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SHORT COMMUNICATION

The SIFT-MS fingerprint of *Vitis vinifera* L. cv. Syrah berries is stable over the second part of maturation under warm conditions of climate

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ABSTRACT

Wine grape breeding for fungal resistance has been very dynamic worldwide over the last decade. The quick phenotyping of genotype quality traits, including aroma composition, remains challenging. Selected ion flow tube mass spectrometry (SIFT-MS) could be particularly valuable for this usage. Due to the high number of seedlings to phenotype and the low availability of berries, the sampling strategy can hardly rely on time-consuming destructive methods such as the measurement of classical maturity parameters (i.e., sugar concentration). To investigate the impact of the sampling time on the SIFT-MS fingerprint, berries from *Vitis vinifera* L. Syrah were collected in 2020, a season characterised by warm climatic conditions, at seven times during maturation and analysed by SIFT-MS using O_2^+ as reagent ion. This fingerprint has proved to be stable from 28 days after mid-veraison. This finding greatly simplifies the sampling procedure for future berry phenotyping, which can only rely on non-destructive data (lapse of time after mid-veraison date). For most *m/z*, a decrease in abundance was observed during the maturation, which could be the consequence of volatile emission or an increase in non detectable bound compounds. Further studies would be necessary to assess the full grape aroma potential, to better understand the mechanisms involved, and to evaluate our approach over more than one season.

KEYWORDS: SIFT-MS, fingerprint, *Vitis vinifera* L. Syrah, maturation, grape breeding, high throughput phenotyping

INTRODUCTION

Vitis vinifera L. is one of the most widely grown and economically important grapevine species in the world, mainly as a consequence of the high quality of its wines (Vivier and Pretorius, 2002). However, it is susceptible to abiotic and biotic stresses such as pests or fungal diseases. These pathogens can be chemically fought or through crossbreeding with resistant or tolerant genotypes (Töpfer *et al*., 2011). Crossbreeding for wine grape biotic resistance has been very dynamic across Europe in the second part of the 19th century due to the introduction of phylloxera (*Daktulosphaira vitifoliae*). It led to the development of hybrid direct producers (HDPs) that interestingly also exhibited cross-tolerance to downy mildew (*Plasmopara viticola*) and powdery mildew (*Erysiphe necator*) (Alleweldt and Possingham, 1988). However, these genotypes were associated with poor quality wines, which prevented the continuation of related breeding programs in most countries, with the exception of Germany and Hungary (Alleweldt and Possingham, 1988). Nowadays, grape breeding for fungal resistance is experiencing a resurgence of interest worldwide because of the societal pressure towards the reduction of pesticide use. Breeding programs based on controlled sexual reproduction typically generate 50,000 seedlings a year and last between 25 to 30 years from the initial crossing to the release of new cultivars on the market. The use of marker-assisted selection (MAS), notably markers related to mildew resistance, can help the screening and accelerate the process for up to 10 years by quickly reducing to about 5000 the number of plants to phenotype (Töpfer *et al*., 2011).

Despite the identification of quantitative trait loci (QTLs) for berry and wine quality (Doligez *et al*., 2006; Eibach *et al*., 2002; Hausmann *et al*., 2018), the evaluation of quality traits remains by far one of the most time-consuming steps. Grape aroma compounds imparting wine typicity are considered some of the most important molecules driving wine quality and appreciation (Zhu *et al*., 2016). In this context, there is a high demand within the grape research community for high throughput technology to quickly assess the varietal aroma composition of a large amount of genotypes.

Selected ion flow tube mass spectrometry (SIFT-MS) is a technology commercially available since 2008 that has the advantage of offering real-time headspace analysis and high sensitivity (Smith and Španěl, 2005). This device based on soft ionisation using eight different reagent ions for the most recent equipment (H_3O^+, NO^+, O_2^+, NO_3^-, NO_2^-, O^-, O_2^- and OH^-) can analyse a sample headspace and determine relative abundances in Selected Ion Monitoring (SIM) or scan mode (Hera *et al*., 2017).

