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APPLICATION OF GAS CHROMATOGRAPHY-ION MOBILITY SPECTROMETRY(GC-IMS) TO CHARACTERIZE VOLATILE SIGNATURES OF FETEASCĂ NEAGRĂ WINES FROM THE IGP ȘTEFAN VODĂ REGION

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Abstract. Wine aroma is a key determinant of quality and typicity, shaped by complex mixtures of volatile compounds. Traditional methods such as GC-MS provide detailed chemical information but are often time consuming and less suited for rapid terroir studies. This study hypothesized that gas chromatography-ion mobility spectrometry (GC-IMS) can differentiate wines from neighboring vineyards within the same protected geographical indication (PGI). The objective was to evaluate its applicability for profiling volatile compounds in wines from three vineyards of the PGI Ștefan Vodă region in Moldova. Microvinification was carried out with Fetească Neagră grapes harvested at technological maturity in 2022, and the resulting wines were analyzed by GC-IMS. Three dimensional spectra, two dimensional projections, differential mapping, and fingerprint plots revealed vineyard specific volatile profiles. Wine from Purcari was characterized by higher levels of esters, Cimișlia by carbonyls and terpenes, and Căușeni by higher alcohols and acetate esters. These results confirm that GC-IMS can capture subtle vineyard level differences and provide unique chemical fingerprints.

Keywords: *Fetească Neagră, wine aroma, volatile compounds, Ștefan Vodă, gas chromatography-ion mobility spectrometry.*

Rezumat. Aroma vinului este un determinant esențial al calității și tipicității, fiind modelată de amestecuri complexe de compuși volatili. Metodele tradiționale, precum GC-MS, oferă informații chimice detaliate, dar sunt adesea consumatoare de timp și mai puțin adecvate pentru studii rapide asupra terroirului. Acest studiu a emis ipoteza că cromatografia gazoasă cu spectrometrie de mobilitate ionică (GC-IMS) poate diferenția vinurile provenite din vii învecinate, aflate în cadrul aceleiași regiuni cu indicație geografică protejată (IGP). Obiectivul a fost evaluarea aplicabilității acestei metode pentru profilarea compușilor volatili din vinurile a trei vii din regiunea cu IGP Ștefan Vodă din Republica Moldova. Microvinificarea a fost realizată cu struguri Fetească Neagră recoltați la maturitate tehnologică în 2022, iar vinurile obținute au fost analizate prin GC-IMS. Spectrele tridimensionale, proiecțiile bidimensionale, hărțile diferențiale și diagramele de tip „fingerprint” au evidențiat profiluri volatile specifice fiecărei plantații de viță de vie. Vinul din Purcari s-a caracterizat prin niveluri mai ridicate de esteri, cel din Cimișlia prin compuși carbonilici și terpene, iar cel din Căușeni prin concentrații mai mari de alcooli superiori și de esteri ai acidului acetic. Aceste rezultate confirmă faptul că GC-IMS poate detecta diferențe subtile la nivel de vie și poate furniza amprente chimice unice.

Cuvinte-Cheie: *Fetească Neagră, aroma vinului, compuși volatili, Ștefan Vodă, cromatografia gazoasă cu spectrometrie de mobilitate ionică.*

1. Introduction

Wine's aroma is shaped by a complex mixture of volatile compounds produced from grape material, metabolism during fermentation, and subsequent aging [1,2]. Thousands of volatile compounds have been identified in wine, which can be divided into alcohols, esters, aldehydes, ketones, terpenes, sulfur compounds, and methoxypyrazines [3]. Although many of the volatile compounds are present in low concentrations in wine, with very low odor thresholds, they still contribute to the wine’s aroma.

Advances in analytical chemistry over the past few decades have enabled the study of volatile compounds in wine to become more extensive. Gas chromatography-mass spectrometry (GC-MS) has long been considered the gold standard for qualitative and quantitative analysis [4,5]. More comprehensive methods, such as comprehensive two-dimensional gas chromatography (GC×GC-MS) and proton transfer reaction mass spectrometry (PTR-MS), have further improved resolution and sensitivity [6,7]. However, these methods are generally time-consuming (complex sample preparation, analysis, and data processing). In recent years, gas chromatography-ion mobility spectrometry (GC-IMS) has been considered as an alternative for the analysis of volatile compounds in wine [8]. GC-IMS combines gas chromatographic separation with ion mobility-based detection to provide rapid, highly sensitive measurements and generate two- or three-dimensional “fingerprints” that allow visualization of complex volatile mixtures [9-11].

Previous studies have demonstrated the utility of GC-IMS in food authenticity and quality control, including applications in olive oil, honey, ham, beer, and dairy products [12-14]. In recent years, GC-IMS has been introduced into oenological research and has been shown to be effective in differentiating wines based on grape variety, vintage, and fermentation conditions [15-17]. However, the application of this technique in terroir related studies remains rare, especially at the vineyard level within a single geographical indication.

