SUPPLEMENTARY DATA
Baerenzung dit Baron, T., Chikri, A., Rodrigues, O., Jacques, A., Roland, A., Tavernier, F., Romieu, C., Segura, V., This, D., Bacilieri, R., Doligez, A., Simoneau, T., Coupel-Ledru, A., & Geffroy, O. (2026). Large-scale SIFT-MS volatile profiling of Vitis vinifera berries grown under greenhouse semi-controlled conditions. *OENO One*, *60*(3). https://doi.org/10.20870/oeno-one.2026.60.3.9987

SUPPLEMENTARY DATA

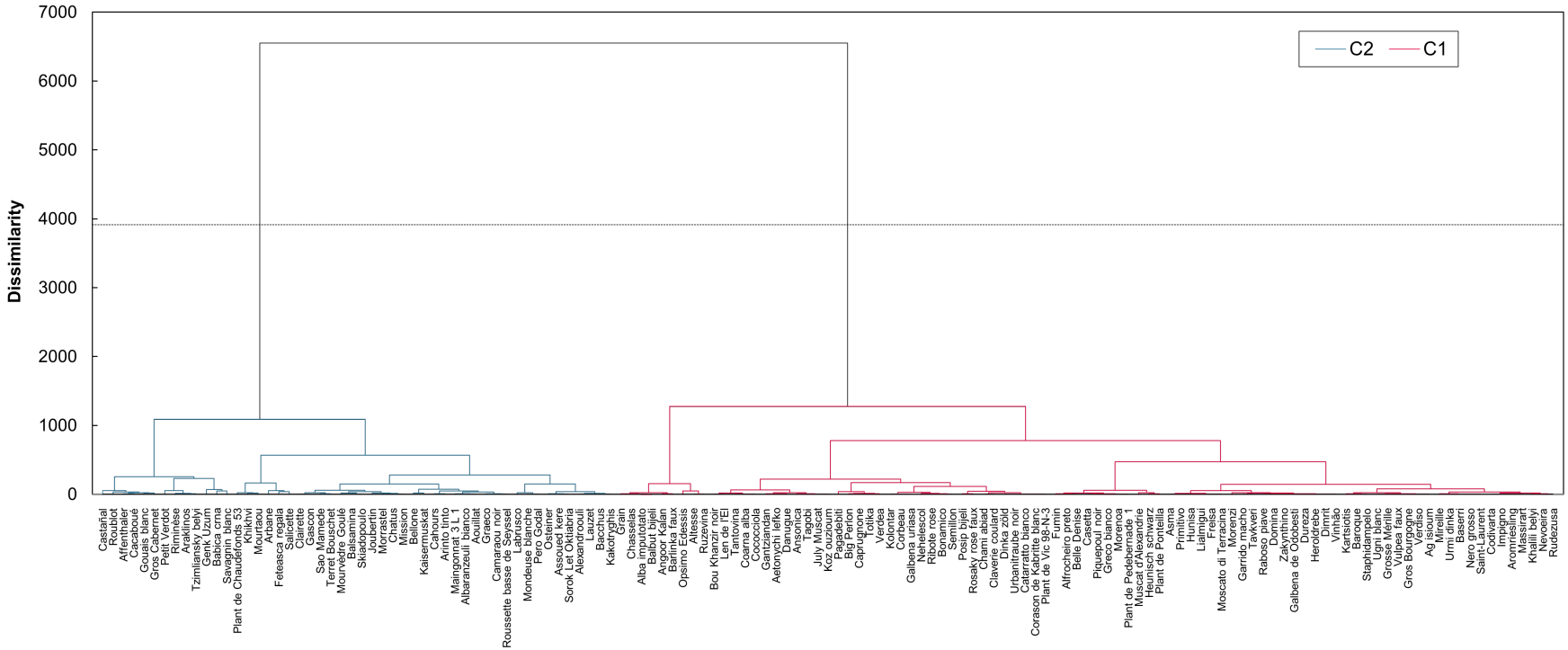


Figure S1. Hierarchical Cluster Analysis (HCA) generated using Euclidean distance and Ward's method on principal component analysis (PCA) coordinates for SIFT-MS abundance data obtained with O_2^+ reagent ion for the 141 sampled varieties. The optimal number of clusters was chosen to maximise the silhouette and Calinski–Harabasz indices.

