

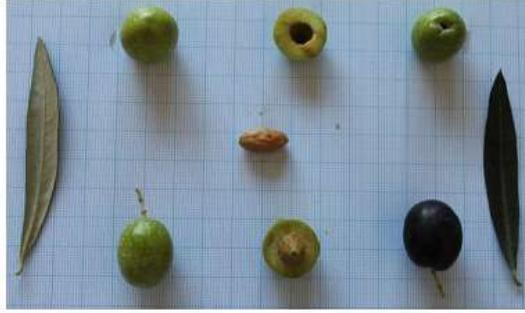
Table S1. Rotated factor loadings, eigenvalues and variances explained of the three first principal components

Variables	Component			Variables	Component		
	PC1	PC2	PC3		PC1	PC2	PC3
β -Sesquiphellandrene	0.985	-0.034	0.093	Heptadecanoic acid	-0.115	-0.082	0.909
Pyran aldehyde	0.985	-0.034	0.095	α -Muurolene	0.014	0.369	0.908
α -Bergamotene	0.981	-0.035	0.090	Hydroxytyrosol	-0.420	0.165	0.889
(E)-3-Hexen-1-ol acetate	0.976	-0.007	0.129	Decanoic acid	-0.326	0.293	0.858
Octanoic acid	0.971	-0.032	0.098	Heneicosanoic acid	-0.449	0.135	0.855
Hexyl acetate	0.918	-0.291	0.067	Vanilic acid	-0.032	0.076	0.851
Trans-ferrulic acid	0.916	-0.182	-0.183	Cyclosativene	0.092	0.262	0.828
1-Hexanol	0.891	0.325	-0.009	a-Copaene	-0.453	0.309	0.821
Caffeic acid	0.872	0.014	-0.250	Stearic acid	-0.356	-0.369	0.765
Tyrosol	0.864	-0.411	-0.201	10-Heptadecanoic acid	0.398	0.370	0.667
Benzaldehyde	0.792	0.239	-0.243	Total phenolic content	-0.898	0.095	-0.269
Free fatty acid	0.788	0.229	0.496	(E)-2-Hexenal	-0.867	0.437	-0.114
Pinoresinol	0.772	-0.287	-0.216	Tricosanoic acid	-0.540	-0.648	-0.132
Chlorophyll	0.761	0.165	-0.039	3-Ethyl-1,5-octadiene	-0.521	0.023	0.188
Luteolin	0.753	0.173	-0.415	Ethanol	-0.506	-0.129	-0.742
4-Hexanedienal	0.747	0.394	-0.172	(E)-2-Decenal	-0.290	-0.907	-0.071
Phenylethanol	0.743	0.277	-0.265	Oleic acid	-0.148	-0.840	0.022
(Z)-3-Hexen-1-ol	0.738	0.195	0.599	3-Hexenal	-0.445	-0.833	0.263
α -Curcumene	0.736	-0.216	0.401	MUFAs	-0.145	-0.831	-0.029
				(E)-4,8-Dimethyl-1,3,7-			
Carotenoids	0.704	0.138	-0.102	nonatriene	-0.494	-0.829	-0.073
Palmitic acid	0.595	-0.051	-0.752	1-Penten-3-ol	-0.185	-0.820	-0.453
11-Eicosenoic acid	0.589	0.183	0.244	(Z)-2-Penten-1-ol	0.314	-0.779	-0.386
p-Qumaric acid	0.507	0.336	-0.717	Docosanoic acid	0.388	-0.734	0.387
PUFAs	0.049	0.935	0.109	1-Pentanol	0.032	-0.716	-0.262
Linoleic Acid	0.086	0.931	0.116	Eicosanoic acid	0.251	-0.695	0.153
Catechin	-0.193	0.879	-0.308	Apigenin	-0.157	-0.539	-0.632
K ₂₇₀	0.016	0.813	0.272	SFAs	0.352	-0.527	-0.306
Linolenic acid	-0.548	0.789	-0.026	9-Hexadecenoic acid	-0.124	0.007	-0.940
(Z)- β -Ocimene	-0.512	0.761	0.006	Pyridine	-0.264	0.488	-0.576
K ₂₃₂	0.311	0.737	-0.276	(E)-2-Heptenal	-0.264	0.489	-0.575
Oleuropin	-0.496	0.717	-0.127	Phenylmethanol	-0.256	0.484	-0.557
Nonanal	0.212	0.579	0.557	2-Ethylhexanol	0.365	0.443	-0.489
Pentadecanoic acid	0.198	0.559	0.434	1,2-Dimethyl benzene	-0.184	0.132	-0.408
(E)-2-Hexen-1-ol	-0.461	0.544	0.609	(E)-2-Pentenal	0.496	-0.289	-0.406
Hexanal	0.027	0.515	0.312	Pentanal	-0.085	0.181	-0.335
5-Ethyl-2(5H)-furanone	0.385	0.506	-0.067	Methylbenzene	-0.086	0.181	-0.335
Total antioxidant capacity	-0.289	0.250	0.918	Peroxide value	0.254	-0.427	0.141
Variance explained of total variance	29.80%	23.89%	21.81%				
Sum of variance		75.50%					
Eigenvalues	22.43	18.82	14.63				

