

Study on extra virgin olive oil: quality evaluation by anti-radical activity, color analysis and polyphenolic HPLC-DAD analysis

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MILL samples	MILL samples	ITA samples	EUR samples
A1	L10	Ar	Aa
B1	L11	Au	Ac
C1	L12	Ca	Ai
C2	L13	Cc	Be
C3	M1	Ce	Cf
L1	P1	Cp	Cm
L2	P2	Ct	Co
L3	P3	Cv	Cr
L4	P4	Ds	Dc
L5	P5	Fb	Dn
L6	S1	Ma	Gi
L7	T1	Pa	Lr
L8	T2	Sa	Sp
L9	U1		

Table S1. Legend of analysed oil samples.

	A1	B1	C1	C2	C3	L1	L2	L3	L4	L5	L6	L7	L8	L9
K₂₃₂	1.72	0.41	0.14	1.97	2.32	-1.21	1.40	0.16	0.10	1.96	1.95	2.07	1.71	1.71
K₂₇₀	0.14	0.15	0.06	0.20	0.28	-1.26	0.27	0.04	0.03	-0.03	0.19	-0.64	-1.04	-1.04
ΔK	-0.004	-0.007	-0.001	-0.009	0.001	-0.003	0.031	-0.003	-0.002	0.053	0.001	-0.037	-0.039	-0.039
Car*	0.018	0.017	0.033	0.028	0.017	0.048	0.042	0.021	0.038	0.015	0.021	0.036	0.038	0.016
Chlor**	0.013	0.001	0.002	0.021	0.009	0.030	0.069	0.012	0.028	0.006	0.015	0.039	0.029	0.012

DPPH***	89.4	29.1	37.7	122.8	34.4	154.0	72.3	71.1	96.1	57.1	237.5	83.4	136.0	41.5
	L10	L11	L12	L13	M1	P1	P2	P3	P4	P5	S1	T1	T2	U1
K₂₃₂	1.22	3.57	1.79	1.50	2.39	0.14	2.32	2.47	3.17	3.17	0.14	0.17	2.79	1.61
K₂₇₀	0.11	0.47	0.12	0.11	0.27	0.04	0.27	0.32	0.42	0.26	0.03	0.03	0.31	0.32
ΔK	-0.003	0.002	0.002	-0.001	-0.003	-0.003	-0.004	0.002	0.001	-0.003	-0.002	0.001	-0.002	0.004
Car*	0.008	0.002	0.021	0.115	0.018	0.061	0.018	0.031	0.005	0.031	0.014	0.023	0.018	0.005
Chlor**	0.005	0.012	0.015	0.100	0.007	0.036	0.016	0.006	0.007	0.014	0.022	0.015	0.015	0.008
DPPH***	57.0	8.3	51.4	43.2	14.7	115.4	7.4	71.4	135.0	85.5	42.7	92.8	39.8	28.3
	Ar	Au	Ca	Cc	Ce	Cp	Ct	Cv	Ds	Fb	Ma	Pa	Sa	
K₂₃₂	2.36	2.56	1.96	0.20	1.93	0.20	0.19	0.17	1.31	1.12	2.78	2.84	2.31	
K₂₇₀	0.22	0.27	0.22	0.09	0.16	0.04	0.03	0.03	0.15	0.14	0.17	0.44	0.21	
ΔK	0.001	0.002	-0.004	-0.002	0.001	-0.070	-0.003	-0.003	-0.002	0.001	-0.005	-0.004	0.003	
Car*	0.018	0.015	0.030	0.023	0.016	0.021	0.029	0.022	0.020	0.034	0.040	0.019	0.033	
Chlor**	0.009	0.038	0.027	0.024	0.012	0.021	-	-	-	0.029	0.034	0.046	0.015	
DPPH***	26.0	15.3	224.9	25.0	259.7	266.1	17.4	17.7	198.2	91.7	38.2	13.4	293.2	
	Aa	Ac	Ai	Be	Cf	Cm	Co	Cr	Dc	Dn	Gi	Lr	Sp	
K₂₃₂	-0.39	2.66	-0.25	-0.01	2.63	1.96	1.66	1.95	2.41	1.52	2.04	-0.04	1.84	
K₂₇₀	0.03	0.21	0.04	0.05	0.16	0.15	0.12	0.19	1.46	0.20	0.25	0.04	0.18	
ΔK	-0.003	-0.004	0.001	-0.003	-0.005	-0.005	-0.003	0.001	0.032	-0.051	0.046	-0.002	0.005	
Car*	0.013	0.017	0.032	0.024	0.029	0.021	0.037	0.019	0.022	0.026	0.026	0.016	0.022	
Chlor**	0.013	0.014	0.015	0.010	0.029	0.013	0.032	0.014	0.018	0.022	-	-	0.015	
DPPH***	40.0	17.9	54.6	31.6	85.5	184.3	54.4	53.5	40.4	38.7	49.5	43.1	143.0	

