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Tracking Wheat Variety and Origin by the Shape Analysis of the Volatiles Fingerprint of Wheat Kernels and Wheat Beers

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Abstract: The Volatile Organic Compounds (VOCs) of common wheat of different origin (variety and altitude of cultivation) and craft wheat beers produced by using the wheat themselves were analyzed by SPME GC-MS. The VOCs of wheat kernels and wheat beers were compared, and 14 common flavor-active compounds were identified. Principal component analysis was used to describe changes in the profile of common volatiles induced by beer processing. A unifying approach by Generalized Procrustes analysis (GPA), which considers the overall characteristics of the datasets, permitted linking the VOCs of wheat to those of beers and to define a common flavor pattern. Despite the beer processing deeply affecting the overall volatilome profile, a consensus map permitted to clearly classify the VOCs profile of five out of six samples. This work revealed that differences in wheat VOCs induced by wheat variety and cultivation site were reflected in different beer aromatic profiles, highlighting the importance of origin on the wheat and beers' flavor. This unifying approach to flavor analysis by GPA could be of help in sight of a certification of origin, since it may contribute not only to the definition of wheat origin but also of the "terroir" of wheat beer thereof.

Keywords: volatile organic compound; SPME GC-MS; wheat craft beer; wheat kernel; aroma profile; wheat varieties; cultivation altitude; terroir; multivariate analysis; Generalized Procrustes analysis

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1. Introduction

Wheat is among the most important cereal crops, and its worldwide production makes it the second world's most important grain after corn [1]. Currently, wheat is the most widely grown crop in the world and its world trade is greater than for all other crops combined. This is likely due to wheat's agronomic adaptability to different latitudes and altitudes, growth temperatures, humidity conditions, and types of soils [2].

Wheat is also the most important food grain source, and thereby also occupies a central place in human nutrition. More than the 90% of the wheat produced in the world is common wheat (*Triticum aestivum* L.), which can be classified as "hard" or "soft", depending on grain hardness, and is mostly used for breadmaking [3] whilst the rest of the production consists of durum wheat (*Triticum turgidum* subsp. *durum* (Desf.) Husn.).

Nowadays, there is an increasing interest in wheat volatiles variation due to species [4,5] and variety [6–8]. Since wheat is cultivated over a wide range of altitudes (from 0 to 4570 m a.s.l.) and in different geographical locations characterized by different climates and soils [2], some authors also studied the effect of cultivation area and altitude on VOCs profile [6,9–11].

Since selected compounds characterizing the VOCs profile of wheat were found also in wheat flour and bread, as well as in semolina, pasta, and wheat beer [12–16], a deeper knowledge of VOCs profile evolution along the wheat foods chain is crucial both for the improvement of the quality of wheat products and their quality control since they contain several flavor-active volatiles.

Most of the studies focused on VOCs of wheat or wheat flours, and their derivatives were aimed to track selected compounds along the food processing chain [12,13,16].

The aim of this work was to study the changes of the volatilome from wheat to wheat beer by a unifying approach that considers the overall profile of the volatiles.

To this purpose, common wheat varieties grown in different geographical locations sited between 70 and 1200 m a.s.l. within the Abruzzo region (Italy) and wheat beers obtained by them were analyzed by solid phase microextraction (SPME) coupled with gas chromatography-mass spectrometry (GC-MS), and the obtained datasets were processed with multivariate statistics.

2. Materials and Methods

2.1. Grain Samples

This study involved two common wheat varieties (*Triticum aestivum* L.), genetically distant Solina (a historical landrace, in-situ conserved) and Vittorio (commercial modern variety, registered in 1996). Solina seeds were provided by a local farmer (Azienda Agricola De Santis, Introdacqua, Italy) whereas Agroservice S.p.A. (S. Severino Marche, Italy) provided Vittorio wheat. These grains were cultivated in 2019/2020 in randomized experimental fields sited in Corropoli (F1), Introdacqua (F2), and Rocca Pia (F3), at three different altitudes (70, 500 and 1200 m a.s.l. respectively). Agronomic practices were limited to accomplish organic regime standards. After harvesting, wheat kernels were stored in plastic bins at controlled temperature (18 ± 1 °C). The moisture content of the kernels was measured and was always lower than 13%.

2.2. Wheat Craft Beer Production

The harvested grains (n = 6) were used in the production of wheat craft beers as described by De Flaviis et al. [16]. Briefly, the beers were obtained in a pilot plant (BeerStudioLab, Giulianova, TE, Italy) using Italian pilsner malt (Agroalimentare Sud S.p.A., Melfi, PZ, Italy), Hallertau Hersbrucker hops (Hopsteiner, New York, NY, USA), and a dry ale yeast (US-05, Fermentis by Lesaffre, Marcq en Baroeul, France). Ground kernels were mixed to barley malt just before infusion step in a 4-to-6 ratio. After mashing, the draff was separated by a filter basket and then washed with hot water. Twenty grams of hop pellet were added after 60 min of boiling; then, the rehydrated yeast was inoculated to the wort at a concentration of 1 g L^{-1} for the fermentation step. After secondary fermentation (20 days at 20 °C) in bottles, the craft beers were stored at controlled temperature (18 ± 1 °C) until analysis.