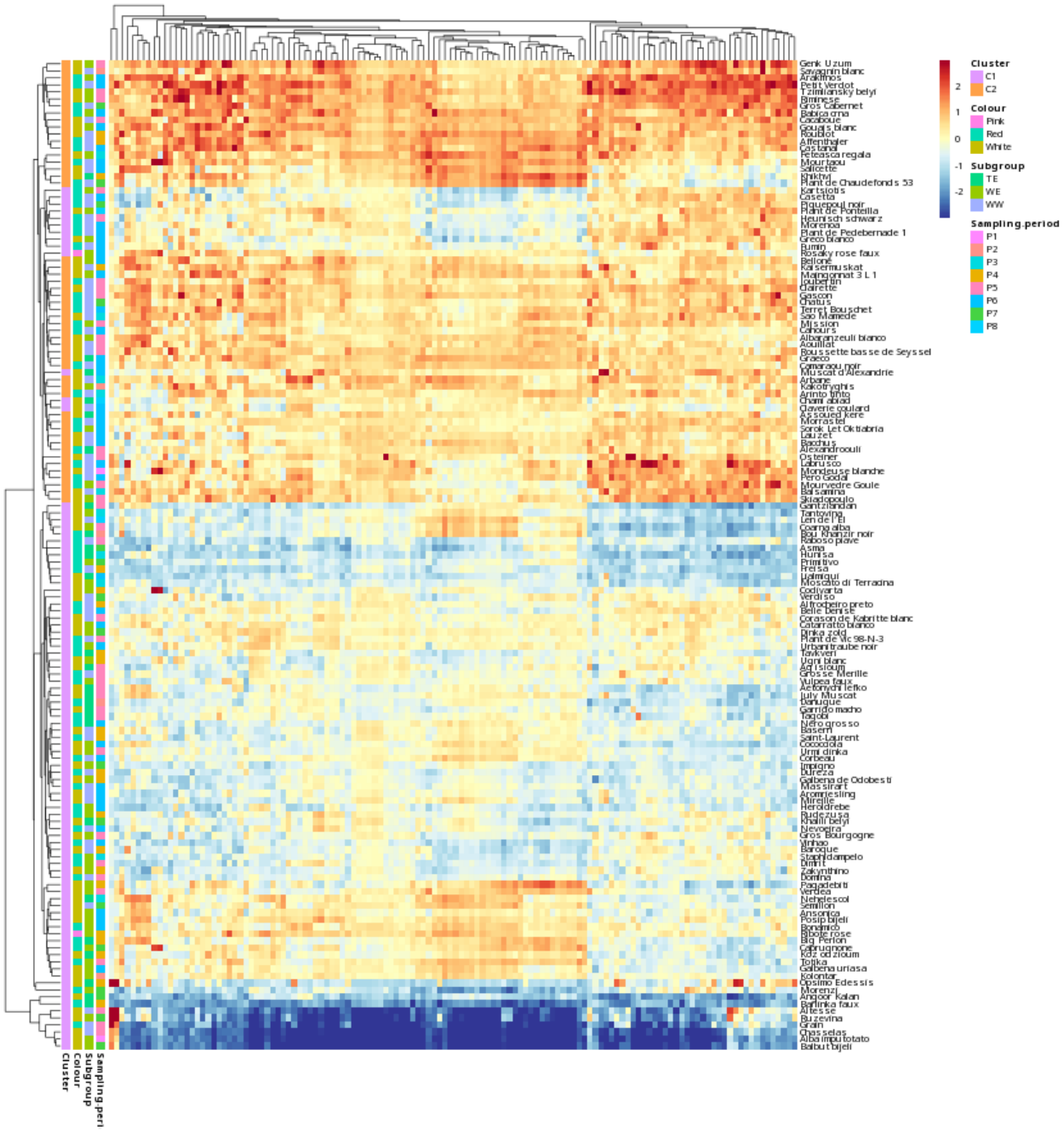


Figure S2. Heatmap of SIFT-MS abundance data obtained with O_2^+ reagent ion for the 141 sampled varieties by cluster identified by PCA followed by HAC, skin colour, subgroup panel, and sampling period. Both samples and abundances at different *m/z* were hierarchically clustered to highlight patterns of similarity.