Table S2. Spectrophotometric data of all analysed samples.

*Carotenoids detected at 470 nm,**Chlorophylls detected at 670 nm and expressed as absorbance of oils solution (100 mg in 5 mL n-hexane); ***expressed as µg equivalents of gallic acid/g of oil

	A1	B1	C1	C2	C3	L1	L2	L3	L4	L5	L6	L7	L8	L9
L*	47.60	54.90	45.50	45.20	56.60	42.30	36.50	51.30	44.00	48.50	49.70	41.60	38.60	43.10
a*	0.80	0.10	2.50	2.90	0.60	2.70	0.70	3.30	3.20	0.90	4.10	4.20	1.00	1.60
b*	18.50	46.80	33.60	30.20	50.50	29.60	13.30	44.00	33.70	20.90	41.30	27.90	17.70	30.60
C* _{ab}	18.50	46.80	33.70	30.50	50.50	29.70	13.35	44.10	33.90	20.90	41.50	28.20	17.80	30.60
h _{ab}	87.70	89.90	85.80	84.60	89.40	84.70	87.00	85.70	84.50	87.70	84.30	81.40	86.60	86.90
	L10	L11	L12	L13	M1	P1	P2	P3	P4	P5	S1	T1	T2	U1
L*	55.90	49.80	51.30	53.30	52.30	43.90	50.00	53.10	56.50	51.30	43.60	47.10	51.10	39.70
a*	0.75	0.00	1.50	1.80	3.70	1.90	4.20	5.00	-1.10	4.70	4.70	3.90	3.30	2.20
b*	48.50	6.40	39.40	47.80	46.50	30.90	42.50	48.00	44.70	45.00	32.30	35.70	43.90	24.10
C* _{ab}	48.50	6.40	39.40	47.80	46.60	30.90	42.70	48.30	44.70	45.20	32.70	35.90	44.00	24.20
h _{ab}	89.20	89.90	87.90	87.90	85.30	86.50	84.40	84.00	91.40	84.00	81.60	83.80	85.80	84.90
	Ar	Au	Ca	Cc	Ce	Cp	Ct	Cv	Ds	Fb	Ma	Pa	Sa	
L*	50.30	53.50	48.00	49.90	46.30	49.80	51.40	50.80	46.40	55.50	47.70	49.20	52.50	
a*	3.70	1.30	4.90	4.90	1.70	4.80	3.60	4.60	2.70	4.40	0.80	3.60	3.20	
b*	42.70	46.40	39.30	42.40	19.00	42.40	44.10	43.60	25.70	52.10	9.10	40.40	46.50	
C* _{ab}	42.80	46.40	39.60	42.60	19.10	42.60	44.30	43.90	25.90	52.20	9.20	40.60	46.60	
h _{ab}	85.00	88.40	82.90	83.40	85.10	83.60	85.30	84.00	84.00	85.10	85.10	85.20	86.30	
	Aa	Ac	Ai	Be	Cf	Cm	Co	Cr	Dc	Dn	Gi	Lr	Sp	
L*	51.80	52.20	52.10	52.80	55.70	51.40	44.00	51.40	49.30	51.40	50.60	51.70	53.30	
a*	3.80	2.80	3.70	3.30	4.50	3.60	3.20	3.60	4.70	4.00	3.70	3.70	2.00	
b*	45.10	45, 6	45.20	46.50	51.90	44.10	31.00	44.10	41.50	44.70	43.30	45.00	47.40	
C* _{ab}	45.30	45.70	45.30	46.60	52.10	44.30	31.20	44.30	41.70	44.80	43.50	45.20	47.40	
h _{ab}	85.20	86.50	85.30	86.00	85.10	85.30	84.10	85.30	83.40	84.80	85.10	85.30	87.60	