2.3. SPME GC-MS Analyses

Volatile compounds were extracted by solid phase micro extraction (SPME-Supelco) coupled with gas chromatography (GC–PerkinElmer Clarus 580) and mass spectrometry (MS-PerkinElmer Clarus SQ8S). A 50/30 µm Divinylbenzene/Carboxen/Polydimethylsiloxane fiber (DVB/CAR/PDMS) with StableFlex core and a Zebron (Phenomenex, Bologna, Italy) capillary column (30 m × 0.25 mm × 0.25 µm) were used. Extraction conditions, GC-MS parameters, and VOCs identification were described in-depth in De Flaviis et al. [10,16] for wheat kernels and wheat beers, respectively. GC-MS analyses were conducted in duplicate. Peak areas were calculated using TurboMass 6.1.0 software and expressed as total ion current (TIC) multiplied 10^{-7}.

2.4. Statistical Analysis

Principal component analysis (PCA) based on the correlation matrix was performed on the dataset with VOCs identified both in wheat kernels and in wheat beers. The dataset was previously row-scaled in order to reduce the magnitude effect due to instrumental factors.

Generalized Procrustes analysis (GPA) is an iterative statistical technique able to compare different spatial representations constructed on the same observations; in particular, it was used to transform two multidimensional configurations (wheat kernel and wheat beer VOCs) so that they became as much alike as possible. Thus, the shape analysis obtained by GPA was used to define a communal volatiles pattern in wheat samples of different origin (variety, cultivation site) and in wheat beers obtained by them. Configuration points were mathematically transformed (scaled, rotated, and/or reflected) by using Commandeur method in order to minimize a specific criterion (basically a root–mean–square difference) between the scores of the reference dataset and the scores of the transformed dataset [17].

Moreover, GPA centroids (Y) of two wheat varieties were modelled along the altitude of wheat cultivation (X) by using a second order polynomial equation in the form:

$$Y = a + bX + cX^2$$

where a, b, and c are mathematical parameters to estimate. Model fitting was performed using the least square criterion and the "Levenberg–Marquadt" algorithm. The goodness of fit of the model was evaluated considering the R^2, the coefficient of variation of the root means square error (CVRMSE), the Akaike's Information Criterion (AIC) and the distribution of residuals. Statistical analyses were performed using XLSTAT software (XLSTAT 2021, Addinsoft, Paris, France).

3. Results and Discussion

3.1. Comparing VOCs in Kernels and Craft Beers

A total of 149 and 31 VOCs were identified in wheat kernels and wheat craft beers, respectively (data not shown). Since the aim of this research work was to find relationships and differences between raw materials and their respective processed food on the basis of aroma profile, a description focused on the individual dataset was avoided. However, a complete list of the molecules (listed in Table S1), their putative origin, and biosynthesis were described in the previous paper independently for wheat kernels [5,10,11] and wheat craft beers [16].

The datasets obtained from the two matrices were somewhat different, both in terms of numbers and chemical compounds, confirming the radical impact of this type of food process on the aroma profile of raw materials. Wheat kernels revealed a volatile profile considerably more complex but relative less intense considering the absolute area under the curve in the chromatograms. On the contrary, the wheat craft beers presented a limited number of compounds, but with higher peak area mostly due to ethyl ester compounds generally found at elevated concentrations in beer [18,19]. The most numerous chemical group in wheat kernel was terpenes, which became the least represented VOC in wheat beer, with only β-Linalool identified, a hop-marker compound deriving partially from the oxidation of β-Myrcene during the boiling process [20]. However, it has been demonstrated that during boiling and fermentation, due to oxidation and enzymatic phenomena, the majority of hop-derived volatiles, especially terpenes, are transformed or even lost [21,22]. It is reasonable to assume that the same process could affect the terpenes deriving from other raw ingredients such as ground wheat.

Concerning wheat beer, the most important chemical group is represented by esters. These compounds are known to derive from yeast metabolism by the enzymatic chemical condensation of fatty acids with ethanol or with higher alcohols (also known as fusel alcohols), which in turn are synthesized along the Ehrlich pathway through transamination, decarboxylation, and the reduction of amino acids [23]. Thus, wheat kernel may influence the final esters composition of beers both because it contains already higher alcohols such as 2-Methyl propanol, 2-Methyl butanol, 3-Methyl butanol, and Phenethyl alcohol and also because it affects the nutritional composition of the wort from which yeasts obtain nutrients.