A recent study highlighted that SIFT-MS could be valuable for discriminating the volatile composition of *Vitis vinifera* berries and, therefore, for the quick phenotyping of grape varieties (Baerenzung dit Baron *et al*., 2022). Cultivars could be easily distinguished based on their SIFT-MS fingerprint scan, notably with O_2^+. The use of this latter single reagent ion which has the highest ability to ionise most organic compounds was particularly relevant to reduce the time of analysis to 3 minutes. The SIFT-MS technology enabled discrimination of low and high aroma producers and to connect cultivars, in most cases, according to their parentage relationship. In this former research, grape varieties were sampled at three different dates according to their theoretical timing of veraison (Baerenzung dit Baron *et al*., 2022). One cultivar was collected at the three sampling dates to investigate the impact of maturity on the whole volatile fingerprint. These three samples were all included in the same cluster of varieties, supporting the hypothesis of a higher impact of the cultivar on SIFT-MS grape fingerprint than at the time of sampling.

However, in the perspective of further use of this methodology for the quick phenotyping of new varieties, the impact of the sampling date on the SIFT-MS volatilome would deserve to be investigated deeper. This would enable one to establish a reliable berry sampling strategy based on non-destructive phenological data (lapse of time after mid-veraison date). Indeed, the adaptation of the date of sampling and measurement to typical maturity parameters such as sugar concentration is hardly implementable due to the high number of individuals to phenotype and the low quantity of grapes available for each genotype, at best a couple of clusters borne by one single plant. The aim of this research work was to study the impact of seven sampling times over maturation on the SIFT-MS fingerprint of *Vitis vinifera* L. cv. Syrah.

MATERIALS AND METHODS

1. Vineyard site and grape sampling

The 0.51-ha vineyard from where the grapes were sourced was located in the southwest of France (lat. 43° 50′ 25″ N; long. 01° 50′ 57″ E) and was typical of the area with 2.20 m × 1 m vine spacing. The block was planted in 2002 with Syrah, the most widely grown cultivar in the vineyards of Occitanie, according to FranceAgriMer (www.franceagrimer.fr). It was grafted on Gravesac rootstock and was trained with vertical shoot positioning on a single Guyot pruning system. The orientation of the vine rows was north-east to south-west. The soil was mechanically managed under the vines and by grass cover in the inter-row area. Samples composed of 100 berries were first collected every third day from the end of July to the beginning of August 2020 to determine mid-veraison (50 % of soft berries), and then in triplicate at seven times during maturation to investigate the impact of sampling time on SIFT-MS fingerprint. Grapes were sampled on 6, 20 and 28 August 2020, 3, 10, 17 and 25 September 2020 which corresponds to mid-veraison (50 % ver.), 14 days after mid-veraison (50 % ver.+14d), 22 days after mid-veraison (50 % ver.+22d), 28 days after mid-veraison (50 % ver.+28d), 35 days after mid-veraison (50 % ver.+35d), 42 days after mid-veraison (50 % ver.+42d) and 50 days after mid-veraison (50 % ver.+50d), respectively. The commercial harvest of the vineyard took place on 15 September. Samples

were always collected from the same fifty vine plants spread over three rows, from both sides of the row and several parts of the bunch (50 berries from each side of the row). Crop load was estimated at around 3 kg per vine (150 kg for the whole sampling area), which indicates that the whole amount of grapes harvested over the seven sampling dates (2100 berries) is unlikely to impact crop load or leaf area to fruit ratio for each sampled plant and therefore should not induce any bias.