Table S2. Morphological and quality characteristics of the olive plant/fruit variety used in the study [62]

Phenolic compound	Edincik	Ayvalık	Domat	Uslu	Gemlik
<i>Flower bud</i>					
Length	short	Medium	medium	medium	short
Number of flowers	small	medium	small	small	small
<i>Leaf</i>					
Shape	long-elliptical	long-elliptical	long-elliptical	long-elliptical	long-elliptical
Length	long	medium	medium	medium	medium
Width	medium	medium	medium	medium	medium
<i>Fruit</i>					
Weight	medium	medium	extra-large	medium	medium
Shape	oval	oval	elliptical	oval	oval
Symmetry	symmetrical	symmetrical	symmetrical	slight-symmetrical	slight-symmetrical
Widest point	towards tip	central	central	central	central
Fruit tip	round	round	round	pointed	round
Stem part	cut	round	round	round	cut
<i>Stone</i>					
Weight	medium	medium	large	large	medium
Shape	elliptical	oval	long	elliptical	oval
Symmetry	symmetrical	symmetrical	symmetrical	asymmetric	slight-symmetrical
Widest point	towards tip	near-end	central	central	towards tip
Stone tip	pointed	pointed	pointed	pointed	round
Stem part	pointed	cut	pointed	pointed	round
Surface	rough	rough	rough	rough	rough
Tip point	pinpoint	pinpoint	pinpoint	pinpoint	pinpoint
<i>Quality features</i>					
Number of fruits (kg)	311	291	140	260	273
Pulp ratio (%)	89	89	88	88	86
Stone ratio (%)	11	11	12	12	14
Oil ratio (%)	low (<18%)	high (>22%)	low (<18%)	low (<18%)	high (>22%)

Edincik



Ayvalik



Domat



Uslu



Gemlik



Figure S1. Fruits, leaves and seeds of olive varieties used [63]

Materials and Methods

Phenolic compounds (PC) analysis

The analysis of phenolic fractions in samples was carried out using a Water Alliance e2695 HPLC (Waters, Milford, MA, USA) system, consisting of a photodiode array detector (PDA) (Waters 2996, Milford, MA, USA) and an inertSustain C18 (5 μ m, 4.6 x 250 mm, GL Sciences, Tokyo, Japan). The phenolic extract was filtered through a 0.45 μ m polyvinylidene fluoride (PVDF) syringe filter before the injection into the system. The operational procedures of the HPLC were performed as described by Veneziani et al. (2018) [8], with some modifications. The mobile phases were ultrapure water acidified to pH 2.10 with phosphoric acid (A) and methanol: acetonitrile (90:10, v/v) mixture (B). The flow rate was 1.0 mL/min and the total run time was 73 min. The elution gradient was as follows: 95% A and 5% B for 2 min, 75% A and 25% B in 8 min, 60% A and 40% B in 10 min, 50% A and 50% B in 16 min, 0% A and 100% B in 14 min. This last composition was sustained for 10 min and then returned to the initial composition within 13 min. The quantification PC was performed with calibration curve for each available commercial standard. The phenolic alcohols (hydroxytyrosol, tyrosol), oleuropein, phenolic acids (*p*-qumaric, *t*-ferulic, caffeic and vanilic acids), catechin and pinosresinol were detected at 280 nm, while apigenin and luteolin were detected at 335 nm. Results were expressed as mg.kg⁻¹.

Volatile compounds (VC) analysis

A 2 g of oil sample was weighed in a 20 mL SPME vial (Supelco) and 10 μ L of isobutyl acetate (500 mg.L⁻¹) solution was added as an internal standard (IS). The vial was closed with a screw cap with a silicone septum and placed into the tray of the autosampler. The rest of SPME operations were applied on the autosampler. The sample vial was maintained in the heating block at 40 C° for 30 min under an agitation at 220 rpm. Then, a divinylbenzene/carboxen/polydimethylsiloxane (DVB/CAR/PDMS) fiber (2 cm, 50/30 μ m, Supelco) was inserted to the vial and exposed to the headspace of the vial at the same conditions for 25 min.

After extraction, the VC were desorbed thermally from the fiber in the injection port of the GC at 250 C° for 5 min, with a splitless mode. The separation was achieved with a DB-HeavyWax column (0.25 μ m, 60 m x 0.25 mm) (Agilent Technologies). Hydrogen was used as the carrier gas at a flow rate 1.05 ml.min⁻¹. The oven temperature was first kept at 40 C° for 2 min, then increased to 80 C° at a rate of 3 C°.min⁻¹ and held at this temperature for 1 min. and then was programmed to 240 C° at a rate of 5 C°.min⁻¹ and held at this temperature for 6 min. The temperatures of ion source and the interface of MS were 201 C° and 250 C°, respectively. Electron ionizing (EI mode) energy was recorded at 70 eV. Mass scanning range was m/z 20-450.

The identification of VC was performed by comparing their mass spectra with those of NIST11 and Wiley9 mass spectral libraries and literature. Additionally, the many identifications were confirmed by comparing VC retention indices (Kovats Index) with those available in the literature. The quantifications of VC were calculated by matching the peak area of each compound to the calibration curves of IS, and expressed as mg per kg of sample.