smell	15,14,11,18
TERPENES (n=3)						
Geraniol	88	120	2-180	40	Apple, apricot, berry, rose	21,14,8,16,17
Linalool	28	30	1-57	6	Floral, citrus, woody	12,14,8,16,20,17
Nerolidol	42	38	2-89	15	Apple, green, citrus, woody, rose	12,14,8,20
ESTERS (n=4)						
Ethyl hexanoate	195	132	2-600	1	Apple, banana, pineapple, wine-like	19,21,12,22,13,14,15,16,20,17
Ethyl octanoate	749	532	12-1850	194	Apricot, banana, floral, pear	11,18,19,21,12,22,13,14,15,16,20,17
Ethyl acetate	44300	44685	149-161520	5000	Anise, pineapple	11,18,19,12,14,15
Isoamyl acetate	757	614	57-2990	30	Banana, pear, sweet	11,18,19,22,13,14,17
ACIDS (n=1)						
Isobutyric acid	590	475	103-1193	0.4-43	Butter, acid, rancid	14,16,17

[†] references 6-8

Table 2. List of theoretically "odor-active" volatile compounds (17) found in the literature dealing with *Monastrell* red wines

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.

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