2. Physico-chemical parameters and weather measurements

For each 100-berry sample, 50 g were used for SIFT-MS analysis and the rest for the determination of physico-chemical parameters. In this latter subsample, the number of berries was first counted to determine berry weight. Grape samples were then crushed, the juice was centrifuged for 1 min at 5600 *g* and the supernatant was used for the analyses. Sugar concentration (°Brix) was estimated with an MA885 Wine Refractometer (Milwaukee, Wisconsin, USA), and pH was measured using a PHM 210 MeterLab pH meter (Radiometer, Copenhagen, Denmark). Titratable acidity (TA) expressed as g/L of tartaric acid was determined according to the method of the Organisation Internationale de la Vigne et du Vin (OIV, 2009) using a 1 M NaOH solution.

As climatic conditions over the sampling period are likely to impact physico-chemical parameters and particularly berry weight, rainfall and mean daily air temperature were also monitored daily since 2005 by a CimAGRO weather station (Cimel Electronique, Paris, France) placed within 200 m of the experimental site. These data were used to calculate the average mean temperature and cumulative rainfall between 6 August and 25 September for 2020 and for the 2005-2020 period.

3. Sample preparation and SIFT-MS measurements

Sample preparation and SIFT-MS measurements were performed according to the protocol proposed by Baerenzung dit Baron *et al*. (2022), which can be summarised briefly here.

After crushing, 50 g of grapes were transferred into a 1 L Schott bottle (Verres Vagner, Toulouse, France) sealed with a Teflon-secured screw cap. Then, it was kept for 6 h at room temperature and transferred to a water bath for 40 min at 40 °C. These conditions that did not saturate the device analysis potential were determined in previous research (Baerenzung dit Baron *et al*., 2022).

SIFT-MS measurements were conducted using a Voice 200 Ultra model (Syft Technologies, Christchurch, NZ) in full scan mode (from *m/z* 15 to 250) using O_2^+ as a reagent ion. The injection was conducted using N_2 flow as a carrier gas (Alphagaz, Air Liquide, 99.9999 %, Paris, France) with a nitrogen flow rate set at 2.0 TorrL/s. The sample headspace was introduced by a calibrated capillary at a sampling flow rate of 0.3 TorrL/s. The analytes reacted with the selected precursor in the flow tube kept at 119 °C and 0.06 kPa

Instrumental repeatability was estimated at 7 % and reproducibility at 10 %. LabSyft 1.6.2. software (Syft Technologies) was used for data acquisition and analysis.

4. Data treatment

SIFT-MS data were pre-treated by removing masses with an *m/z* ratio below 100 and abundance below noise following the procedure proposed by Baerenzung dit Baron *et al*. (2022).

Then SIFT-MS data, together with physico-chemical parameters, were subjected to a one-way analysis of variance (ANOVA) treatment using XLSTAT software (Addinsoft, Paris, France). Fisher's least significant difference (LSD) test was used as a post-hoc.

A principal component analysis (PCA) was performed on SIFT-MS significant variables ($P < 0.05$) using ClustVis online software (http://biit.cs.ut.ee/clustvis).

RESULTS AND DISCUSSION

1. Berry maturity and weather conditions

Results show a steady evolution of the measured physico-chemical parameters over the sampling period (Table 1). As could be expected, sugar concentration increased

TABLE 1. Results (mean and standard deviation of three observations) and significance of physico-chemical parameters analysed on berries sampled at seven times during maturation, from mid-veraison (50 % ver.). Different letters within a column indicate significantly different means at $P < 0.05$ by the Fisher test.

Time of sampling	Sugar concentration (°Brix)	Titratable acidity (g/L as tartaric acid)	pH	Berry weight (g)
50 % ver.	13.0 ± 0.1 e	16.95 ± 0.36 a	2.80 ± 0.02 e	1.31 ± 0.11 bc
50 % ver.+14d	18.3 ± 0.6 d	15.90 ± 1.31 a	3.12 ± 0.03 d	1.57 ± 0.17 a
50 % ver.+22d	20.0 ± 0.9 c	12.75 ± 1.40 b	3.25 ± 0.02 c	1.21 ± 0.10 c
50 % ver.+28d	21.9 ± 0.6 b	11.25 ± 0.90 b	3.25 ± 0.02 c	1.31 ± 0.12 bc
50 % ver.+35d	22.5 ± 0.4 b	8.44 ± 0.15 c	3.32 ± 0.03 b	1.40 ± 0.08 ab
50 % ver.+42d	24.9 ± 0.2 a	4.77 ± 0.16 d	3.46 ± 0.04 a	1.37 ± 0.06 bc
50 % ver.+50d	25.1 ± 0.7 a	4.90 ± 0.28 d	3.49 ± 0.06 a	1.27 ± 0.11 bc
P	< 0.0001	< 0.0001	< 0.0001	< 0.05