Table S3. Colorimetric data of the analysed samples.

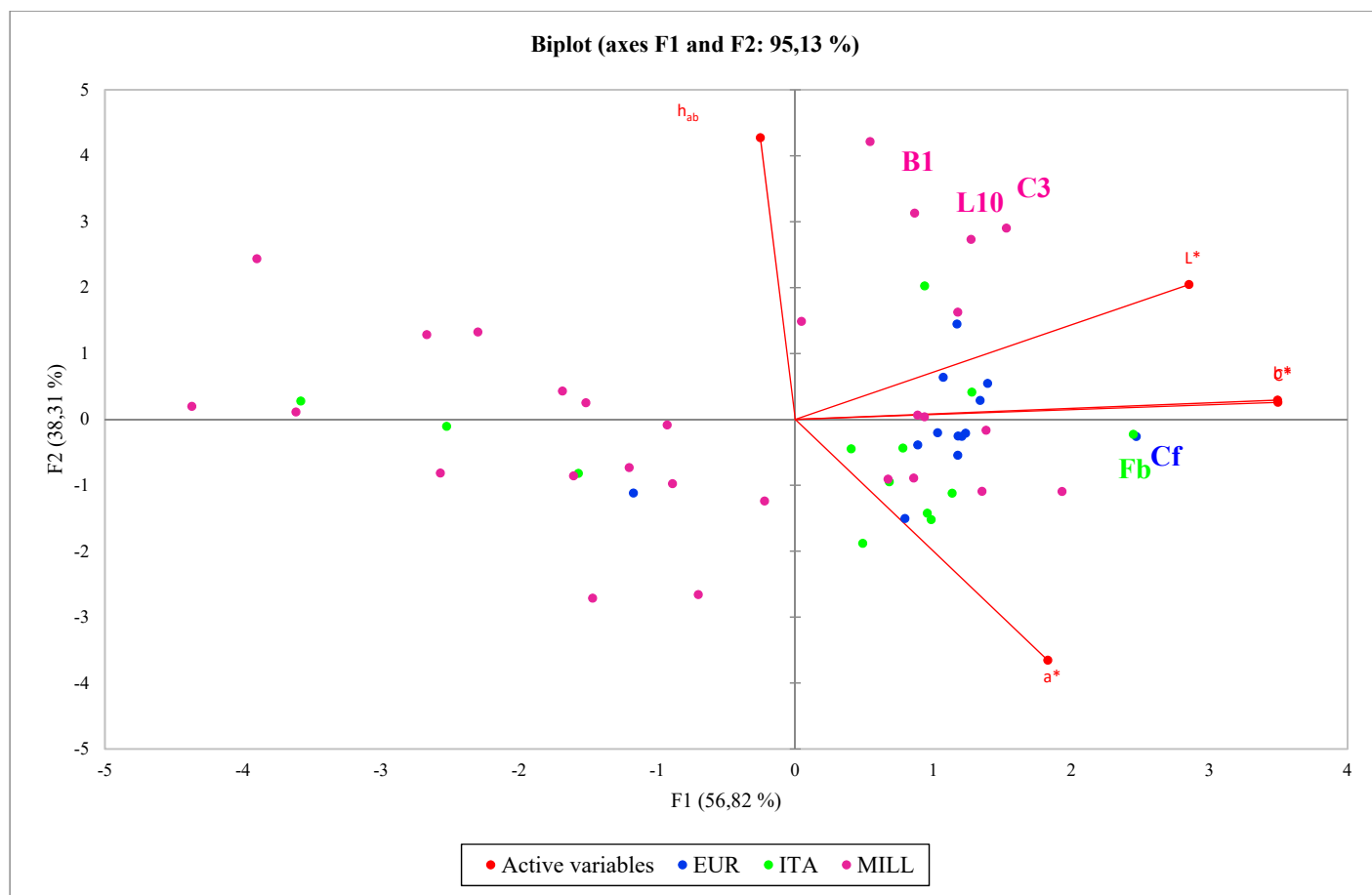


Figure S1. Principal component analysis (PCA) of all analysed samples.

