

# Volatile Compound and Sensory Analysis for the Characterization of an Italian White Wine from “Inzolia” Grapes

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**Abstract** The research evidences the importance of linking chemical and sensory data for the wine characterization; in particular, the Italian white wine made from Inzolia grapes has been considered. Inzolia is one of the most widespread native white grapes in Sicily (Italy), and wine samples from two different areas (Monreale and Sambuca di Sicilia) have been analyzed. A headspace solid-phase microextraction/gas chromatography–mass spectroscopy method has been developed, and 56 volatile components, esters, fatty acids, alcohols, and terpenes have been identified; the method allows also the quantification of the main components, namely, ethyl octanoate (banana, fruit, fat) (257.2–541.6 mg/l) and ethyl decanoate (fruity, oily, floral; 171.8–272.0 mg/l). A good repeatability in terms of retention times and peak areas resulted. Sensory analysis was performed by ten trained judges that evaluated eight attributes: two referring to appearance (yellow color and yellow reflex), four referring to aroma (fruity, banana, ripened apple, and floral), and two referring to oral perception (acid and pungent). The volatile constituents and the aroma sensory attributes were in agreement.

**Keywords** Wine Characterization · HS-SPME/GC–MS · Volatile Composition · Sensory Analysis · Multivariate Analysis · Inzolia White Wine

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## Introduction

The aroma profile is important in wine, as it contributes to the quality of the final product; it is due to the combined effects of several volatile compounds mainly alcohols, aldehydes, esters, acids, monoterpenes, and other minor components already present in the grapes or being formed during the fermentation and maturation process. All these compounds are responsible for their so-called bouquet on sniffing the headspace from a glass and the odor/aroma component (palate/aroma) of the overall flavor perceived on drinking. Several factors, such as environment (climate and soil), ripeness and grape variety, winemaking as fermentation conditions, and ageing, influence the type and amount of volatile compounds.

Recently, the availability of new analytical techniques, such as the solid-phase microextraction (SPME), that allow the determination of the low-level components in complex mixtures has advanced the understanding of the aroma wine composition. Using SPME, wines from different countries, Germany, (De la Calle Garcia et al. 1998; Ong and Acree 1999) Portugal, (Alves et al. 2005) Greece, (Demyttenaere et al. 2003; Karagiannis et al. 2000) Spain, (Mestres et al. 2002), and Italy (Begala et al. 2002; Bonino et al. 2003), have been analyzed.

The aromatic component of a wine is, moreover, closely related to its sensory quality, which is determined by the consumer's acceptability (Vilanova 2006; Varela and Gàmbara 2006). Recently, sensory analysis has defined its role in the oenological industry identifying the causes of variation of perceived quality, the corrective actions thereby becoming instrument of quality control (Muñoz 2002; Lawless 1995; Moskowitz 1995).

Inzolia is one of the most widespread native white grapes in Sicily (Italy), and it is commonly blended with

Grillo and Catarratto white grapes to make the famous sweet dry “Marsala” wine. As to the best of our knowledge, the information reported in literature on Inzolia wine are limited (Randazzo et al. 1998; Dugo et al. 1994); the present work aimed at its characterization using both aroma volatile and sensory analysis. The analytical approach used for the extraction of aroma volatile compounds was the SPME, already successfully used for the wine characterization, followed by capillary gas chromatography–mass spectroscopy (GC–MS) analysis. The sensory assessment of the Inzolia wine samples followed three steps: visual inspection, smelling, and tasting in the mouth. Quantitative volatile data were matched up to sensory ones.

## Materials and Methods

### Sampling

Twelve samples of Inzolia wine from two different Sicilian vineyards, Monreale (sample numbers 1 to 6) and Sambuca di Sicilia (sample numbers 7 to 12), both in the province of Palermo, have been considered. The wines from 2006 vintage were stored at cellar temperature and analyzed 2 months after the production. Chemical and sensory analyses have been performed, each in triplicate. pH, titratable acidity, and alcohol content were determined according to AOAC methods (1990).