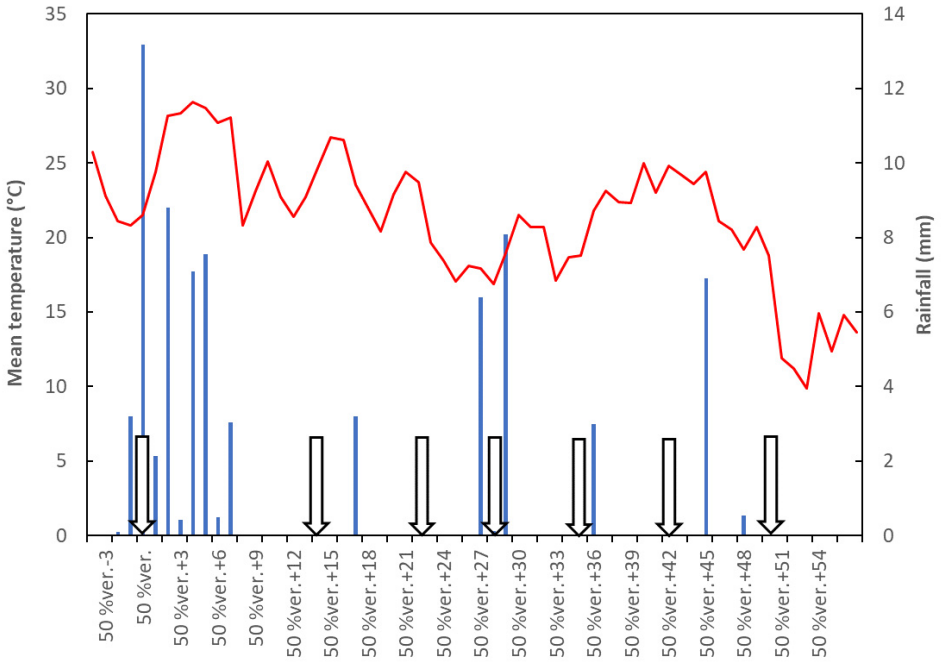

FIGURE 1. Daily mean temperature (red line) and rainfall (blue bar) over the sampling period. Sampling dates are symbolised by arrows.

through accumulation in hexoses while TA decreased through malate catabolism (Coombe, 1992). Trivially, this latter phenomenon was also accompanied by an increase in pH. It is worth mentioning that the changes in sugar content and TA level were particularly marked between 50 % ver.+35d and 50 % ver.+42d. This could be the consequence of the warmer and dryer conditions of climate experienced over this lapse of time (Figure 1) that might have enhanced the speed of maturation (Scholasch and Rienth, 2019). It can be noticed that the climatic conditions were generally warm over the studied period, with mean temperatures surpassing 20 °C in most cases and even approaching 30 °C just after veraison. Indeed, the average temperature that reached 22.3 °C for the sampling period was warmer than those recorded for the 2005-2020 period (20.1 ± 1.2 °C), while cumulative rainfall was in the same range (57.7 mm for 2020; 78.7 ± 43.8 mm for 2005-2020). The 2020 season was an early vintage with a 15-day advance in phenology, and these data might not completely reflect the differences in temperature observed during maturation between the studied season and the other vintages, during which maturation occurs later and under likely cooler conditions.