Table S1. Cultivar names, accession IDs, passport data, cluster assignment, basic berry parameters for the studied varieties (n = 141). TE, WE, and WW stand for Table East, Wine East, and Wine West, respectively. NS, not specified.

Full cultivar name	Accession ID (Vassal)	Subgroup panel	Skin colour	Sampling period	Cluster	Sugar concentration (°Brix)	pH	Berry weight (g)
Aetonychi lefko	2281	TE	White	P5	C1	13.9	3.93	9.2
Affenthaler	1583	WW	Red	P4	C2	15.4	3.35	2.5
Ag isioum	2687	TE	White	P1	C1	10.2	4.10	2.0
Alba imputotato	44	WE	White	P5	C1	18.9	3.94	4.8
Albaranzeuli bianco	2342	WE	White	P5	C2	16.3	3.73	4.5
Alexandroouli	2500	TE	Red	P4	C2	12.5	3.58	2.2
Alfrocheiro preto	50	WW	Red	P5	C1	13.9	3.37	2.6
Altesse	167	WW	White	P7	C1	16.0	3.96	1.8
Angoor Kalan	3657	TE	NS	P6	C1	14.6	3.48	12.2
Ansonica	1307	WE	White	P5	C1	17.8	3.86	5.0
Aouillat	403	WW	White	P6	C2	11.6	3.31	3.3
Araklinos	1805	WE	Red	P3	C2	17.1	4.30	1.5
Arbane	219	WW	White	P6	C2	12.7	4.01	2.0
Arinto tinto	3364	WW	Red	P7	C2	15.3	3.59	3.0
Aromriesling	601	WW	White	P6	C1	20.0	3.94	3.1
Asma	3262	TE	Red	P6	C1	11.7	3.41	4.9
Assoued kere	1695	TE	White	P6	C2	19.5	3.78	1.8
Babica crna	3746	WE	Red	P7	C2	9.4	4.04	3.0
Bacchus	2725	WW	White	P3	C2	16.0	3.60	2.6
Balbut bijeli	1888	WE	White	P4	C1	7.3	3.04	4.8
Balsamina	3009	WW	White	P4	C2	16.4	4.04	2.4
Barlinka faux (Almeria)	3602	TE	Red	P4	C1	6.6	2.77	7.9
Baroque	380	WW	White	P6	C1	18.2	4.30	2.5
Baserri	2890	WW	White	P6	C1	11.9	3.45	2.6
Belle Denise	3499	WW	Red	P4	C1	11.2	3.52	2.8
Bellone	1338	WE	White	P6	C2	13.6	3.51	2.7
Big Perlon	3061	TE	Red	P2	C1	8.6	3.51	5.4
Bonamico	1354	WE	Red	P5	C1	12.0	3.77	3.0
Bou Khanzir noir	1909	TE	Red	P6	C1	16.0	3.90	6.7
Cacaboué	2070	WW	White	P6	C2	21.8	4.02	2.3
Cahours	3093	WW	Red	P7	C2	18.0	3.96	2.6
Camaraou noir	411	WW	Red	P6	C2	22.0	4.35	2.6
Caprugnone	3316	WE	Red	P6	C1	18.0	3.97	6.5
Casetta	3181	WW	Red	P6	C1	17.5	3.57	2.1
Castañal	3379	WW	Red	P8	C2	14.4	4.14	2.8
Catarratto bianco	1304	WE	White	P5	C1	18.0	3.29	4.1
Chami abiad	3221	TE	White	P7	C1	15.4	3.39	2.6
Chasselas	585	WW	White	P5	C1	15.9	3.85	3.8
Chatus	129	WW	Red	P6	C2	16.9	3.41	3.1
Clairette	26	WW	White	P5	C2	11.4	3.95	2.5
Claverie coulard	1217	WW	White	P6	C1	14.6	3.67	3.2
Coarna alba	749	WE	White	P4	C1	14.4	3.61	7.3
Cococciola	2348	WE	White	P5	C1	10.0	3.12	5.8
Codivarta	2972	WE	White	P6	C1	13.3	3.50	3.2
Corason de Kabritte blanc	3148	WW	White	P2	C1	12.2	3.27	2.7
Corbeau	157	WW	Red	P5	C1	13.7	3.66	4.7
Danugue	666	TE	Red	P7	C1	11.3	3.54	6.8
Dimrit	2107	WE	Red	P5	C1	14.5	3.20	3.5
Dinka zöld	1628	WE	White	P4	C1	12.7	3.34	3.7
Domina	3464	WW	Red	P3	C1	13.0	2.95	3.4
Dureza	4218	WW	Red	P4	C1	11.9	3.41	3.8
Feteasca regala	2247	WE	White	P6	C2	18.1	3.68	2.2
Freisa	1245	WW	Red	P4	C1	10.2	3.30	4.3
Fumin	2371	WW	Red	P6	C1	12.5	3.33	3.0
Galbena de Odobesti	2136	WE	White	P5	C1	12.8	3.59	4.0