### Sensory Analyses

For the sensory analysis, 25 judges were recruited from students of the Department of Food Science and Technology, University of Catania (Italy). The candidates were submitted to preliminary tests to determine their sensory performance on basic tastes and the aromas associated with wines. The sensory profile was constructed using a selected panel of ten judges (ISO 13299, 2003) trained over five sessions. A list of attributes was selected on the basis of the frequency (%) of the terms used by the judges in several sessions. Reference standards (Noble et al. 1987) were available to define attributes. The final set consisted of eight attributes: two referring to appearance (yellow pale, yellow reflex), four referring to aroma (fruity, banana, ripened apple, floral), and two referring to oral perception (acid, pungent). The different attributes were quantified using a nine-point intensity scale (ISO 4121, 2003). Each judge evaluated 36 wines in 12 sessions each with three wines. All evaluations were conducted from 10:00 to 12:00 A.M. in individual booths (ISO 8589, 1988). Thirty milliliters of each wine was served at  $22 \pm 1$  °C (room temperature) in glasses (ISO 3591, 1977) labeled with a three-digit code and covered to prevent volatile loss. The

order of presentation was randomized among judges and sessions. Water was provided for rinsing between wines.

### Volatiles Extraction: HS-SPME

A 40-ml vial was filled with 20 ml of each sample. The vial was equipped with a “mininert” valve (Supelco, Bellefonte, PA, USA) that allowed the introduction of the fiber without piercing any septum. The septumless “mininert” vial permitted to avoid extraneous peaks due to possible septum bleeding. Extraction was performed in the headspace vial kept at 30 °C using a commercially available fiber housed in its manual holder (Supelco, Bellefonte, PA, USA). All extractions were carried out using a DVB/CAR/PDMS fiber, of 50/30- $\mu\text{m}$  film thickness (Supelco, Bellefonte, PA, USA). The liquid sample was equilibrated for 15 min and then extracted for 20 min. During the extraction, the sample was continuously stirred. After sampling, the SPME fiber was introduced onto the splitless injector of the HRGC/MS using the conditions reported below. The fiber was kept in the injector for 3 min for thermal desorption of the analytes onto the capillary GC column. The split-splitless injector port was maintained at 260 °C. No artifacts were observed after a SPME analysis of water performed as blank analysis.

### Volatiles Analysis: GC–MS

A Varian 3800 gas chromatograph directly interfaced with a Varian 2000 ion trap mass spectrometer (Varian Spa, Milan, Italy) was used to analyze the volatile components. The conditions were as follows: injector temperature, 260 °C; injection mode, splitless; capillary column, CP-Wax 52 CB, 60 m, 0.25 mm i.d., 0.25- $\mu\text{m}$  film thickness (Chrompack Italy, s.r.l. Milan, Italy); oven temperature, 45 °C held for 5 min, then increased to 80 °C at a rate of 10°C/min and to 240 °C at 2°C/min; carrier gas, helium at a constant pressure of 10 psi; transfer line temperature, 250 °C; acquisition range, 40–200  $m/z$ ; scan rate, 1  $\mu\text{s}^{-1}$ . Each component was identified using mass spectral data, NIST’98 (NIST/EPA/NIH Mass Spectra Library, version 1.7, USA), linear retention indices, literature data, and the injection of standards where available. The linear retention indices (LRI) were calculated according to Van den Dool and Kratz (1963). The peak area of each component in total ion current chromatograms was determined during three replicates, and the average value was calculated.

The repeatability of the developed method was determined by analyzing three different samples of the same wine under identical experimental conditions; the absolute peak area obtained for each component identified during the three different analyses was tabulated, and the coefficient of variation (CV, %) was calculated. This was <10%

for all the components identified as previously reported (Verzera et al. 2004).