In order to enhance as much as possible the contribution of wheat volatiles to the beer flavor profile, the craft beers were made with reduced concentrations of hops and yeast and with the maximum level (40%) of wheat allowed by Italian legislation (Legge n. 1354/1962, art.1, c. 4). This technological approach permitted obtaining wheat beers having 14 VOCs in common with wheat kernels (Table 1) of which were: five alcohols, three organic acids, two aldehydes, and two esters. In order to better visualize and describe this dataset, a PCA was computed. In particular, Figure 1 shows the results of a PCA highlighting a clear separation between kernels and beers on the basis of common volatiles along the first component (accounting for the 69.9% of the total variance). Wheat kernels were characterized by Decanoic acid (fatty odor), Pentanoic acid (cheesy odor), 2-Nonanone (fruity odor), 1-Hexanol-2-ethyl (citrus odor), 1-Octanol (waxy odor), Nonanal (aldehydic odor), Decanal (aldehydic odor), 1-Decanol (fatty odor), and Ethyl dodecanoate (waxy odor), whereas Styrene (balsamic odor), Phenylethyl alcohol (sweet odor), 1-Butanol-2-methyl (roasted odor), Octanoic acid (fatty odor), and Ethyl decanoate (waxy odor) characterized wheat beers. Wheat kernels were distinguished by mainly oxidative compounds (alcohols and aldehydes) that in beers were found in a relatively lower amount. Along the second component, it was possible to observe the separation of wheat samples on the basis of the altitude of cultivation, confirming that utilizing only a little chunk of the datasets, pedo-climatic conditions were key factors in the VOCs expression in wheat [5,11]. On the contrary, the common VOCs characterizing wheat beers were mainly molecules synthetized by yeast (higher alcohols and an ester), but, interestingly, they were already present in the raw material. Among them, Phenethyl alcohol, having the highest Flavor Dilution (FD) factor and an Odor Activity Value (OAV) greater than one [24], is considered an important odorant in Bavarian wheat beer; our results thus suggests that the wheat used in beer production may contribute to this important odor, classified as "rose" or "sweet" type [25].