There is still debate about whether GC-IMS can replace traditional GC-MS for detailed chemical characterization [18]. Some researchers argue that GC-IMS has limitations in terms of compound identification and quantification and is best considered a complementary tool [19]. While others emphasize its advantages in terms of speed, sensitivity to trace volatile substances (e.g., methoxypyrazines, volatile sulfur compounds), and pattern recognition capabilities, which are closely related to authenticity of origin studies [20]. It is hypothesized that GC-IMS would be able to differentiate between wines from neighboring vineyards under the same PGI, providing a unique chemical fingerprint associated with the specific terroir of the vineyard.

The aim of this study was therefore to evaluate the applicability of GC-IMS for profiling volatile compounds in wines from three vineyards located in the IGP Ștefan Vodă region of

Moldova, with a focus on assessing its value as a rapid and informative tool for vineyard level discrimination.

2. Materials and Methods

This research was conducted in three vineyards located within the IGP Ștefan Vodă region: Purcari, Cimișlia, Căușeni. The Fetească Neagră grape harvest in the 2022 vintage, sampling showed a sugar content of 255 g/L. For microvinification, 3 kg of grapes per trial were destemmed and crushed, and 100 mg/dm^3 potassium metabisulfite (PMS) was added. After must clarification, 80 mg/dm^3 of commercial *Saccharomyces cerevisiae* yeast was inoculated. During alcoholic fermentation, pigeage and remontage were performed twice daily, and the must density was continuously monitored. When the density decreased to 1010 - 1020 g/dm^3, 25 mg/dm^3 of lactic acid bacteria were added to initiate malolactic fermentation. Upon completion of malolactic fermentation, the wines were racked, treated with 50 mg/dm^3 PMS, and bottled in 750 mL glass bottles.

The analysis of volatile organic compounds was performed using a GC-IMS instrument FlavourSpec® (G.A.S., Germany), equipped with an automatic CTC-PAL 3 injection system. An aliquot of 1 g of wine was placed in a 20 mL headspace vial, incubated at 60 °C for 20 min, and then injected, with each sample analyzed in triplicate. The headspace injection conditions were as follows: incubation temperature 60 °C, incubation time 20 min, injection volume 100 μL, splitless mode, incubation agitation speed 500 rpm, and injector needle temperature 85°C. GC conditions included a column temperature of 60 °C and high-purity nitrogen as the carrier gas (≥99.999%). The initial flow rate was 2.0 mL/min (held for 2 min), increased linearly to 10.0 mL/min within 8 min, then to 100.0 mL/min within 10 min, and held for 20 min, giving a total run time of 40 min; the drift gas flow was 75.0 mL/min, and the injector temperature was 80°C. IMS conditions included a tritium ionization source, a drift tube length of 53 mm, an electric field strength of 500 V/cm, a drift tube temperature of 45°C, high purity nitrogen (≥99.999%) as the drift gas, and positive ion mode. Data processing was carried out using VOCal software, with compound identification based on retention time and drift time matched against the built in NIST 2020 GC retention index and IMS drift time libraries. The Reporter and Gallery Plot modules were used to generate three dimensional spectra, two dimensional spectra, various maps, and fingerprint plots.

All samples were measured in triplicate, and the VOC content results are expressed as mean values ± standard deviation. Statistical analysis was first performed in Excel for raw data organization, followed by subsequent processing in R package (version 4.4.3). R package is a programming language and statistical computing environment widely used for data analysis. One-way analysis of variance (ANOVA) was used to evaluate differences among vineyards, and Tukey's post hoc test was applied for multiple comparisons. Differences were considered statistically significant at $p < 0.05$.

3. Results

Figure 1 shows a three-dimensional GC-IMS spectrum, with drift time on the X-axis, retention time on the Y-axis, and signal intensity on the Z-axis. It is immediately apparent that the main diagonal line (representing the reaction ion peak and its associated cluster) is consistent across all spectra. At the same time, subtle differences in the distribution and intensity of secondary peaks were evident. In particular, the front region of the spectra (corresponding to lower retention times) contained multiple minor clusters with variable intensities across samples, suggesting vineyard specific variations in light volatiles, such as alcohols and esters. Although the overall complexity appeared comparable, these local differences justified further visualization through two dimensional projections, as illustrated in Figure 2.

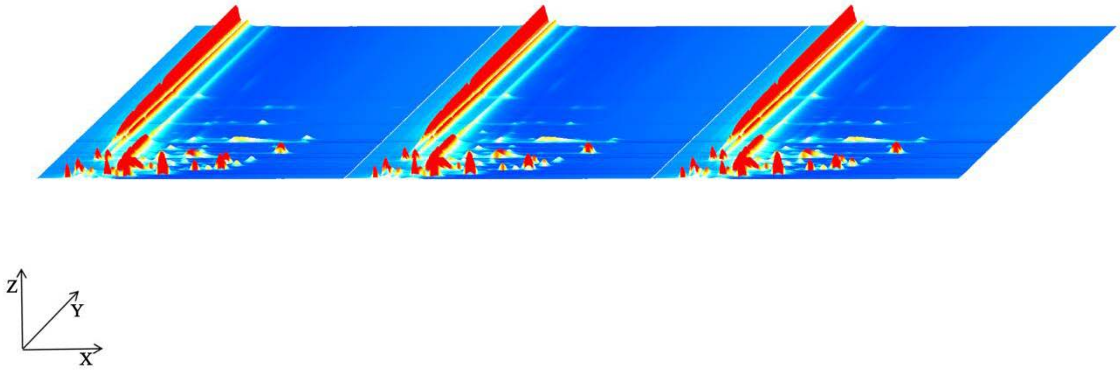

Figure 1. Three-dimensional GC-IMS spectra of wines from three vineyards in the IGP Ștefan Vodă region.