### Quantitative Analysis

The main compounds were quantified in the samples analyzed; each peak quantified was required to have a minimum signal to noise ratio (*S/N*) of 10. Quantitative results were obtained using the method of standard additions. Hexyl acetate, ethyl butanoate, ethyl hexanoate, ethyl octanoate, ethyl decanoate, (*Z*)-ethyl-4-decenoate, 3-methylbutyl acetate (isoamyl acetate), 3-methylbutyl hexanoate (isoamyl hexanoate), 3-methylbutyl octanoate (isoamyl octanoate), butyl octanoate, diethyl succinate, 3-methyl-1-butanol (isoamyl alcohol),  $\beta$ -phenylethyl alcohol, 1-hexanol, (*Z*)-3-hexen-1-ol, hexanoic acid, octanoic acid, and decanoic acid were purchased from Sigma-Aldrich s.r.l. (Milan, Italy) of the highest purity available, whereas  $\beta$ -phenylethyl acetate was purchased from Panreac (Barcelona, Spain). Standard solutions were added to multiple aliquots of a sample wine. The sample alone was analyzed, too. The quantification was based on a calibration curve that was generated by plotting the detector response versus the amount spiked of each standard. Each sample measurement was repeated three times. To quantify (*Z*)-ethyl-3-decenoate, (*E*)-ethyl-4-decenoate, and 4-hexenyl acetate, being standards not available, it was used as the calibration curve of the ester with the most similar peak area.

### Statistical Analysis

Sensory data were statistically analyzed using FIZZ software. Both sensory and chemical data were submitted to variance analysis (ANOVA) using the Statgraphic plus software (v5.1). Duncan's multiple-range test was applied to the chemical data to determine the presence of significant differences between the analyzed samples; the model was statistically significant with a *P* value less than 0.05.

## Results

Table 1 reports the mean values of pH, titratable acidity, and the alcohol content for each of the analyzed sample. The sensory analysis (Fig. 1) described the aroma of the Inzolia wine as fruity, banana, ripened apple, and floral; each term showed similar scores. Only yellow reflex attribute was significantly different between the samples from the two different production areas.

As regards the volatile fraction, 56 components were identified in each sample analyzed, specifically esters, fatty acids, alcohols, monoterpenes, and aromatic compounds. Table 2 reports all the identified components together with their retention times (RT) and linear retention indices (LRI) calculated on CP-Wax 52 CB column. Table 3 shows the quantified components and their amount (mg/l) in the analyzed samples.

Esters constituted the main class of substances; they constituted more than 95% of the total volatile fraction. Ethyl esters of fatty acids and acetates of higher alcohols were the dominating esters in the analyzed wine: linear and branched, saturated and unsaturated methyl, ethyl, butyl, isoamyl esters of fatty acids from C<sub>2</sub> to C<sub>16</sub> have been identified. In our samples, the main components were ethyl octanoate (banana, fruit, fat; 257.2–541.6 mg/l) and ethyl decanoate (fruity, oily, floral; 171.8–272.0 mg/l).

Among the less represented components, isoamyl acetate (banana; 8.2–15.1 mg/l) and 4-hexenyl acetate (banana; 0.4–1.3 mg/l) have been identified, too. Other important aroma compounds were diethyl succinate (3.3–6.7 mg/l) described as wine and fruit and  $\beta$ -phenylethyl acetate (1.2–3.2 mg/l) as rose and honey.

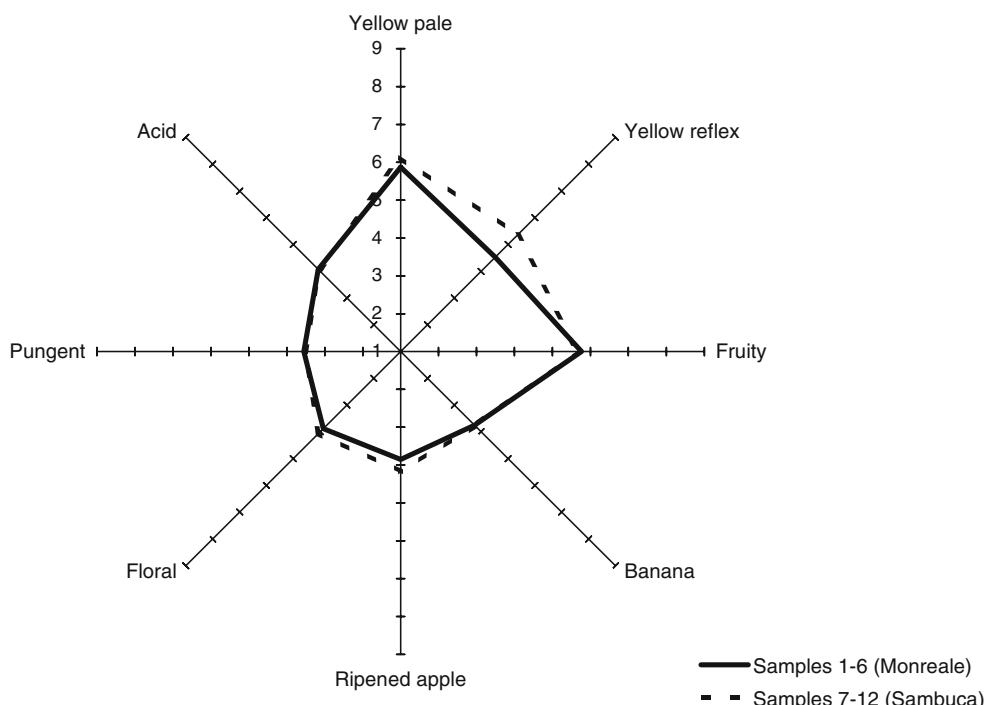
As regards esters, no statistically significant differences resulted for most of components among the analyzed samples, excluding, for example, ethyl octanoate whose amount resulted significantly higher in samples 8 and 12 (Monreale) and  $\beta$ -phenylethylacetate that was present in a higher amount in all the samples from Monreale.