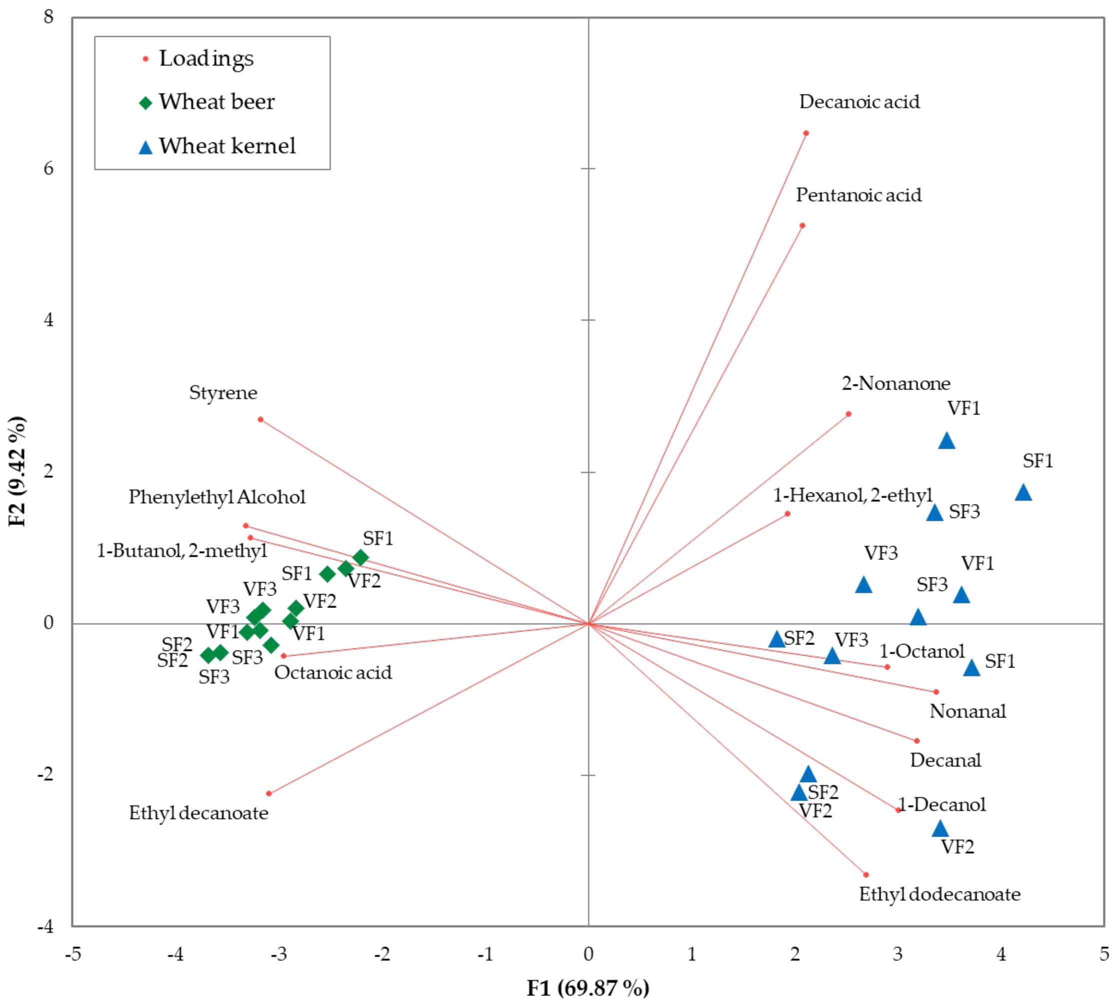

Figure 1. PCA biplot of common VOCs identified in wheat kernels and wheat beers. Score nomenclature: (V) Vittorio wheat; (S) Solina wheat; F1: 70 m a.s.l.; F2: 500 m a.s.l.; F3: 1200 m a.s.l.

Table 1. Absolute peak areas, expressed as mean ± standard deviation, for common VOCs between wheat kernel and wheat beer dataset.

		Wheat Kernel						Wheat Beer					
Chemical Class	**VOCs**	**SF1**	**VF1**	**SF2**	**VF2**	**SF3**	**VF3**	**SF1**	**VF1**	**SF2**	**VF2**	**SF3**	**VF3**
Alcohol	2-Methyl-1-butanol	0.077 ± 0.001	0.000 ± 0.000	0.016 ± 0.022	0.100 ± 0.125	0.181 ± 0.013	0.286 ± 0.021	0.664 ± 0.026	0.855 ± 0.046	0.753 ± 0.013	0.772 ± 0.001	0.763 ± 0.007	0.586 ± 0.011
Benzene derivative	Styrene	0.001 ± 0.000	0.000 ± 0.000	0.001 ± 0.001	0.000 ± 0.000	0.002 ± 0.001	0.002 ± 0.003	0.154 ± 0.008	0.134 ± 0.021	0.192 ± 0.018	0.171 ± 0.005	0.145 ± 0.028	0.181 ± 0.006
Organic acid	Pentanoic acid	0.348 ± 0.197	0.192 ± 0.090	0.074 ± 0.041	0.068 ± 0.043	0.141 ± 0.096	0.097 ± 0.092	0.019 ± 0.008	0.016 ± 0.002	0.017 ± 0.002	0.014 ± 0.000	0.041 ± 0.008	0.051 ± 0.001
Alcohol	2-Ethyl-1-hexanol	0.810 ± 0.228	0.294 ± 0.149	0.078 ± 0.042	0.227 ± 0.209	0.317 ± 0.013	0.536 ± 0.063	0.006 ± 0.000	0.006 ± 0.001	0.098 ± 0.027	0.138 ± 0.008	0.107 ± 0.003	0.016 ± 0.001
Alcohol	1-Octanol	0.543 ± 0.197	0.681 ± 0.016	0.497 ± 0.022	1.120 ± 0.021	1.933 ± 0.178	2.102 ± 0.064	0.064 ± 0.002	0.062 ± 0.006	0.051 ± 0.001	0.055 ± 0.001	0.054 ± 0.006	0.062 ± 0.004
Ketone	2-Nonanone	0.110 ± 0.047	0.041 ± 0.058	0.073 ± 0.009	0.147 ± 0.208	0.188 ± 0.025	0.141 ± 0.199	0.020 ± 0.001	0.000 ± 0.000	0.000 ± 0.000	0.010 ± 0.002	0.000 ± 0.000	0.000 ± 0.000
Aldehyde	Nonanal	4.040 ± 0.185	4.213 ± 0.281	2.209 ± 0.252	4.343 ± 0.402	5.244 ± 0.336	7.116 ± 0.067	0.032 ± 0.007	0.013 ± 0.002	0.013 ± 0.002	0.010 ± 0.004	0.055 ± 0.051	0.059 ± 0.001
Alcohol	Phenethyl Alcohol	0.345 ± 0.008	0.402 ± 0.103	0.093 ± 0.028	0.518 ± 0.114	0.732 ± 0.145	1.561 ± 0.240	1.630 ± 0.158	1.459 ± 0.010	1.431 ± 0.052	1.686 ± 0.086	1.524 ± 0.202	1.665 ± 0.004
Organic acid	Octanoic acid	0.068 ± 0.059	0.022 ± 0.010	0.744 ± 0.255	0.511 ± 0.524	0.080 ± 0.013	0.068 ± 0.013	0.734 ± 0.110	0.474 ± 0.058	0.559 ± 0.064	0.564 ± 0.006	0.876 ± 0.069	1.141 ± 0.025
Aldehyde	Decanal	1.247 ± 0.296	0.675 ± 0.170	0.561 ± 0.095	1.145 ± 0.149	0.775 ± 0.117	1.074 ± 0.039	0.017 ± 0.004	0.012 ± 0.003	0.006 ± 0.000	0.007 ± 0.001	0.019 ± 0.011	0.012 ± 0.000
Alcohol	1-Decanol	0.541 ± 0.097	0.417 ± 0.100	0.184 ± 0.042	0.838 ± 0.230	0.300 ± 0.011	0.527 ± 0.194	0.016 ± 0.001	0.015 ± 0.000	0.015 ± 0.001	0.000 ± 0.000	0.013 ± 0.001	0.018 ± 0.001
Organic acid	Decanoic acid	0.101 ± 0.040	0.080 ± 0.013	0.036 ± 0.022	0.098 ± 0.018	0.155 ± 0.014	0.074 ± 0.027	0.013 ± 0.004	0.009 ± 0.001	0.014 ± 0.000	0.009 ± 0.003	0.021 ± 0.002	0.035 ± 0.001
Ester	Ethyl decanoate	0.085 ± 0.081	0.028 ± 0.023	0.193 ± 0.211	0.433 ± 0.128	0.107 ± 0.079	0.175 ± 0.094	0.180 ± 0.012	0.331 ± 0.040	0.330 ± 0.030	0.259 ± 0.033	0.329 ± 0.020	0.395 ± 0.021
Ester	Ethyl dodecanoate	0.321 ± 0.284	0.237 ± 0.232	0.150 ± 0.168	0.441 ± 0.120	0.354 ± 0.271	0.177 ± 0.150	0.000 ± 0.000	0.011 ± 0.001	0.018 ± 0.003	0.009 ± 0.001	0.012 ± 0.001	0.014 ± 0.001