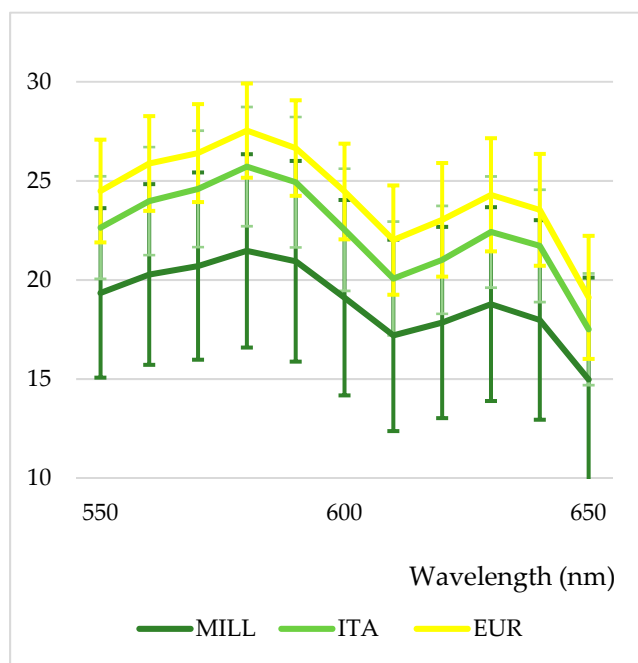
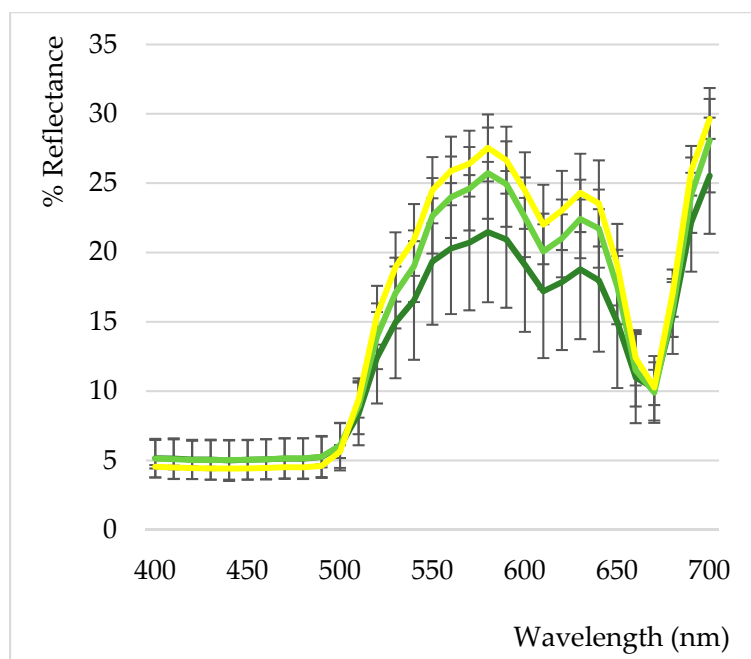


Figure S2. Reflectance curves of selected samples.