Galbena uriasa	2472	WE	White	P5	C1	15.5	3.80	4.2
Gantziandan	2902	TE	White	P5	C1	14.3	3.55	8.5
Garrido macho	1972	TE	White	P5	C1	13.5	3.64	6.4
Gascon	226	WW	Red	P6	C2	14.6	3.81	3.0
Genk Uzum	789	WE	White	P6	C2	16.0	3.93	1.8
Gouais blanc	211	WE	White	P5	C2	12.5	3.65	3.2
Graeco	3224	TE	White	P6	C2	15.6	4.09	3.1
Grain	3112	WW	Red	P5	C1	11.4	3.12	4.0
Greco bianco	2373	WE	White	P7	C1	9.2	3.16	2.2
Gros Bourgogne	80	WE	White	P5	C1	15.0	3.62	2.3
Gros Cabernet	1232	WW	Red	P6	C2	17.3	3.78	2.0
Grosse Mérille	3509	WW	Red	P5	C1	13.2	3.64	2.9
Heroldrebe	2745	WE	Red	P3	C1	11.7	3.47	3.8
Heunisch schwarz	1576	WW	Red	P7	C1	15.4	3.80	2.6
Hunisa	2903	TE	Red	P5	C1	9.5	3.27	7.5
Impigno	2057	WE	White	P5	C1	14.4	3.59	3.9
Joubertin	154	WW	Red	P4	C2	11.6	3.75	3.3
July Muscat	2282	TE	White	P2	C1	13.3	3.55	6.2
Kaisermuskat	613	WW	White	P5	C2	15.7	3.73	3.7
Kakotryghis	3167	WE	White	P7	C2	18.6	3.85	2.1
Kartsiotis	1784	WE	Red	P4	C1	12.8	3.70	1.9
Khalili belyi	657	TE	White	P2	C1	18.2	4.13	2.3
Khikhvi	2279	TE	White	P4	C2	16.8	3.49	3.1
Kolontar	744	WE	White	P6	C1	11.2	3.43	5.0
Koz ouzioum	2635	TE	White	P6	C1	14.4	3.60	6.9
Labrusco	2953	WW	Red	P8	C2	9.3	3.80	1.2
Lauzet	424	WW	White	P6	C2	18.5	3.85	1.9
Len de l'El	446	WW	White	P6	C1	17.8	4.25	4.9
Lialmigui	2844	TE	White	P6	C1	14.4	3.55	6.7
Maingonnat 3 L 1	2543	WE	White	P6	C2	13.5	3.37	5.0
Massirart	3016	WW	Red	P5	C1	13.2	3.64	4.2
Mireille	2713	WW	White	P1	C1	14.0	4.10	3.1
Mission	1827	WE	Red	P6	C2	11.5	3.96	2.1
Mondeuse blanche	176	WW	White	P7	C2	9.9	3.65	1.1
Morenoa	3521	WW	Red	P6	C1	19.5	3.80	1.7
Morenzi	3412	WE	Red	P3	C1	6.0	2.83	3.6
Morrastel	9	WW	Red	P6	C2	12.5	3.58	2.3
Moscato di Terracina	577	WE	White	P5	C1	12.2	3.49	5.3
Mourtaou	2968	WW	Red	P6	C2	17.1	3.94	2.7
Mourvèdre Goulé	3164	WE	Red	P3	C2	12.3	3.74	1.9
Muscat d'Alexandrie	308	TE	White	P6	C1	19.6	3.85	2.1
Nehelescol	727	TE	White	P6	C1	18.6	4.16	5.2
Nero grosso	3176	TE	Red	P4	C1	10.0	3.26	3.3
Nevoeira	3366	WW	Red	P5	C1	17.1	3.26	3.8
Opsimo Edessis	1769	TE	White	P4	C1	10.0	3.09	6.9
Osteiner	3471	WW	White	P6	C2	17.9	4.08	2.3
Pagadebiti	114	WE	White	P6	C1	11.7	3.34	5.3
Pero Godal	3376	WW	Red	P3	C2	10.7	3.66	1.4
Petit Verdot	328	WW	Red	P7	C2	19.9	4.00	1.7
Piquepoul noir	11	WW	Red	P7	C1	14.4	3.92	2.0
Plant de Chaudefonds 53	3082	WW	Red	P6	C2	14.8	3.98	3.8
Plant de Pedebernade 1	3099	WW	Red	P8	C1	13.6	3.78	1.4
Plant de Ponteilla	3090	WE	White	P6	C1	12.0	4.01	2.9
Plant de Vic 98-N-3	3308	WW	Red	P7	C1	17.6	3.60	4.3
Posip bijeli	1654	WE	White	P5	C1	16.4	3.90	4.4
Primitivo	1277	WE	Red	P4	C1	10.9	3.59	5.1
Raboso piave	1266	WW	Red	P5	C1	15.1	2.84	3.2
Ribote rose	3310	WE	Pink	P6	C1	13.8	3.93	3.5
Riminèse	124	WE	White	P4	C2	12.8	3.58	2.9
Rosaky rose faux	3403	WE	Pink	P5	C1	14.9	3.46	5.5
Roublot	227	WW	White	P4	C2	13.5	3.68	2.4
Roussette basse de Seyssel	3551	WW	White	P7	C2	20.8	4.19	1.8
Rudezusa	1636	WE	Red	P4	C1	13.8	3.66	3.1
Ruzevina	1653	WE	White	P6	C1	15.1	4.13	2.8
Saint-Laurent	203	WW	Red	P3	C1	11.0	3.19	2.9
Salicette	830	WW	White	P2	C2	10.1	3.79	3.2
Sao Mamede	3591	WW	White	P7	C2	18.0	3.80	2.3
Savagnin blanc	257	WW	White	P5	C2	19.8	3.87	2.2
Semillon	332	WW	White	P5	C1	18.1	3.90	4.1
Skiadopoulo	2316	WE	White	P6	C2	14.5	3.42	2.0