**Table 1** Average values of physicochemical parameters of the analyzed Inzolia wine samples

Sample	Production Area	pH	Titratable acidity (g/l)	Alcohol (%/vol)
1	Monreale	3.35±0.02 a	5.30±0.06 b	11.73±0.12 ab
2	Monreale	3.32±0.03 a	5.95±0.06 ab	11.23±0.06 ab
3	Monreale	3.34±0.01 a	6.10±0.04 a	11.23±0.06 ab
4	Monreale	3.24±0.03 a	5.86±0.06 ab	10.40±0.00 b
5	Monreale	3.23±0.03 a	6.28±0.11 a	10.60±0.00 b
6	Monreale	3.26±0.01 a	6.30±0.08 a	10.87±0.06 b
7	Sambuca	3.38±0.02 a	5.93±0.15 a	10.67±0.06 b
8	Sambuca	3.39±0.01 a	5.43±0.14 b	10.70±0.00 b
9	Sambuca	3.49±0.01 a	5.70±0.04 ab	11.37±0.06 ab
10	Sambuca	3.45±0.02 a	5.86±0.02 ab	12.10±0.10 a
11	Sambuca	3.48±0.01 a	5.70±0.14 ab	11.67±0.06 ab
12	Sambuca	3.46±0.01 a	6.06±0.06 a	11.50±0.00 ab

Different letters in the same row indicate significant differences at *P*<0.05 by Duncan's multiple-range test.

**Fig. 1** Sensory analysis of the analyzed Inzolia wine samples



**Table 2** Compounds identified in the analyzed Inzolia wine samples

Compounds	RT	LRI
Ethyl butanoate	12.43	1,033
Ethyl 3-methylbutanoate	13.39	1,063
Isoamyl acetate	15.32	1,120
Ethyl 2-butenate	16.98	1,162
Limonene	18.33	1,192
Isoamyl alcohol	18.40	1,199
Terpinolene	18.70	1,206
Ethyl hexanoate	19.90	1,231
Isoamyl butanoate	21.29	1,261
Hexyl acetate	21.87	1,274
(Z)-Ethyl 3-hexenoate	21.98	1,276
(E)-Ethyl 3-hexenoate	23.07	1,299
4-Hexenyl acetate	23.89	1,315
Ethyl heptanoate	24.73	1,331
(Z)-Ethyl 2-hexenoate	25.33	1,342
1-Hexanol	25.39	1,343
2-Methylpropyl hexanoate	25.68	1,349
(Z)-3-Hexen-1-ol	27.11	1,376
(E)-3-Hexen-1-ol	27.16	1,377
Methyl octanoate	27.78	1,388
Nonanal	28.20	1,396
Ethyl octanoate	30.46	1,436
1-Heptanol	31.09	1,448
Acetic acid	31.18	1,450
Isoamyl hexanoate	31.64	1,458
Furfural	32.09	1,467
(Z)-Ethyl 3-octenoate	33.15	1,483
Propyl octanoate	35.13	1,517
Ethyl nonanoate	36.10	1,535
Butyl octanoate	37.03	1,549