S: Solina wheat beer; V: Vittorio wheat beer; F1: 70 m a.s.l.; F2: 500 m a.s.l.; F3: 1200 m a.s.l.

3.2. Generalized Procrustes Analysis

In order to analyze jointly both the wheat and beer VOCs datasets without losing useful information, improving data visualization, and reducing block-variance inequalities due to a strong difference in terms of number of variables, a multitable statistical approach was chosen. Thus, a GPA was carried out by using wheat kernel (6 samples × 2 replicates × 149 variables) and wheat beer (6 samples × 2 replicates × 31 variables) datasets as configurations to obtain a common volatile profile as much alike as possible. GPA results are shown graphically through the consensus and correlation maps interpretable similarly to PCA scores and the loadings plot, respectively [26]. In Figure 2a, the consensus coordinates are shown along the first two components (accounting for the 83% of the total consensus variance), whereas in Figure 2b, the third and fourth components are shown (accounting for the 12% of the total consensus variance). The kernel and the beer samples VF3, SF1, SF3, and VF2 (highlighted in figure by polygonal dashed lines) are clearly separated among them in the first two components of the consensus space, while the third and fourth components classify the sample SF2. Thus, the combination of wheat variety and cultivation site generated a distinguishable and unique volatile profile at least for five samples, of which differences are reflected from kernels' to beers' VOCs.

In Figure 3, the correlations between variables (VOCs) and factors (F1 and F2) are shown. To improve the readability of the graph, only the VOCs with a correlation higher than 0.7 are shown. Interestingly, Linalool oxide found in kernels resulted in being correlated to β-Linalool found in beers (negatively correlated to the first component). Indeed, Lermusieau et al. [27] suggested that the final concentration of Linalool in beer may depend on the amount of linalool glycosides hydrolyzed by Linalool oxide in fermentation.

Even if not all the samples generated consensus individually, by looking at the centroids in Figure 4, it was possible to observe a clear separation between groups, in particular between Solina and Vittorio wheat. As a consequence, the consensus scores suggest that the two analyses are interchangeable for discrimination purposes on the basis of wheat varieties.