As a consequence of these warm conditions, the sugar concentration was already high at 50 % ver.+42d, reaching 24.9 ± 0.2 °Brix. Between 50 % ver. and 50 % ver.+14d, and to a lesser extent, between 50 % ver.+28d and 50 % ver.+35d, an increase in berry weight was noticed. Despite that xylem is known to be dysfunctional from veraison and that berries become less sensitive to soil moisture (Scholasch and Rienth, 2019), this could be related to some rainfall events that provoked a significant water inflow.

2. SIFT-MS fingerprint

Among the 150 ions monitored by SIFT-MS with *m/z* between 100 and 250, 61 showed an abundance above noise and 59 were significantly impacted by the sampling date (Table 2).

For the seven sampling dates, several groups of masses were observed with the highest abundances around *m/z* 105, 119 and 147, which is in accordance with previous SIFT-MS results obtained on *Vitis vinifera* berries (Baerenzung dit Baron *et al.*, 2022). Even if such masses could be related to several ions, such as $C_7H_5O^+$ for *m/z* 105 that originates from the ionisation of benzaldehyde (Španěl *et al.*, 1997), they are also commonly related to the fragmentation of terpenoids (Amadei and Ross, 2011).

The aroma of Syrah grapes and wines has been the subject of much research worldwide (Geffroy *et al.*, 2020b; Morère *et al.*, 2020; Mayr *et al.*, 2014; Segurel, 2005). These works highlighted that rotundone, 3-mercaptohexanol, dimethyl sulfide (DMS), β-damascenone and other glycosidic precursors were the key compounds involved in the varietal aroma of this cultivar. 3-Mercaptohexanol, which is found in grapes in a non-volatile form bound to amino acids or glutathione, is a priori not detectable through SIFT measurements (Roland *et al.*, 2011). The same remark can be made for the largest part of DMS, which is mainly produced in wine by degradation of *S*-methylmethionine (Segurel, 2005) and for most glycosidic precursors, including β-damascenone although a minority of these latter compounds can also be present under a free aglycone form in grapes (Ugliano and Moio, 2008). Despite the high fragmentation ability of O_2^+, ionisation with this reagent ion is always known to generate one