	A1	B1	C1	C2	C3	L1	L2	L3	L4	L5	L6	L7	L8	L9
Hydroxytyrosol	32.2	4.88	3.56	35.6	1.27	3.43	5.68	6.12	5.19	BDL	4.98	14.4	19.7	3.8
Tyrosol	39.1	BDL	10.5	8.84	5.76	3.84	19.7	6.53	5.78	3.31	7.08	11.9	7.91	8.89
Ferulic acid	BDL	BDL	BDL	BDL	0.32	BDL	0.42	0.44	BDL	BDL	BDL	BDL	BDL	0.56
Oleuropein and derivatives	30.43	22.93	4.23	5.22	22.56	16.5	9.77	18.54	13.16	8.58	3.33	6.48	53.24	3.54
Flavonols	0.99	0.63	BDL	BDL	0.64	0.06	0.12	0.21	0.7	0.27	BDL	BDL	0.71	BDL
	L10	L11	L12	L13	M1	P1	P2	P3	P4	P5	S1	T1	T2	U1
Hydroxytyrosol	4.64	BDL	13.10	3.65	2.95	8.34	BDL	5.84	3.07	BDL	2.28	10.70	13.50	BDL
Tyrosol	1.75	3.66	5.16	2.32	1.45	13.80	2.66	11.50	16.60	9.24	15.30	7.07	15.90	5.23
Ferulic acid	BDL	BDL	4.09	BDL	BDL	1.33	BDL	BDL	0.71	BDL	BDL	BDL	BDL	BDL
Oleuropein and derivatives	BDL	14.50	5.36	16.47	3.32	41.20	6.48	2.82	22.42	13.46	5.98	22.20	52.33	4.07
Flavonols	BDL	0.18	0.03	0.24	0.12	0.57	0.04	0.09	0.26	0.24	0.23	BDL	0.17	0.58
	Ar	Au	Ca	Cc	Ce	Cp	Ct	Cv	Ds	Fb	Ma	Pa	Sa	
Hydroxytyrosol	14.10	9.50	6.01	4.71	6.06	13.30	20.20	BDL	15.40	1.75	16.60	2.36	12.50	
Tyrosol	8.36	13.50	11.60	12.50	BDL	2.22	27.20	11.50	22.60	2.52	12.70	7.72	BDL	
Ferulic acid	0.86	0.77	0.91	0.89	BDL	0.50	1.04	0.83	BDL	BDL	0.36	0.46	1.04	
Oleuropein and derivatives	BDL	24.80	37.58	30.40	23.70	56.20	55.20	16.95	70.40	0.82	44.50	18.59	43.00	
Flavonols	0.25	0.41	0.50	0.18	0.44	BDL	0.52	0.30	0.23	0.13	0.32	0.63	1.33	
	Aa	Ac	Ai	Be	Cf	Cm	Co	Cr	Dc	Dn	Gi	Lr	Sp	
Hydroxytyrosol	5.38	4.68	5.58	17.10	8.80	BDL	13.00	10.10	9.04	10.50	9.25	10.90	9.04	
Tyrosol	5.60	31.40	9.03	14.60	4.78	4.87	20.00	13.80	10.50	13.20	11.60	9.49	22.70	
Ferulic acid	0.58	BDL	0.71	0.70	BDL	BDL	BDL	0.50	0.34	0.30	0.28	0.64	1.49	

Oleuropein

7.54 12.29 26.00 24.10 2.17 9.13 21.70 21.42 33.20 21.30 20.22 69.60 21.24

and derivatives

Flavonols

0.05 0.05 0.24 0.53 BDL 0.33 0.28 0.30 0.48 0.28 0.46 1.29 0.64

BDL* below detection limit

Table S4. HPLC-DAD analysis of the analysed samples.