The two-dimensional GC-IMS spectra (Figure 2) provides a clearer picture of the distribution of volatile compounds than the three-dimensional plots. While the overall spectral structure of the three samples is similar, there are differences in the peak intensities, particularly in the region with lower drift times, which are typically associated with light compounds such as alcohols and esters.

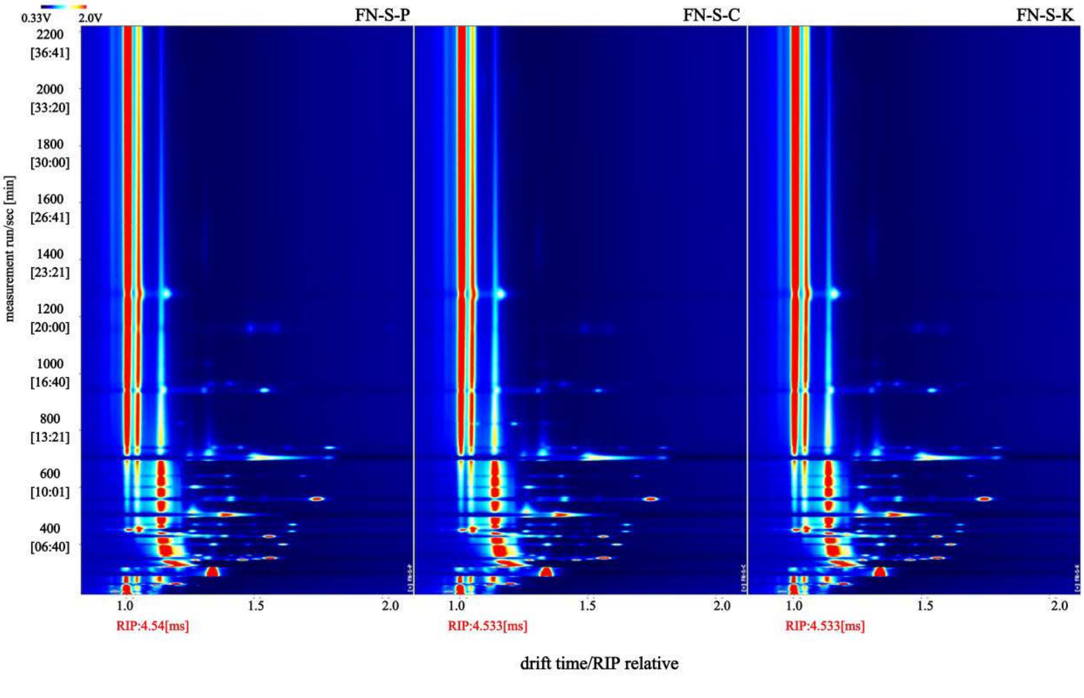

Figure 2. Two-dimensional GC-IMS spectra of wines from three vineyards in the IGP Ștefan Vodă region. (FN-S-P: Purcari, FN-S-C: Cimișlia, FN-S-K: Căușeni).

To further highlight these variations, differential mapping was performed using the spectrum of FN-S-P (Purcari) as the reference (Figure 3). In the differential plots, the red vertical line at drift time 1.0 corresponds to the normalized reaction ion peak (RIP), with the vertical axis representing gas chromatographic retention time(s) and the horizontal axis representing relative drift time (normalized, a.u.). Each point adjacent to the RIP peak corresponds to a volatile organic compound, and the color gradient from blue to red indicates signal intensity, with deeper colors denoting higher peak responses. In comparative analysis, a white background indicates no difference between the target and reference compounds, while red represents higher concentrations of the compound and blue represents lower concentrations. The results showed that compared to the Purcari sample, Cimişlia and Căușeni showed weaker signals in the intermediate drift time region, which may be related to aldehydes and esters. Overall, the combination of two-dimensional visualization and differential mapping demonstrated that GC-IMS is a powerful tool for capturing and emphasizing subtle vineyard specific variations in wine aroma profiles.