**Table 2** (continued)

Compounds	RT	LRI
Methyl decanoate	39.59	1,593
Diethylene glycol	40.75	1,612
Butanoic acid	41.40	1,623
Ethyl decanoate	42.21	1,637
1-Nonanol	43.06	1,652
Isoamyl octanoate	43.28	1,655
Diethyl succinate	44.17	1,670
(Z)-Ethyl 4-decenoate	45.17	1,687
(Z)-Ethyl 3-decenoate	45.88	1,699
(E)-Ethyl 3-decenoate	46.88	1,717
Propyl decanoate	47.13	1,721
$\beta$ -Phenylethyl acetate	52.43	1,813
Hexanoic acid	53.79	1,840
Ethyl dodecanoate	53.92	1,840
Geranyl acetone	54.59	1,853
Isoamyl decanoate	54.85	1,857
(Z)-Ethyl 3-dodecenoate	56.89	1,895
Phenylethyl alcohol	57.57	1,907
Phenol	62.56	2,001
2-Propyl tetradecanoate	64.30	2,034
(E)-Cinnamaldehyde	64.54	2,040
Ethyl tetradecanoate	64.78	2,045
Octanoic acid	65.07	2,050
1-Tridecanol	65.72	2,063
Ethyl hexadecanoate	75.35	2,161
Decanoic acid	75.45	2,163

TR Retention time, LRI linear retention index calculated on CP-WAX 52 CB column

**Table 3** Average volatile composition (mg/l) as main components and classes of substances of the analyzed Inzolia wine samples