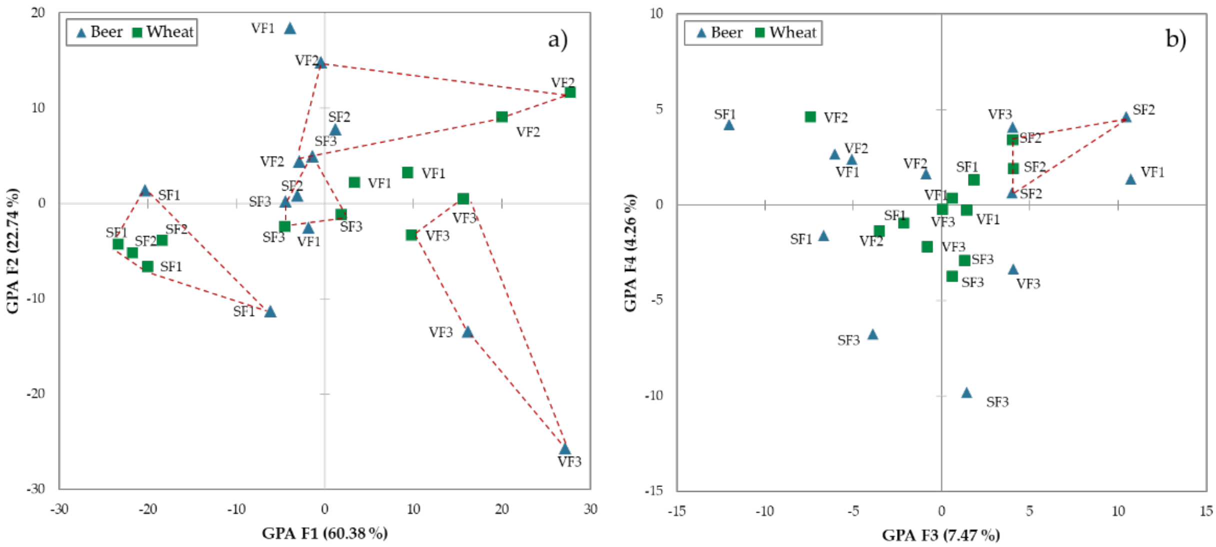

Figure 2. Consensus map, presented by configuration (wheat kernels and wheat beers), obtained by GPA along the F1 and F2 components (**a**); F3 and F4 components (**b**). Score nomenclature: (V) Vittorio wheat; (S) Solina wheat; F1: 70 m a.s.l.; F2: 500 m a.s.l.; F3: 1200 m a.s.l.

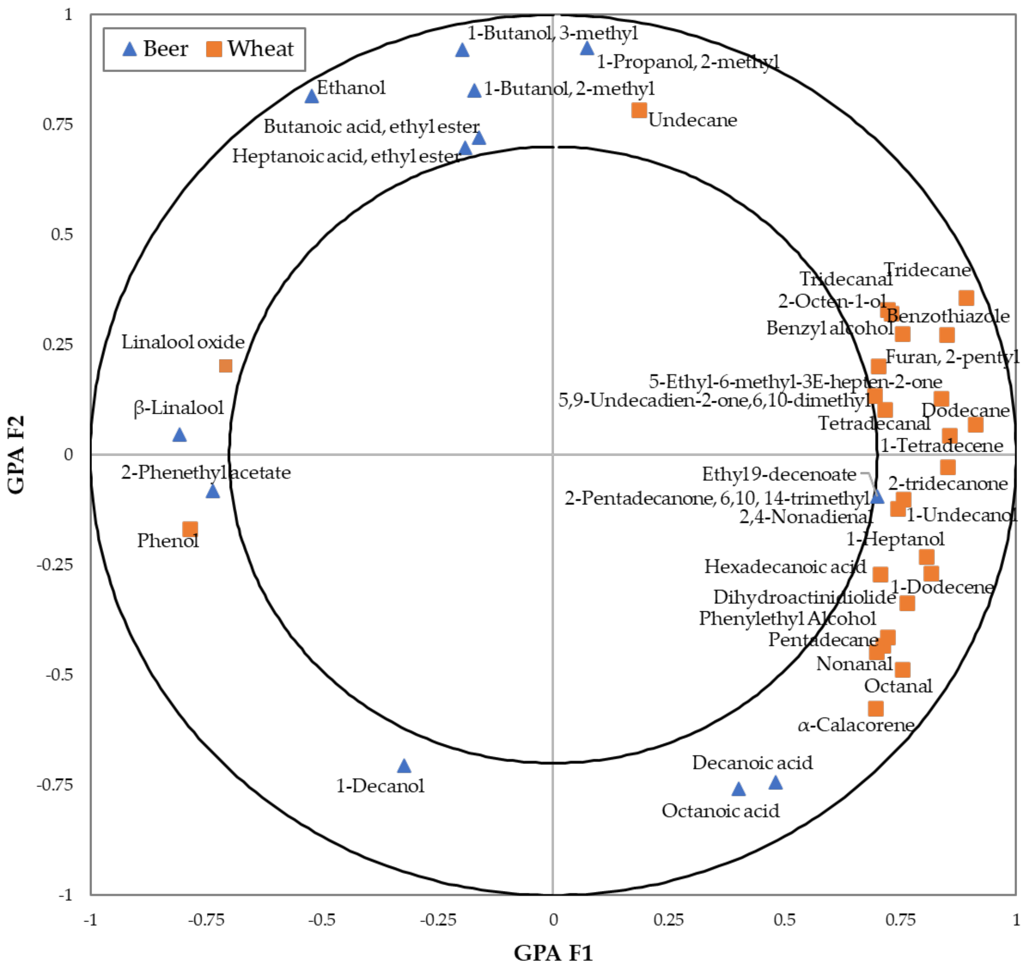

Figure 3. GPA correlations between dimensions in the initial consensus configuration and the first two factors by using GC-MS datasets.