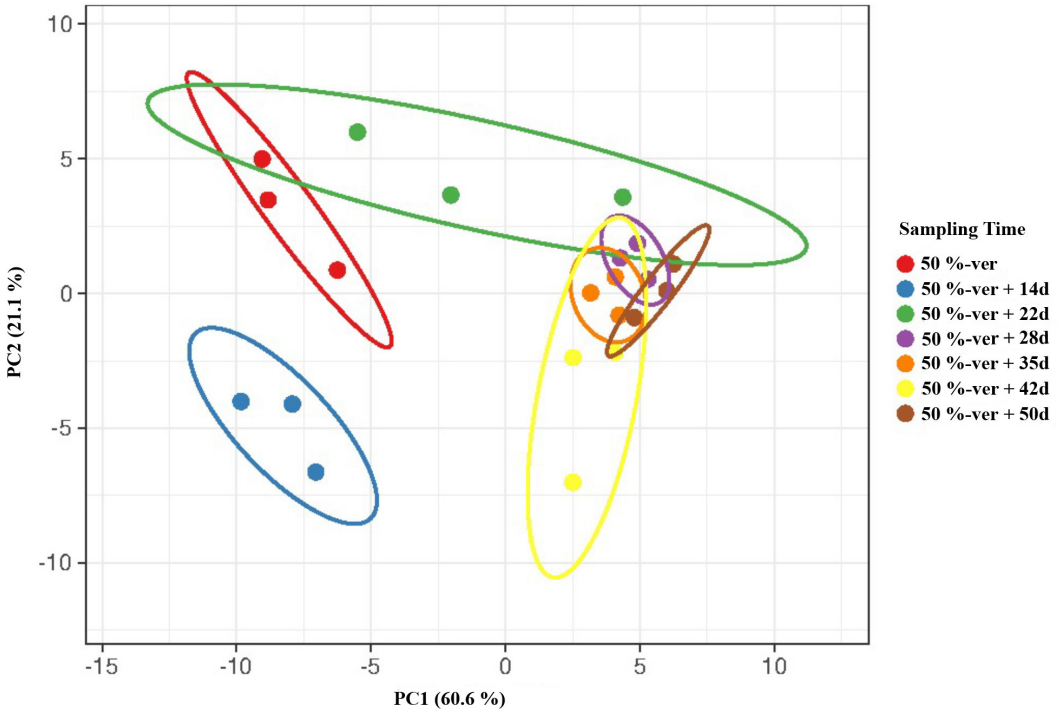

FIGURE 2. Factor scores with 95 % confidence ellipse for a principal component analysis (PCA) performed on the SIFT-MS abundance data using O_2^+ as reagent ion for berries sampled seven times during maturation, from mid-veraison (50 % ver.).

molecular ion (Smith and Panel, 2005). If this were the case for β-damascenone and rotundone, a signal would have been expected at *m/z* 190 and 218, respectively. The absence of a signal might be the consequence of concentration levels below the limit of detection of the SIFT-MS device, from 100 ppt to 1 ppb in a gas phase (Lehnert *et al*., 2019). This might be particularly the case for rotundone as the warm climatic conditions experienced during the studied vintage were not favourable to the biosynthesis of this molecule (Geffroy *et al*., 2020a). By removing masses below 100, the data pretreatment has contributed to removing potential molecular ions of DMS whose signal would have been expected at *m/z* 62. On the hand, it cannot be excluded that free DMS, whose concentration in Syrah juices is known to be in the ppb range (Segurel, 2005), would have also been below the limit of detection. On the other hand, SIFT-MS is known to create molecular clusters and adducts, notably with water molecules (Lehnert *et al*., 2019). It cannot be discarded that a signal related to DMS could be recorded with *m/z* above 100. The identification of such compounds would require more work using the DMS standard.

The PCA plot shows that the volatile composition of berries determined by SIFT-MS measurements greatly varied from 50 % ver. to 50 % ver.+28d but remained stable from this latter sampling date (Figure 2). Such a finding is in accordance with previous work highlighting a high similarity in SIFT-MS fingerprint between Sémillon samples harvested at three different times from 40 days after mid-veraison (Baerenzung dit Baron *et al*., 2022). It is particularly interesting for future high throughput berry phenotyping as it indicates that maturity does not need to be carefully monitored for physico-chemical parameters and that berries can be harvested for SIFT-MS measurements from 50 % ver.+28d. The fact that the sample harvested at 50 % ver.+42d exhibited a slightly different fingerprint remains unclear but could be related to the sudden increase in temperature previously described.

In most cases, a decrease in abundance was noticed during maturation (Table 2). Large changes in berry volatile composition involving translocation, accumulation, or metabolism mechanisms have been previously reported during this period (Robinson *et al*., 2014). To our knowledge, alkyl-methoxypyrazines are one of the rare grape aroma compounds whose concentration is known to decrease over maturation (Lei *et al*., 2018). Such a decrease cannot be observed for 3-isobutyl-2-methoxypyrazine (IBMP), whose molecular ion is not detected at *m/z* 166. An abundance reduction can be noticed at *m/z* 152, which could be related to 3-isopropyl-2-methoxypyrazine (IPMP). However, this hypothesis is unlikely as IPMP is generally found in grapes at a lower abundance than IBMP (Lei *et al*., 2018). For the other masses, the decrease in abundance could be the consequence of volatile emissions (Rice *et al*., 2019) or an increase in non-detectable glycosidically-bound compounds, as reported for monoterpenols (Fenoll *et al*., 2009). Further work, including additional preparation steps which are not essential for our study objective, would be necessary to improve the existing model and to access the full aroma potential of grapes through either acid or enzymatic hydrolysis of bound compounds (Dziadas and Jeleń, 2016).