	Odor threshold ( $\mu\text{g/l}$ )	Monreale samples											
		1	2	3	4	5	6	7	8	9	10	11	12
<b>Esters</b>													
Ethyl butanoate	20 (Ferreira et al. 2000)	1.84 b <sup>a</sup>	1.45 a	1.89 b	1.65 ab	2.13 b	1.41 a	1.07 a	2.10 b	1.23 a	1.32 a	2.16 b	1.95 b
Isoamyl acetate	30 (Ferreira et al. 2000)	10.61 a	8.25 a	8.94 a	8.43 a	11.21 a	10.70 a	15.12 b	14.50 b	14.41 b	13.48 ab	13.97 ab	14.72 b
Ethyl hexanoate	14 (Ferreira et al. 2000)	52.79	54.28	46.09	57.65	50.27	43.38	47.95	70.97	53.57	58.33	55.21	63.76
Hexyl acetate	1,500 (Maarse 1991)	1.86 a	1.94 a	1.59 a	1.71 a	1.56 a	1.79 a	2.54 ab	4.05 b	3.39 b	2.71 ab	4.50 b	3.88 b
Ethyl octanoate	580 (Maarse 1991)	474.22 b	357.77 a	434.08 b	374.84 a	445.67 b	410.64 b	343.72 a	514.02 b	257.18 a	360.63 a	454.48 b	541.58 b
Isoamyl hexanoate		1.35 a	1.26 a	1.46 a	1.126 a	1.71 ab	1.17 a	1.12 a	1.81 ab	1.40 a	1.103 a	2.32 b	2.01 b
Butyl octanoate		0.97	0.81	1.02	0.64	1.06	0.78	0.79	1.04	0.80	0.88	0.93	1.07
Ethyl decanoate	200 (Ferreira et al. 2000)	237.98	207.53	233.57	171.79	229.58	175.54	263.75	250.25	228.87	204.48	202.70	271.96
Isoamyl octanoate	125 (Ferreira et al. 2000)	2.68 ab	1.63 a	2.42 ab	2.51 ab	2.143 ab	1.90 a	2.11 ab	3.01 b	3.00 b	1.89 a	2.57 ab	2.53 ab
Diethyl succinate	200,000 (Maarse 1991)	5.10 ab	4.43 a	5.49 ab	6.67 b	5.29 ab	4.50 a	3.32 a	5.72 b	3.81 a	3.88 a	5.01 ab	5.21 ab
(Z)-Ethyl 4-decenoate		66.98	57.23	71.25	66.44	56.46	57.53	47.06	49.59	44.19	56.67	59.04	69.88
(Z)-Ethyl 3-decenoate		2.69 b	1.90 ab	2.40 b	3.08 b	2.27 ab	2.15 ab	1.35 a	1.78 a	1.42 a	2.51 b	1.84 a	1.44 a
(E)-Ethyl 3-decenoate		1.42 b	1.28 ab	1.74 b	1.40 b	1.15 a	1.35 ab	0.79 a	1.01 a	1.01 a	1.47 b	1.62 b	1.76 b
$\beta$ -Phenylethyl acetate	250 (Guth 1997)	1.33 a	1.24 a	1.41 a	1.23 a	1.29 a	1.26 a	3.16 b	2.79 b	1.90 ab	2.23 ab	2.44 b	2.82 b
4-Hexenyl acetate		0.49 a	0.38 a	0.39 a	0.45 a	0.49 a	0.43 a	0.77 b	1.34 c	1.22 c	0.58 ab	1.22 c	1.32 c
All		862.33	701.45	813.78	699.67	812.32	714.56	734.69	924.04	617.45	712.24	810.03	985.96
<b>Alcohols</b>													
Isoamyl alcohol	30,000 (Guth 1997)	20.37 c	14.66 b	16.44 bc	19.36 c	23.75 c	15.09 bc	6.61 a	10.54 ab	6.96 a	6.02 a	14.49 b	11.87 b
1-Hexanol	8,000 (Ferreira et al. 2000)	0.93 b	0.62 a	0.75 ab	0.80 ab	1.05 b	0.66 a	0.71 ab	0.77 2ab	0.57 a	0.56 a	0.93 b	0.98 b
(Z)-3-Hexen-1-ol	400 (Guth 1997)	0.34 a	0.19 a	0.42 ab	0.23 a	0.27 a	0.19 a	0.29 a	0.65 b	0.26 a	0.26 a	0.78 b	0.49 ab
$\beta$ -Phenylethyl alcohol	300 (Cabaroğlu and Canbas 2002)	5.98 bc	5.21 b	7.19 c	5.54 bc	7.08 c	4.13 b	5.60 bc	4.46 b	4.33 b	2.35 a	6.60 b	5.81 bc
All		27.63	20.69	24.81	25.94	32.16	20.07	13.22	16.43	12.13	9.20	22.81	19.17
<b>Acids</b>													
Hexanoic acid	3,000 (Guth 1997)	1.76 bc	0.64 a	1.55 b	0.66 a	2.08 c	1.15 b	2.43 c	1.74 bc	2.44 c	2.21 c	2.57 c	1.75 bc
Octanoic acid	7,000 (Guth 1997)	3.21 b	4.04 b	2.75 ab	1.56 a	4.33 b	1.26 a	7.50 c	8.52 c	6.94 c	6.31 c	8.43 c	6.33 c
Decanoic acid	15,000 (Guth 1997)	0.62 ab	0.17 a	0.46 a	0.17 a	1.41 b	0.23 a	2.28 c	2.47 c	2.42 c	2.39 c	2.39 c	2.32 c
All		6.77	4.85	4.78	2.40	7.83	2.64	12.22	12.74	11.81	10.92	13.40	10.40

<sup>a</sup> Analysis of variance; different letters in the same row indicate significant differences at  $P < 0.05$  by Duncan's multiple-range test.

**Table 4** Principal components loading autoscaled data

Compound	PC1	Compound	PC2
Octanoic acid	0.356415	Isoamyl alcohol	0.622957
Hexyl acetate	0.351888	(Z)-Ethyl 3-decenoate	0.499437
Decanoic acid	0.3516	Isoamyl hexanoate	0.458278
4-Hexenyl acetate	0.346692	(Z)-3-Hexen-1-ol	0.33653
Isoamyl acetate	0.3402	Decanoic acid	-0.135349
$\beta$ -Phenylethyl acetate	0.336972	$\beta$ -Phenylethyl acetate	-0.0876075
Hexanoic acid	0.294701	Hexyl acetate	0.0773916
(Z)-3-Hexen-1-ol	0.279456	Octanoic acid	-0.0714023
Isoamyl hexanoate	0.261393	Hexanoic acid	0.0300493
Isoamyl alcohol	-0.148638	4-Hexenyl acetate	0.0254995
(Z)-Ethyl 3-decenoate	-0.143787	Isoamyl acetate	0.0241069