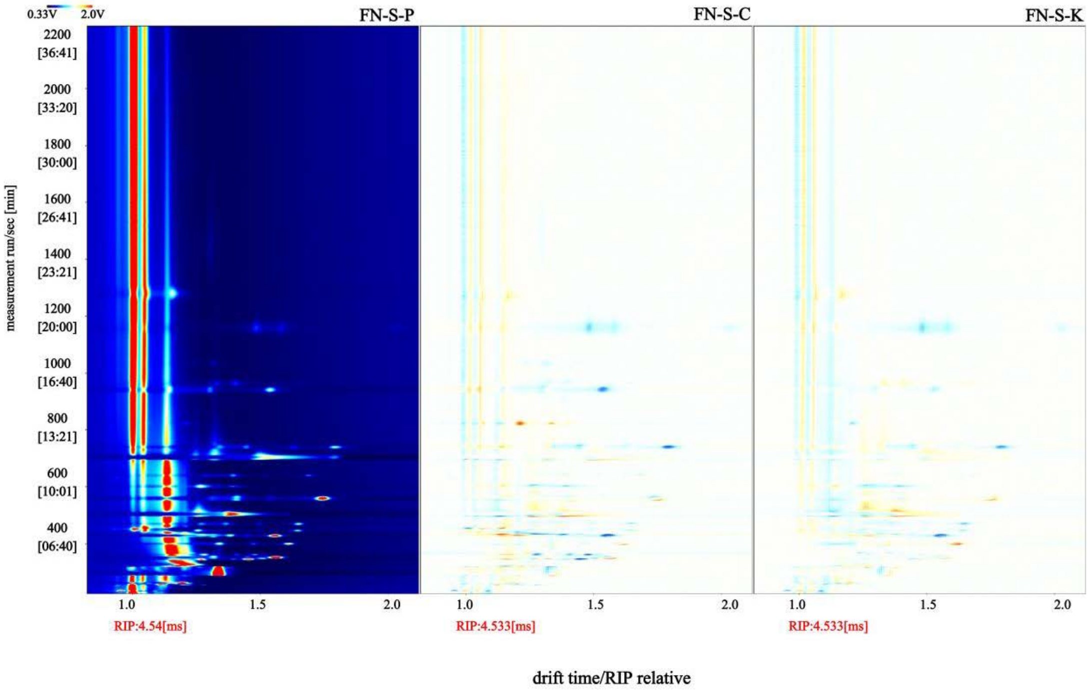

Figure 3. Difference maps of GC-IMS spectra (from left to right: Purcari, Cimişlia, Căușeni).

Volatile compounds were identified by matching their RI and Dt values with the NIST (2020) and VOCal IMS libraries, as summarized in Table 1. A total of 44 peaks were detected across the three samples, corresponding to 33 volatile compounds (where M denotes monomer and D denotes dimer).

Table 1

Details of Volatile Compounds

Peak#	RI*	Rt* (s)	Dt*（RIPrel）	Compound
1	1720.5	2016.961	1.09249	γ-Butyrolactone
2	1720.3	2016.456	1.20485	Acetophenone
3	1509.6	1278.873	1.15744	Acetic acid
4	1462.8	1155.942	1.49214	Ethyl octanoate-M
5	1462.2	1154.366	2.02767	Ethyl octanoate-D
6	1410.6	1032.574	1.32225	(E)-2-Hexenol
7	1410.2	1031.615	1.24315	Z-3-Hexenol
8	1367.9	941.534	1.14236	Ethyl lactate-M
9	1367.9	941.534	1.53785	Ethyl lactate-D
10	1379	964.533	1.33118	1-Hexanol-M
11	1377.7	961.658	1.64119	1-Hexanol-D

Continuation Table 1

12	1306	823.661	1.21126	Terpinolene
13	1305.4	822.573	1.40112	Octanal
14	1255.5	742.174	1.34641	Ethyl hexanoate-M
15	1255.5	742.174	1.8005	Ethyl hexanoate-D
16	1230.8	705.804	1.24902	3-Methyl-1-butanol-M
17	1230.4	705.166	1.48865	3-Methyl-1-butanol-D
18	1182.5	631.148	0.94264	1-Penten-3-ol
19	1168.6	601.796	1.26543	1-Butanol-M
20	1169.2	603.072	1.38799	1-Butanol-D
21	1146.1	557.13	1.31358	Isoamyl acetate-M
22	1146.7	558.406	1.75236	Isoamyl acetate-D
23	1116.9	504.169	1.25559	2-Methyl-1-propanol-M
24	1117.3	504.807	1.36829	2-Methyl-1-propanol-D
25	1095.6	469.075	1.27091	Ethyl 3-methylbutanoate-M
26	1095.6	469.075	1.66154	Ethyl 3-methylbutanoate-D
27	1079.2	447.38	1.25449	Ethyl 2-methylbutanoate-M
28	1079.2	447.38	1.65278	Ethyl 2-methylbutanoate-D
29	1065.1	429.514	1.24793	1-Propanol
30	1064.1	428.237	1.56415	Ethyl butanoate
31	1040.5	400.162	1.33875	2-Methylpropyl acetate-M
32	1041.1	400.8	1.61339	2-Methylpropyl acetate-D
33	1012.3	368.896	1.35625	2-Pentanone
34	1006.3	362.515	1.41315	Pentanal
35	1005.7	361.877	1.48209	Propyl acetate
36	997	352.944	1.56525	Ethyl isobutyrate
37	989	346.563	1.45801	Ethyl propanoate
38	957.6	323.592	1.12319	Ethanol
39	918	296.792	1.34094	Ethyl acetate
40	861.5	262.336	1.1965	Methyl acetate
41	852.5	257.231	1.11225	Acetone
42	832.7	246.384	1.06301	Propanal
43	810.9	234.898	0.95796	Dimethyl sulfide
44	1305.7	823.211	1.07067	3-Hydroxy-2-butanone

*RI - retention index; Rt - retention time; Dt - drift time; RIPrel - normalized relative to the RIP (reaction ion peak).