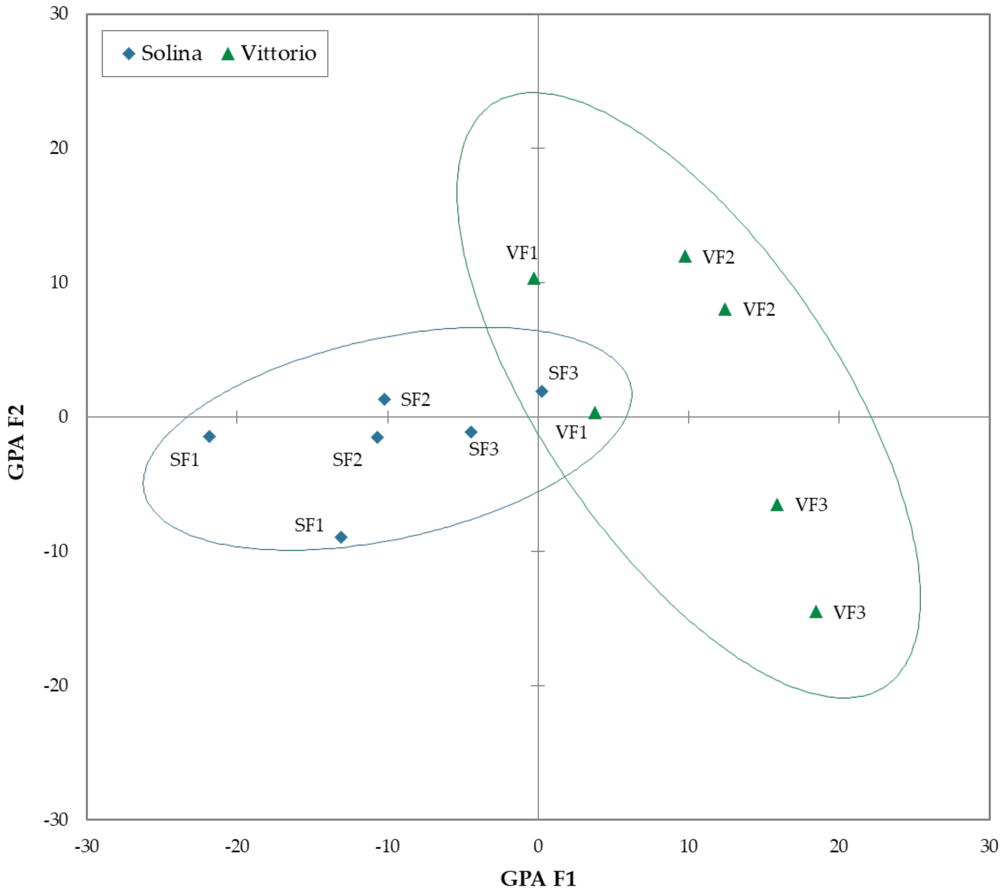

Figure 4. GPA plot of centroid coordinates by using GC-MS datasets, along the first and second factors. Score nomenclature: (V) Vittorio wheat; (S) Solina wheat; F1: 70 m a.s.l.; F2: 500 m a.s.l.; F3: 1200 m a.s.l. The ellipses indicate the 95% confidence limit.

Thus, genotype, was considerable the first root of consensus between the GC-MS analyses conducted on wheat kernels first and then on wheat beers. These findings are in accordance with the results of De Flaviis et al. [11].

De Flaviis et al., in [11] analyzing the VOCs of wheat kernels for two consecutive years, reported a greater effect on VOCs profile due to genetical factors rather than cultivation altitude. In particular, as shown in Figure 3, Solina wheat was characterized by β-Linalool and 2-Phenethylacetate in beer whereas it was in kernel by Phenol and Linalool oxide. These two compounds could be assumed as marker of beers made with Solina wheat as confirmed by PLS-DA computed by De Flaviis et al. on the same beer samples [16]. As regards Vittorio wheat, several VOCs found in kernels were positively correlated to the first component, of which mainly aldehydes, alcohols, ketones, and alkanes, suggesting a more complex aromatic profile of this variety, whereas only Ethyl-9-decenoate distinguished Vittorio beers.

Considering beer odor types, Solina was characterized by two molecules with floral notes (β-Linalool and 2-Phenethylacetate) while Vittorio was characterized by a molecule with a fruity note (Ethyl-9-decenoate).

Within each wheat variety, a second classification may be observed on the basis of altitude of wheat cultivation, again along the first component. To better visualize the discrimination due to farm origin, a regression was performed using altitude as an independent variable (X) and the GPA scores on the first component as variable to predict (Y) for Solina and Vittorio wheat separately. After a first explorative linear regression, a second order polynomial equation was chosen as a mathematical model on the basis of the observation of the residuals distribution in the residuals plot. The regression results, shown in Figure 5, highlighted a good fit with a R^2 of 0.94 and 0.83 for Vittorio and Solina wheat, respectively. Vittorio scores were fitted better than Solina as confirmed by the CVRMSE (22% and 40%, respectively) and AIC (13.5 and 20.7, respectively) indexes.