TABLE 2. SIFT-MS abundance results (mean of three observations) and significance of product ions using O_2^+ as reagent ion for berries sampled seven times during maturation, from mid-veraison (50 % ver.). Different letters within a row indicate significantly different means at $P < 0.05$ by the Fisher test.

Part 1/2

m/z	50 % ver.	50 % ver.+14d	50 % ver.+22d	50 % ver.+28d	50 % ver.+35d	50 % ver.+42d	50 % ver.+50d	P
100	4090 a	2620 bc	3679 ab	1904 d	1561 cd	820 d	1061 d	< 0.0001
101	13428 a	7 752 b	11686 a	5388 bcd	5610 bc	2193 d	3673 cd	< 0.0001
102	1098 a	664 bc	832 b	400 de	456 cd	187 e	286 de	< 0.0001
103	4462 a	5441 a	2478 b	1491 bc	1882 bc	2438 bc	1297 c	< 0.0001
104	998 b	1273 a	591 c	241 d	388 cd	506 cd	310 d	< 0.0001
105	3382 b	6280 a	1648 c	779 c	1469 c	3677 b	1322 c	< 0.0001
106	213 bc	381 a	131 cd	93 d	104 cd	254 b	79 d	< 0.01
107	8024 b	13606 a	2662 c	1001 c	3658 c	8379 b	2379 c	< 0.0001
108	376 b	633 a	128 c	51 c	149 c	398 b	143 c	< 0.0001
109	170 d	1028 b	220 d	203 d	579 b	448 bc	222 cd	< 0.0001
111	139 c	1584 a	86 c	140 c	188 bc	451 b	189 bc	< 0.0001
115	298 a	242 ab	112 c	101 c	102 c	171 bc	92 c	< 0.0001
116	537 ab	391 b	600 a	200 c	222 c	132 c	174 c	< 0.0001
117	5643 a	4074 b	3631 b	1356 c	1463 c	836 c	900 c	< 0.0001
118	1933 a	1676 a	1559 a	528 b	829 b	699 b	506 b	< 0.0001
119	12938 a	8112 bc	11308 ab	4593 d	4866 cd	2529 d	3179 d	< 0.0001
120	900 a	464 bc	669 ab	260 cd	159 d	157 d	151 d	< 0.0001
121	4087 a	3602 ab	2366 cd	2590 cd	1787 cd	2684 bc	1680 d	< 0.01
122	280 a	230 ab	181 bc	197 bc	104 d	149 cd	102 d	< 0.01
123	83 ab	120 a	20 c	16 c	44 bc	77 ab	34 bc	< 0.05
127	329 a	292 a	50 b	112 b	50 b	71 b	70 b	< 0.0001
128	573 a	311 bc	426 ab	202 cd	152 cd	67 d	118 d	< 0.0001
129	453 ab	619 a	314 bc	108 d	208 cd	130 d	110 d	< 0.0001
130	256 a	196 b	170 b	57 cd	91 c	30 d	41 cd	< 0.0001
131	463 a	347 a	210 b	91 bc	111 bc	110 bc	62 c	< 0.0001
133	1389 a	1224 a	451 bc	139 c	440 bc	643 b	254 c	< 0.0001
134	132 ab	171 a	52 c	33 c	46 c	94 bc	33 c	< 0.01
135	632 bc	987 ab	239 cd	80 d	359 cd	1204 a	201 cd	< 0.01
136	112 ab	132 a	20 c	30 c	29 c	106 ab	42 bc	< 0.05
137	110 c	747 a	82 c	31 c	138 c	459 b	102 c	< 0.01
138	23 a	107 a	10 a	70 a	39 a	87 a	46 a	ns
139	177 c	2392 a	118 c	248 c	423 bc	1882 ab	337 bc	< 0.05
140	33 c	177 a	1 c	68 bc	46 c	130 ab	33 c	< 0.01
141	400 a	267 ab	218 bc	103 cd	81 cd	74 d	52 d	< 0.01
142	256 a	167 ab	147 bc	60 c	112 bc	47 c	53 c	< 0.01
143	2101 a	1378 b	1226 b	284 c	496 c	229 c	301 c	< 0.0001
144	724 a	828 a	568 a	123 b	257 b	124 b	157 b	< 0.0001
145	10311 a	11031 a	5700 b	1207 c	3060 bc	1526 c	1529 c	< 0.0001
146	1281 a	1468 a	767 b	193 c	454 bc	290 c	221 c	< 0.0001
147	12703 a	15696 a	6170 b	1552 c	4238 bc	3392 bc	2254 c	< 0.0001
148	1212 b	1517 a	494 c	148 d	384 cd	291 cd	216 cd	< 0.0001
149	3527 b	6938 a	1331 c	657 c	1559 c	3887 b	1100 c	< 0.0001
150	282 b	581 a	99 c	37 c	48 c	328 b	66 c	< 0.0001