Linear saturated fatty acids from C<sub>2</sub> to C<sub>10</sub> have been identified. In the analyzed samples, octanoic acid (1.3–8.5 mg/l) was the main component; hexanoic (0.6–2.6 mg/l) and decanoic (0.2–2.5 mg/l) followed. Statistically significant differences have been observed between the samples of the two areas; specifically, Monreale samples showed the highest amount of volatile fatty acids. Moreover, all fatty acids were present at levels below the odor threshold both in Monreale and in Sambuca samples, with the exception for octanoic acid in samples 7, 8, and 11 (Monreale).

Linear and branched saturated aliphatic alcohols from C<sub>5</sub> to C<sub>13</sub> have been identified. In our samples, isoamyl alcohol (6.0–23.8 mg/l; fruit, wine) was the main component;  $\beta$ -phenylethyl alcohol (2.4–7.2 mg/l) followed. Among alcohols, 1-hexanol and *cis* and *trans*-3-hexenol have been identified; C<sub>6</sub> alcohols were present at concentrations below their odor thresholds in all cases, except for (Z)-3-hexen-1-ol in samples 3, 8, 11, and 12. The content of alcohols is significantly different between the samples of the two areas; samples from Sambuca showed lower values.

Aldehydes were quantitatively very scant; so these substances were not quantified. Only nonanal, 2-furfural, and cinnamaldehyde have been identified.

Among monoterpenes, limonene, terpinolene, and geranyl acetone have been identified. These compounds were present in a very little amount in all the analyzed samples.

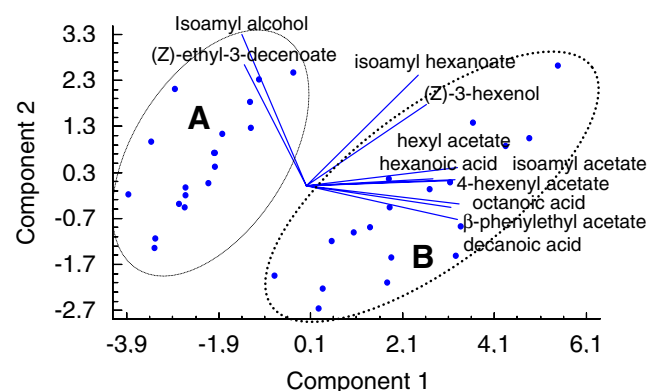
As previously discussed, statistically significant differences were found between the average content of some components in Sambuca and Monreale wine samples by ANOVA and Duncan's multiple-range test (Table 3), even if a multivariate pattern recognition approach resulted more effective in recognizing differences among the samples analyzed. Multivariate analysis techniques have been recently used to assess wine authenticity and for the classification according to their geographical origin (Arvanitoyannis et al. 1999; Kallithraka et al. 2001).

The regression analysis was performed for selecting those components most important in differentiating samples; significant compounds ( $P < 0.01$ ) resulted: isoamyl acetate, hexyl acetate, isoamyl hexanoate, (Z)-ethyl-3-

decenoate,  $\beta$ -phenyl ethyl acetate, 4-hexenyl acetate, isoamyl alcohol, (Z)-3-hexen-1-ol, hexanoic acid, octanoic acid, and decanoic acid.

Principal component analysis was thus performed to calculate the total variance contained in the 11 constituents considered for all the samples analyzed. Principal components 1 (PC1), 2 (PC2), and 3 (PC3) represented 90% of the total variance: 65% of the total variance for PC1, 17% for PC2, and 8% for PC3. Table 4 reports the significant component loadings in decreasing order of importance for PC1 and PC2.