After merging the monomer and dimer signals, GC-IMS detected a total of 33 volatile compounds, including 9 alcohols, 12 esters, 4 aldehydes, 3 ketones, 1 acid, 1 sulfur compound, 1 terpenoid, and 2 others. Among them, 3-hydroxy-2-butanone and γ-butyrolactone were classified as “Others”. The former, although possessing the dual characteristics of a hydroxyketone, contributes to wine aroma mainly through its involvement in the metabolic conversion of diacetyl, rather than behaving as a typical alcohol or ketone. The latter belongs to the lactone family, whereas the esters identified in this study were predominantly straight- and branched-chain acetate esters and ethyl esters of fatty acids. It is noteworthy that γ-butyrolactone has previously been reported as a natural constituent of wines and other beverages.

In Figure 4, each row represents all the selected signal peaks detected in each sample, while each column corresponds to the same volatile compound across different samples.

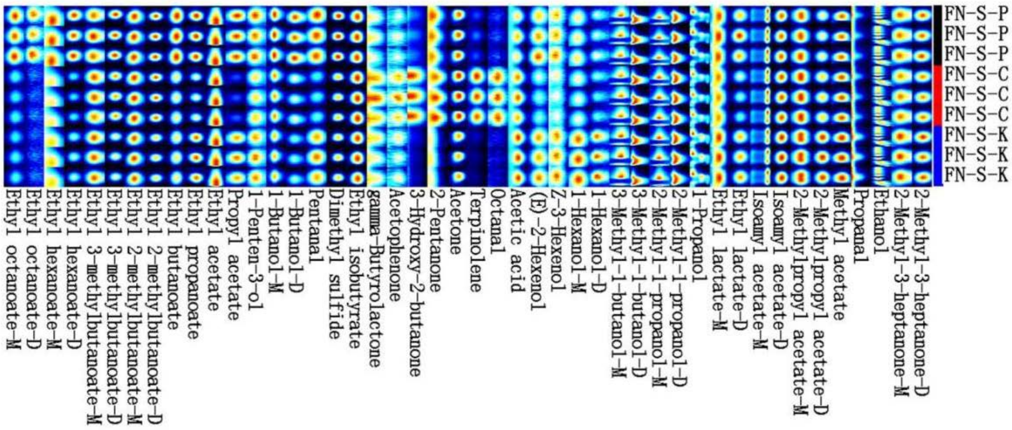

Figure 4. Fingerprint of GC-IMS spectra (FN-S-P: Purcari, FN-S-C: Cimișlia, FN-S-K: Căușeni).

This visualization provides a comprehensive overview of the volatile composition of each wine and highlights the differences among samples. The suffixes M and D indicate the monomer and dimer forms of the same compound, respectively, whereas numerical labels correspond to unidentified signal peaks. Distinct differences can be observed in the relative abundance of various compounds:

Purcari characteristic of higher levels of ethyl octanoate, ethyl hexanoate, ethyl 3-methylbutanoate, ethyl 2-methylbutanoate, ethyl butanoate, ethyl propanoate, ethyl acetate, propyl acetate, 1-penten-3-ol, 1-butanol, pentanal, and dimethyl sulfide.

Cimișlia showed higher contents of ethyl isobutyrate, γ-butyrolactone, acetophenone, 3-hydroxy-2-butanone, 2-pentanone, acetone, terpinolene, and octanal.

Căușeni was characterized by higher levels of acetic acid, (E)-2-hexenol, (Z)-3-hexenol, 1-hexanol, 3-methyl-1-butanol, 2-methyl-1-propanol, 1-propanol, ethyl lactate, isoamyl acetate, isobutyl acetate, methyl acetate, and propanal.

These findings indicate that each vineyard wine exhibited a unique “chemical fingerprint”, underscoring the influence of vineyard specific terroir conditions on the volatile composition of wines.

Table 2

Peak Volumes (Intensities) of Volatile Compounds in Three Vineyards of Ștefan Vodă IGP

Compound	Purcari		Cimișlia		Căușeni	
	Peak volume	Peak volume %	Peak volume	Peak volume, %	Peak volume	Peak volume, %
Acetic acid	4603.65	1.86	5226.08	2.09	5448.58	2.20
(E)-2-Hexenol	193.60	0.08	136.75	0.05	196.77	0.08
Z-3-Hexenol	211.94	0.09	181.59	0.07	220.85	0.09
1-Hexanol	507.53	0.21	448.71	0.18	663.51	0.27
3-Methyl-1-butanol	15480.93	6.27	15712.53	6.30	16009.63	6.46
1-Penten-3-ol	58.71	0.02	55.98	0.02	62.85	0.03
1-Butanol	2931.02	1.19	2398.23	0.96	2171.67	0.88
2-Methyl-1-propanol	16099.42	6.52	17596.70	7.05	18063.53	7.29
1-Propanol	6993.47	2.83	6703.38	2.69	7480.40	3.02
Ethanol	145719.85	58.98	150535.34	60.32	145413.44	58.68