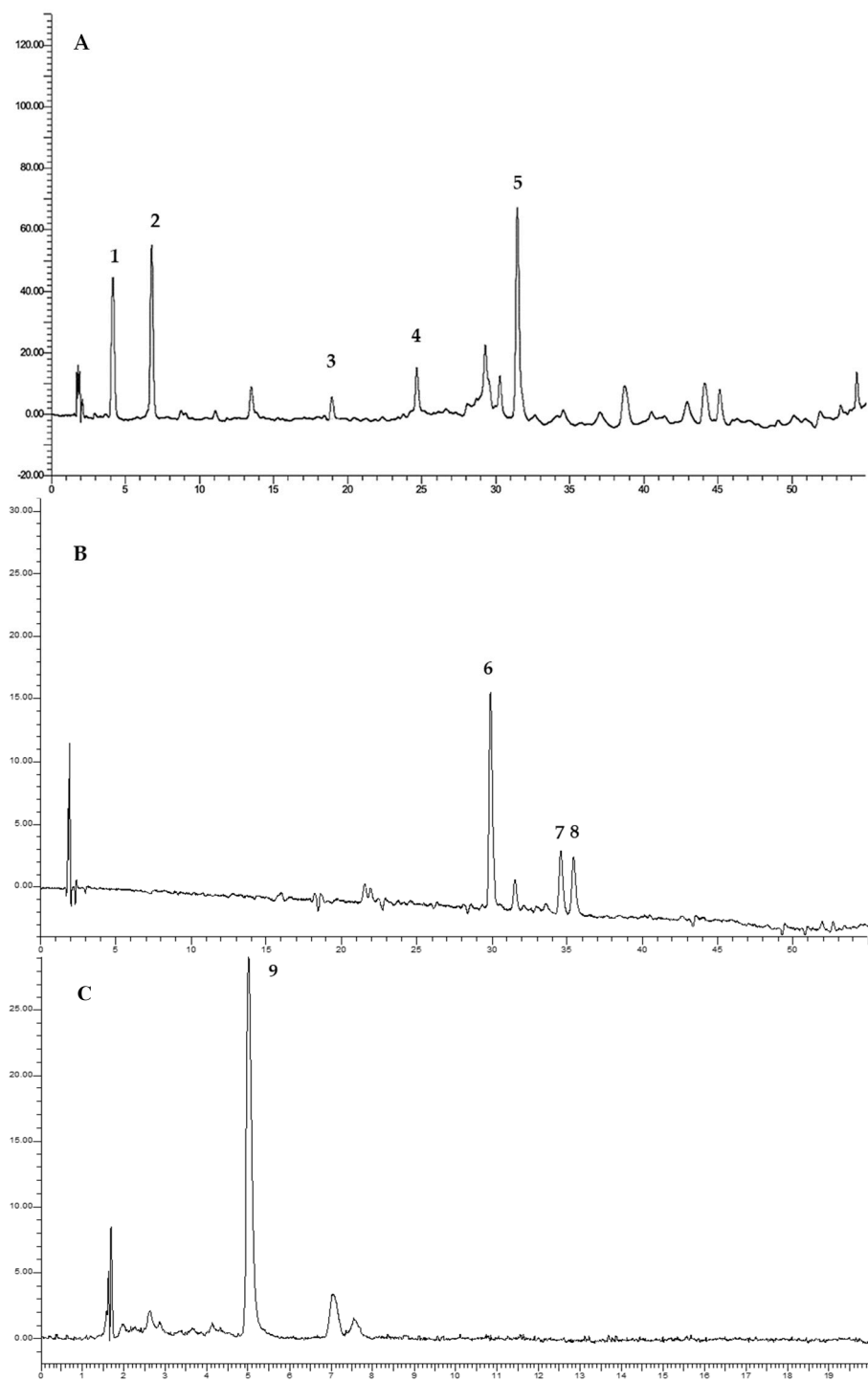


Figure S3. Example chromatograms of a selected sample: (Panel A, 280 nm, hydroxytyrosol (1), tyrosol (2), ferulic acid (3), oleuropein (4) and oleuropein derivative (5); Panel B, 360 nm, quercetin-3-D-galactoside (6), quercetin derivative (7), kaempferol derivative (8); Panel C, 450 nm, lutein (9)).