As listed in Table 4, the constituents that contribute most to PC1 were octanoic acid, hexyl acetate, decanoic acid, 4-hexenyl acetate, isoamyl acetate, and  $\beta$ -phenylethyl acetate and to PC2 isoamyl alcohol were (Z)-ethyl-3-decenoate and isoamyl hexanoate. A graphic display of loadings for PC1 and PC2 is shown in Fig. 2. The figure shows that the Sambuca wine samples were grouped because of isoamyl alcohol and (Z)-ethyl-3-decenoate and the Monreale wine samples because of isoamyl acetate, hexyl acetate, isoamyl hexanoate,  $\beta$ -phenyl ethyl acetate, 4-hexenyl acetate, (Z)-3-hexen-1-ol, hexanoic acid, octanoic acid, and decanoic acid.



**Fig. 2** Principal component analysis (PC1 and PC2) involving quantities of eleven constituents in the samples analyzed. *A* Sambuca wine samples; *B* Monreale wine samples

## Discussion

The data obtained give useful information for the Inzolia characterization. The SPME/GC–MS technique allowed for the identification and quantization of a large number of components belonging to different classes of substances and well known among wine volatiles, mainly esters, fatty acids, and alcohols.

ANOVA and multivariate analysis techniques aided in the interpretation of chemical data obtained for volatile components of samples from different origin areas.

Esters of all kinds are regarded as especially important to wine flavor and are usually secondary aromas arising from the fermentation and sometimes tertiary aromas arising from ageing where alcohol–acids rearrangements can occur (Clarke and Bakker 2004). They are responsible for the fruity note which is defined as the sweet odors occurring generally in ripe fruits such as banana, pear, melon, etc.; particularly, isoamyl acetate, which has a low olfactive threshold, is responsible for the sweet character in almost all fruity notes.

The total amount of alcohols constitutes 2–3% of the total volatile fraction in all the analyzed samples. The alcohols (C<sub>4</sub> upwards), mainly the branched-chain compounds, together with the normal straight-chain compounds, as well as the benzenoid alcohol phenylethanol, are known as fusel oils and are usually present in fair quantity. They have a characteristic pungent odor and, at high concentration (>300 mg/l), are negative quality factors; but, at lower levels, they add to the desirable aspects of wine flavor. The presence of  $\beta$ -phenylethyl alcohol which arises from a Strecker degradation of the amino acid phenylalanine could give the wines a rose-like aroma. C<sub>6</sub> alcohols are less represented; these compounds originally present in the grape must decrease in wine as a result of fermentation (Vermin et al. 1993); they are very important impact substances occurring in many fruits and vegetables, and their flavor note is described as the odor of the freshly cut grass or ground leaves and green plant materials (Ashurst 1999).

The aliphatic acids, as previously discussed, are less represented in our samples. Besides producing a sour and fresh taste in the mouth, the volatile acids are also potent examples of fatty rancid flavor if present in a sufficient amount.

The low amount of substances such as 2-furfural and cinnamaldehyde was expected, as Inzolia samples were analyzed 2 months after the production; in fact, different authors affirmed the increase of substances such as furfural and vanillin in aged wines (Perez-Prieto et al. 2003). 2-Furfural has typical burnt sugar and caramel notes, and it arises from the Maillard reactions. Cinnamaldehyde (spicy, warm, sweet, cinnamon) is widely used in bakery goods

and alcoholic beverage to give them typical spicy herba-ceous notes and arises from a degradation of the amino acid phenylalanine via cinnamic acid. As regards monoterpenes, the low amount according to Palomo et al. (2006) evidenced less terpene compounds in wines with high ester concentration.

From the sensory analysis, the scores of the four attributes for the 12 different wine samples were rather homogenous, and this suggested that these attributes are characterizing feature to the Inzolia wine. The aroma of the Inzolia wine was mainly described as fruity; the attributes fruity, banana, and ripened apple are due to the high amount of ethyl and acetate esters. In fact, ethyl esters of medium-chain fatty acids and acetates tend to present fruity aromas and may play a major sensory role, especially in neutral grape varieties containing negligible amounts of terpenes (Cabaroglu and Canbas 2002; López et al. 2002). The floral attribute is probably correlated to the presence of  $\beta$ -phenylethyl acetate and  $\beta$ -phenylethyl alcohol; their amount was higher than the odor threshold in all the samples. In conclusion, the correlation between sensory data and volatile composition makes major contribution to wine characterization.

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