Continuation Table 2

Octanal	33.63	0.01	92.71	0.04	29.88	0.01
Pentanal	176.73	0.07	85.37	0.03	172.79	0.07
Ethyl propanoate	1658.27	0.67	1024.43	0.41	1551.60	0.63
Propanal	146.51	0.06	161.03	0.06	187.57	0.08
Ethyl octanoate	1497.40	0.61	759.96	0.30	732.84	0.30
Ethyl lactate	4005.18	1.62	3329.80	1.33	4005.56	1.62
Ethyl hexanoate	1730.79	0.70	932.32	0.37	1101.09	0.44
Isoamyl acetate	8000.17	3.24	8078.06	3.24	8494.70	3.43
Ethyl 3-methylbutanoate	1456.43	0.59	1298.07	0.52	1123.80	0.45
Ethyl 2-methylbutanoate	1468.79	0.59	1456.44	0.58	1321.14	0.53
Ethyl butanoate	2676.76	1.08	1608.67	0.64	1709.32	0.69
2-Methylpropyl acetate	2058.90	0.83	2278.15	0.91	2726.21	1.10
Propyl acetate	247.95	0.10	77.85	0.03	224.19	0.09
Ethyl isobutyrate	3684.68	1.49	3916.21	1.57	3755.78	1.52
Ethyl acetate	18839.30	7.63	18099.56	7.25	18560.51	7.49
Methyl acetate	2620.18	1.06	2810.98	1.13	2985.51	1.20
Acetophenone	349.79	0.14	415.67	0.17	371.04	0.15
2-Pentanone	89.89	0.04	98.94	0.04	60.81	0.02
Acetone	1699.29	0.69	1818.96	0.73	1508.18	0.61
Dimethyl sulfide	1041.23	0.42	773.49	0.31	762.15	0.31
Terpinolene	263.33	0.11	787.63	0.32	157.19	0.06
γ-Butyrolactone	443.88	0.18	513.54	0.21	492.11	0.20
3-Hydroxy-2-butanone	60.15	0.02	151.35	0.06	50.97	0.02

Table 2 shows the peak volumes (intensities) of volatile compounds in Fetească Neagră wines from three vineyards of Ștefan Vodă IGP.

Alcohols are among the most important compounds in wine. The results showed that ethanol content was highest (58.68% to 60.32%), significantly exceeding that of the other VOCs. Esters are among the most important volatile aroma compounds in wine. Within the acetate ester group, ethyl acetate, isoamyl acetate, ethyl lactate, ethyl isobutyrate, ethyl butanoate, and methyl acetate were detected. Within the acetate ester group, ethyl acetate, the most common volatile ester, generally contributes fruity aromas at moderate concentrations. Its content from7.25% to 7.63%. Isoamyl acetate was one of the predominant esters detected, imparting intense banana and pear aromas. Its content from3.24% to 3.43%. Within the ethyl ester group of fatty acids, ethyl lactate is an important compound detected in this study, contributing roundness and slightly creamy notes to wine, content from1.33% to 1.62%. Ethyl hexanoate and ethyl octanoate, typical fatty acid ethyl esters that impart fruity and floral aromas.

Ketones are generally identified at low concentrations in wine. The content of acetone went from 0.61% to 0.69%. The content of 2-pentanone from 0.02% to 0.04%.

Dimethyl sulfide (DMS) was the only sulfur-containing compound detected in this study, with the highest content in 0.42% and the lowest in 0.31%. DMS, as a volatile sulfur compound, is further influenced by matrix effects: for instance, when added alone to deodorized wine, it is typically associated with off odors, but when combined with fruity aroma compounds, DMS can enhance overall complexity, imparting sweet fruity notes and green olive nuances to the wine.

Terpinolene, a monoterpene, generally imparts citrus, resinous, herbal, and subtle floral aromas to wine, and in grape varieties, it is primarily synthesized via the mevalonate pathway. However, terpenes are usually found in low concentrations in red wines due to the lower precursor content in red grape varieties, as well as the prolonged skin contact and higher phenolic levels during fermentation, which may suppress their expression. In this study, terpinolene ranged from 0.06% to 0.32%, suggesting that the Fetească Neagră variety may have relatively high terpene precursor levels or that this variety can accumulate higher amounts of free-form terpenes during ripening, which are then released during fermentation.

4. Discussion

Although all three vineyards lie in the Ștefan Vodă region, each site has unique attributes (e.g., slight differences in soil minerals, exposure, elevation, or viticultural practices) that can influence grape metabolism and fermentation outcomes, and the differences in subtle volatiles can be traced back to this terroir driven factors. This interpretation is consistent with the concept of terroir, which holds that even small scale environmental and viticultural differences manifest in the wine's chemical profile [21].

Many recent studies support our findings. A study carried out in Ningxia, China, showed that wines from sub regions with different climatic conditions exhibited different aroma profiles, and the temperature and soil nutrients were the main contributors [22]. Similarly, Goulioti et al. [23] found significant differences in the volatile composition and sensory profile of Xinomavro wines from different Greek Protected Designations of Origin (PDOs). Jin et al. [24] compared the volatile compound fingerprints of the variety Beibinghong from six vineyards and found that each region could be distinguished chemically and sensorially. These examples highlight that a wine's location can lead to measurable differences in its aroma compounds.