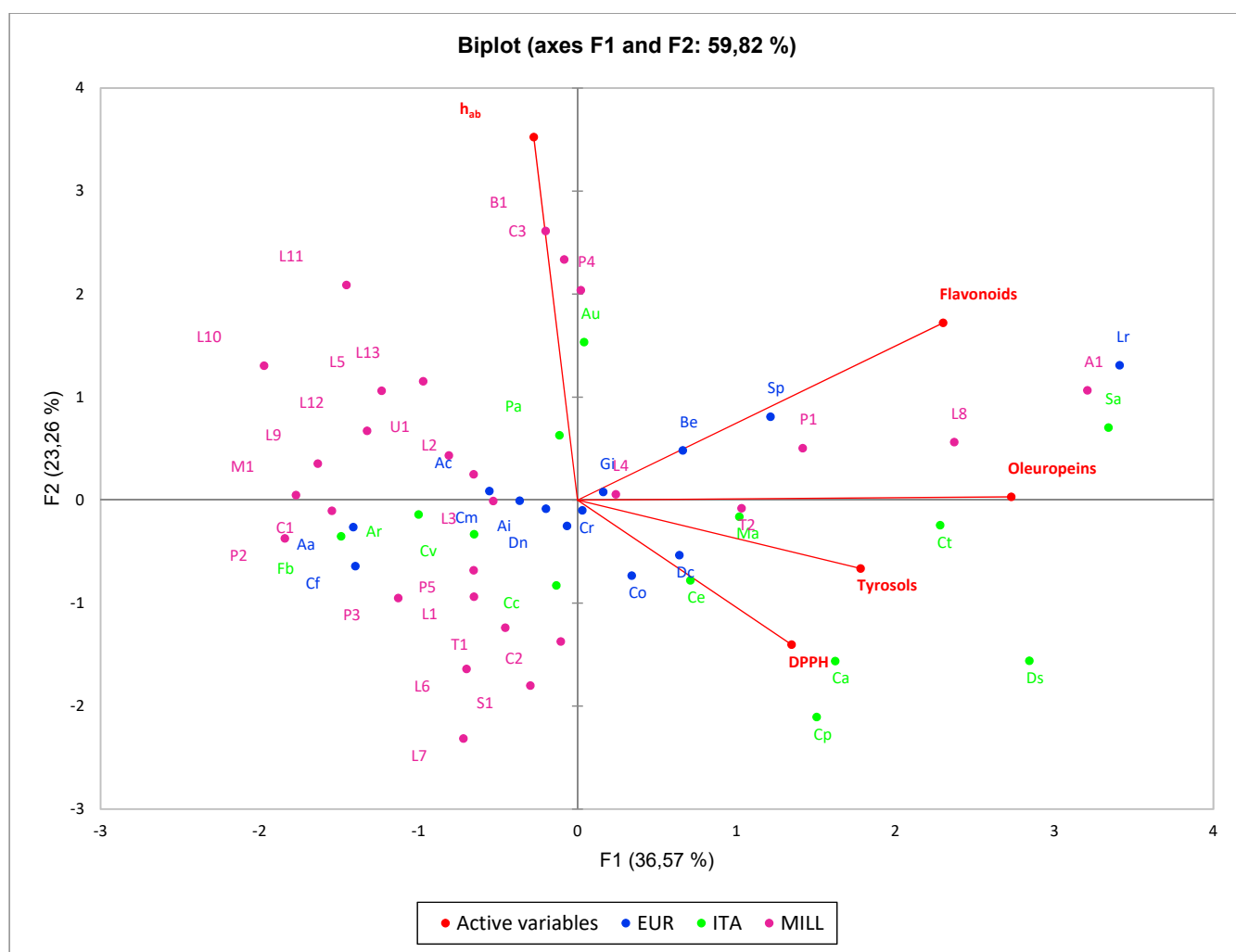


Figure S4. Principal component analysis (PCA) correlating quality variables with h_{ab} .