Part 2/2

m/z	50 % ver.	50 % ver.+14d	50 % ver.+22d	50 % ver.+28d	50 % ver.+35d	50 % ver.+42d	50 % ver.+50d	P
151	47 b	101 a	14 bc	1 c	22 bc	26 bc	27 bc	< 0.01
152	31 ab	53 a	11 b	9 b	20 b	16 b	10 b	< 0.05
153	82 ab	89 a	30 b	47 b	24 b	42 b	30 c	< 0.01
155	132 a	60 b	50 b	68 b	13 b	18 b	28 b	< 0.05
156	100 a	53 bc	71 ab	30 cd	14 d	9 d	14 d	< 0.01
157	233 a	192 ab	126 b	44 c	43 c	19 c	23 c	< 0.0001
159	242 a	248 a	131 b	57 c	49 c	66 c	38 c	< 0.0001
161	516 a	369 ab	459 a	71 c	111 c	223 bc	140 c	< 0.0001
165	87 ab	130 a	61 bc	52 bc	57 bc	67 bc	22 c	< 0.05
167	42 c	331 a	42 c	82 bc	131 bc	156 b	91 bc	< 0.01
181	69 a	70 a	48 a	24 a	40 a	14 a	12 a	ns
189	114 a	71 b	14 c	6 c	7 c	32 c	6 c	< 0.0001
193	36 b	137 a	24 b	22 b	30 b	6 b	14 b	< 0.01
195	22 bc	83 a	71 a	18 bc	50 ab	26 bc	6 c	< 0.05
197	161 a	124 a	177 a	30 b	37 b	17 b	7 b	< 0.01
199	248 a	169 a	262 a	27 b	28 b	11 b	24 b	< 0.01
201	276 a	183 a	242 a	29 b	41 b	16 b	22 b	< 0.01
203	123 a	103 a	96 a	18 b	18 b	21 b	17 b	< 0.0001

ns = non significant.

Our results are only valid for a season characterised by warm climatic conditions during the maturation period. They might not be generalisable and transferable to vintages with cooler conditions. However, it must be pointed out that most of the newly developed genotypes are generally grown during the first years in greenhouses under semi-controlled environmental conditions. Under these growing conditions, temperatures are expected to be warm, and seasonality is likely to have a weaker impact in comparison with field-grown vines.

CONCLUSION

Our work highlighted that the SIFT-MS fingerprint of Syrah berries was stable from 50 % ver. +28 days under warm conditions of climate. This result is particularly relevant for the future high throughput phenotyping of berries under warm conditions of maturation as it enables to simplify the sampling strategy greatly. The proposed strategy only relies on phenological data and does not require accurate monitoring of physico-chemical parameters. In most cases, a decrease in abundance was observed over the maturation period, which could be the consequence of volatilisation or an increase in glycosidically-bound compounds that are not volatile and cannot be detected through SIFT-MS measurements. Additional research would be necessary to test this approach over more than one season or in greenhouses and to improve the model to get access to the full grape aroma potential through preliminary acid or enzymatic hydrolysis preparation step.

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