While the outcomes are encouraging, several limitations of this study should be acknowledged. First, we examined only a single vintage year, which means the observed differences could partially include vintage specific effects. Year to year climatic variability can influence grape composition; thus, our ability to generalize the findings across vintages is limited. Future studies should be carried out in multiple vintages to confirm that the vineyard differentiation holds under different growing seasons. Second, GC-IMS provides limited compound identification. This method is better at pattern recognition (fingerprinting volatiles), but its ability to conclusively identify each peak is constrained by the available spectral library and overlapping signals. Especially, some detected peaks remain unknown, whereas complementary methods like GC-MS would be supplemented to fully characterize the compounds. This limitation means we can pinpoint that "something" differs between vineyards (as shown in the differential maps), but not always name the specific chemical without additional analyses. Third, we did not conduct any sensory analysis in this study. As a result, it is unclear how the chemical differences observed translate to human perceived aroma or flavor differences.

Building on these findings, several avenues for future research are recommended. Expanding the scope to multiple vintages and additional vineyard sites within (and beyond) the Ștefan Vodă IGP will help validate GC-IMS as a robust tool for terroir differentiation. Including more years would clarify the consistency of vineyard specific volatile markers versus vintage induced variability. Similarly, experimental subjects should be expanded to different grape varieties. Another important future direction is to combine gas chromatography-ion mobility spectrometry analysis with sensory evaluation and advanced data analysis techniques. By combining chemical fingerprinting with sensory descriptive analysis or consumer preference testing, researchers can determine which chemical differences are perceptible and crucial for the quality or typicality of wine. In parallel, applying chemometric tools and machine learning can greatly enhance the classification and predictive power of the data. For example, recent studies have shown that combining GC-IMS volatile data with machine learning algorithms (such as artificial neural networks) allowed >95% accuracy in predicting wine quality grades or classifying wines by type [25].

5. Conclusions

This study demonstrates that GC-IMS can effectively differentiate wines from three vineyards in the IGP Ștefan Vodă region of Moldova and reveal vineyard specific volatile fingerprints. The overall volatile composition of the samples was similar, significant differences were observed: FN-S-P wines were enriched in esters (such as ethyl octanoate, ethyl hexanoate, and ethyl acetate) and alcohols (such as 1-butanol and 1-penten-3-ol); FN-S-C wines were characterized by higher levels of carbonyl compounds and terpenes (such as γ-butyrolactone, acetophenone, and terpinolene); whereas FN-S-K wines showed elevated concentrations of higher alcohols and acetate esters (such as 3-methyl-1-butanol, isoamyl acetate, and ethyl lactate). These results confirm that GC-IMS can figure out the vineyard level differences in volatile composition. Although the study was limited to a single vintage, the findings highlight the potential of GC-IMS as a rapid, sensitive, and visual tool for vineyard level discrimination. Future research should include multiple vintages, more varieties, incorporate sensory evaluation, and apply chemometric and machine learning approaches to improve classification reliability.

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References

1. Pittari, E.; Moio, L.; Piombino, P. Interactions between Polyphenols and Volatile Compounds in Wine: A Literature Review on Physicochemical and Sensory Insights. *Appl. Sci.* 2021, 11(3), pp. 1-29.
2. Ilc, T.; Werck-Reichhart, D.; Navrot, N. Meta-analysis of the core aroma components of grape and wine aroma. *Front. Plant Sci.* 2016,7, pp.1-15.
3. Lin, J.; Massonnet, M.; Cantu, D. The genetic basis of grape and wine aroma. *Hortic. Res.* 2019,81(6), pp. 1-24.
4. Louw, S. Recent trends in the chromatographic analysis of volatile flavor and fragrance compounds: Annual review 2020. *Anal. Sci. Adv.* 2021, 2, pp. 157–170.
5. Rossi, L.; Foschi, M.; Biancolillo, A.; Maggi, M. A.; D'Archivio, A. A. Optimization of HS-SPME-GC/MS analysis of wine volatiles supported by chemometrics for the aroma profiling of Trebbiano d'Abruzzo and Pecorino white wines produced in Abruzzo (Italy). *Molecules* 2023, 28(4), pp. 1-18.
6. Lukić, I.; Carlin, S.; Vrhovsek, U. Utility of comprehensive GC× GC gas chromatography in finding varietal markers among volatile compounds in non-aromatic red wines. *Agronomy* 2022, 12(10), pp. 1-21.
7. Boscaini, E.; Mikoviny, T.; Wisthaler, A.; von Hartungen, E.; Märk, T. D. Characterization of wine with PTR-MS. *Int. J. Mass Spectrom.* 2004, 239(2-3), pp. 215-219.
8. Zhu, W.; Benkwitz, F.; Sarmadi, B.; Kilmartin, P. A. Validation study on the simultaneous quantitation of multiple wine aroma compounds with static headspace-gas chromatography-ion mobility spectrometry. *J. Agric. Food Chem.* 2021, 69(49), pp.15020-15035.
9. Chen, K.; Li, S.; Yang, H.; Zou, J.; Yang, L.; Li, J.; Ma, L. Feasibility of using gas chromatography-ion mobility spectrometry to identify characteristic volatile compounds related to brandy aging. *J. Food Compos. Anal.* 2021, 98, pp. 1-12.
10. Geng, D.; Chen, X.; Jin, J.; Lu, D.; Huo, Y.; Chen, B. Optimization of GC-IMS parameters and determination of volatile fingerprint of flavors and fragrances using GC-IMS. *CYTA - J. Food* 2024, 22(1), pp. 1-13.