Sorok Let Oktiabria	2683	WE	Red	P3	C2	10.4	2.93	2.0
Staphidampelo	2317	WE	Red	P5	C1	14.3	3.74	2.9
Tagobi	2659	TE	Red	P3	C1	9.6	3.11	7.3
Tantovina	1620	WE	White	P4	C1	14.9	3.69	5.6
Tavkveri	1218	TE	Red	P6	C1	11.5	3.63	4.7
Terret Bouschet	537	WW	Red	P5	C2	10.9	3.35	3.6
Totika	3455	WE	Red	P5	C1	8.4	3.29	4.2
Tzimliansky belyi	2665	WE	White	P4	C2	15.8	3.91	1.6
Ugni blanc	74	WE	White	P6	C1	11.6	3.60	2.4
Urbanitraube noir	3480	WE	Red	P5	C1	12.7	3.41	3.0
Urmi dinka	3456	WE	White	P5	C1	11.1	3.28	3.9
Verdea	1258	WE	White	P7	C1	17.2	4.12	4.0
Verdiso	1301	WW	White	P6	C1	11.8	3.28	2.0
Vinhão	1483	WW	Red	P5	C1	14.1	2.89	3.3
Vulpea faux	3427	WE	Red	P5	C1	16.8	3.68	2.9
Zakynthino	3000	WE	White	P4	C1	13.4	3.49	2.7