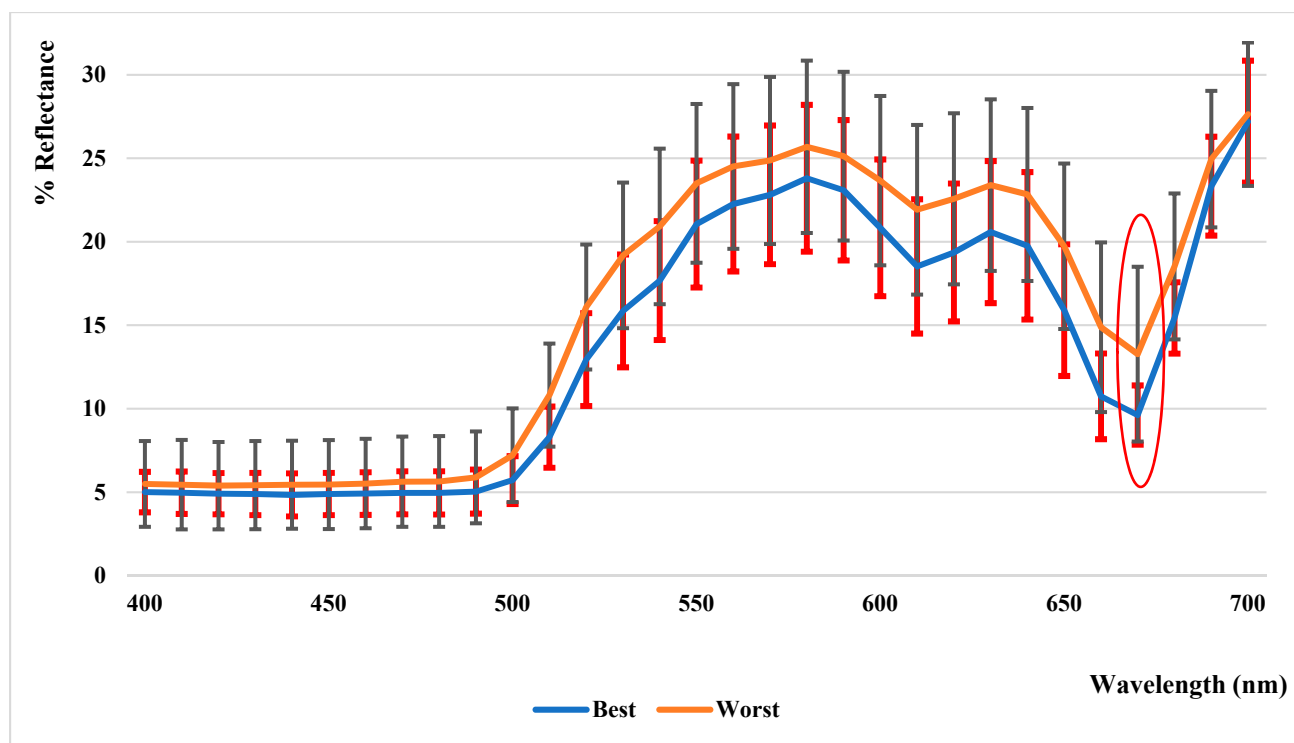


Figure S5. Reflectance curves of the two individuated clusters, associated to best or worst oil quality