11. Capitain, C.; Weller, P. Non-targeted screening approaches for profiling of volatile organic compounds based on gas chromatography-ion mobility spectroscopy (GC-IMS) and machine learning. *Molecules* 2021, 26(18), 5457.
12. del Mar Contreras, M.; Arroyo-Manzanares, N.; Arce, C.; Arce, L. HS-GC-IMS and chemometric data treatment for food authenticity assessment: Olive oil mapping and classification through two different devices as an example. *Food Control* 2019, 98, pp. 82-93.
13. Arroyo-Manzanares, N.; Martín-Gómez, A.; Jurado-Campos, N.; Garrido-Delgado, R.; Arce, C.; Arce, L. Target vs spectral fingerprint data analysis of Iberian ham samples for avoiding labelling fraud using headspace–gas chromatography–ion mobility spectrometry. *Food Chem*. 2018, 246, pp. 65-73.
14. Schwolow, S.; Gerhardt, N.; Rohn, S.; Weller, P. Data fusion of GC-IMS data and FT-MIR spectra for the authentication of olive oils and honeys - is it worth to go the extra mile? *Anal. Bioanal Chem*. 2019, 411(23), pp. 6005-6019.
15. Cao, W.; Shu, N.; Wen, J.; Yang, Y.; Jin, Y.; Lu, W. Characterization of the key aroma volatile compounds in nine different grape varieties wine by headspace gas chromatography–ion mobility spectrometry (HS-GC-IMS), odor activity values (OAV) and sensory analysis. *Foods* 2022, 11(18), 2767.
16. Chen, H.; Bai, S.; Yang, B.; Ren, R.; Tang, Z.; Zhang, Z.; Zeng, Q. Inter-and intra-varietal clonal differences influence the aroma compound profiles of wines analyzed by GC–MS and GC-IMS. *Food Chem. X* 2025, 25, 102136.
17. Zhang, T.; Liao, Z.; Li, Z.; Liu, Y.; Bi, J.; Liu, Y.; Sun, Y; Qin, Y. Revealing the flavor differences of Sauvignon Blanc wines fermented in different oak barrels and stainless-steel tanks through GC-MS, GC-IMS, Electronic, and Artificial Sensory Analyses. *Food Chem. X* 2025, 25, 102188.
18. Parastar, H.; Weller, P. Towards greener volatilomics: Is GC-IMS the new Swiss army knife of gas phase analysis. *TrAC, Trends Anal. Chem*. 2024, 170, 117438.
19. Gao, W.; Yang, X.; Zhu, X.; Jiao, R.; Zhao, S.; Yu, J.; Wang, D. Limitations of GC-QTOF-MS technique in identification of odorous compounds from wastewater: the application of GC-IMS as supplement for odor profiling. *Atmosphere* 2021, 12(2), 265.
20. Capitain, C.; Weller, P. Non-targeted screening approaches for profiling of volatile organic compounds based on gas chromatography-ion mobility spectroscopy (GC-IMS) and machine learning. *Molecules* 2021, 26(18), 5457.
21. Zhou, J.; Cavagnaro, T. R.; De Bei, R.; Nelson, T. M.; Stephen, J. R.; Metcalfe, A.; Gilliham, M; Breen, J.; Collins, C.; Lopez, C. M. R. Wine terroir and the soil bacteria: an amplicon sequencing–based assessment of the Barossa Valley and its sub-regions. *Front. Microbiol*. 2021, 11, 597944.
22. Song, X.; Ling, M.; Li, D.; Zhu, B.; Shi, Y.; Duan, C; Lan, Y. Volatile profiles and sensory characteristics of Cabernet sauvignon dry red wines in the Sub-Regions of the eastern foothills of Ningxia Helan Mountain in China. *Molecules* 2022, 27(24), 8817.
23. Goulioti, E.; Jeffery, D. W.; Kanapitsas, A.; Lola, D.; Papadopoulos, G.; Bauer, A.; Kotseridis, Y. Chemical and sensory characterization of Xinomavro red wine using grapes from protected designations of northern Greece. *Molecules* 2023, 28(13), 5016.
24. Jin, Y.; Shu, N.; Xie, S.; Cao, W.; Xiao, J., Zhang, B.; Lu, W. Comparison of ‘Beibinghong’dry red wines from six producing areas based on volatile compounds analysis, mineral content analysis, and sensory evaluation analysis. *Eur. Food Res. Technol*. 2021, 247(6), pp.1461-1475.
25. Zhou, C; Yu, Y.; Ai, J.; Song, C.; Cui, Z.; Zhou, Q.; Zhao, S.; Rui, H.; Huang, R.; Ao, Z.; Peng, B.; Chen, P.; Feng, X.; Li, D.; Liu, Y. Fruit wines classification enabled by combing machine learning with comprehensive volatiles profiles of GC-TOF/MS and GC-IMS. *Food Res. Int*. 2025, 204, 115890.

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