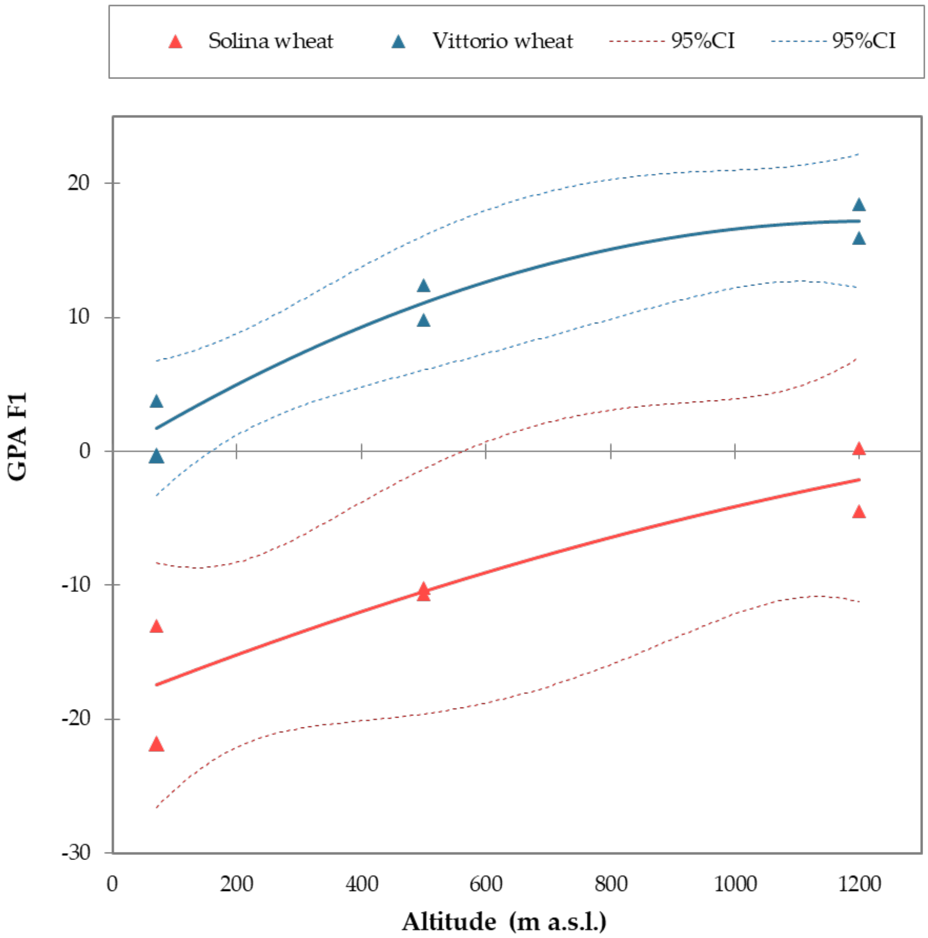

Figure 5. Non-linear regression (second order polynomial equation) of centroid coordinates computed by GPA along altitude. CI: Confidence intervals.

By observing the confidence intervals (Figure 5), it is possible to affirm that the regression model permitted to separate without any overlapping the scores of the first consensus component (between wheat and beers) on the basis of variety and altitude of wheat cultivation. This result suggests that differences in wheat volatiles induced by wheat origin (variety and cultivation site) are reflected in the beers' volatiles profiles.

4. Conclusions

To the authors' knowledge, this work is the first attempt to link the volatiles profile of a prime material, in this case wheat, to that of a processed food produced with the same prime material by using a multivariate approach aimed to match their overall profile (shape analysis).

Despite the beer processing deeply affecting the flavor profile, it was, however, possible to find consensus among the VOCs profile of five different samples (SF1, SF2, SF3, VF2, and VF3) out of six total samples. Moreover, by plotting the scores of the first factor of consensus along altitude of cultivation, it was possible to highlight the effect of origin (variety and cultivation site) on the wheat and beers' VOCs profiles, thus contributing to the definition of the "terroir" of both the prime material and the processed food. In particular, four VOCs were important for Solina wheat discrimination: Phenol and Linalool oxide considering the kernels, whereas β-Linalool and 2-Phenethylacetate (with floral notes) considering the wheat beers. On the contrary, Vittorio wheat was discriminated by several VOCs identified in wheat kernels, while, in wheat beer, only Ethyl-9-decenoate (with fruity note) contributed to its separation.

The data-driven approach proposed in this work could be applied in both quality traits tracking and the identification of products' "terroir" along the food supply chain.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/app12157854/s1, Table S1: VOCs identified in wheat kernels and wheat beers obtained by them. Compounds are ordered by chemical group and subsequently retention time.

Author Contributions: Conceptualization, G.S.; methodology, R.D.F. and V.S.; formal analysis, R.D.F., V.S. and G.S.; investigation, R.D.F. and V.S.; writing—original draft preparation, R.D.F., V.S. and G.S.; writing—review and editing, G.S.; visualization, R.D.F., V.S. and G.S.; supervision, G.S.; project administration, G.S.; funding acquisition, G.S. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest: The authors declare no conflict of interest.

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