

Chemical and ATR-FTIR characterisation of olive oils from small-scale producers in San Lorenzo Maggiore, Southern Italy

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Supplementary figures

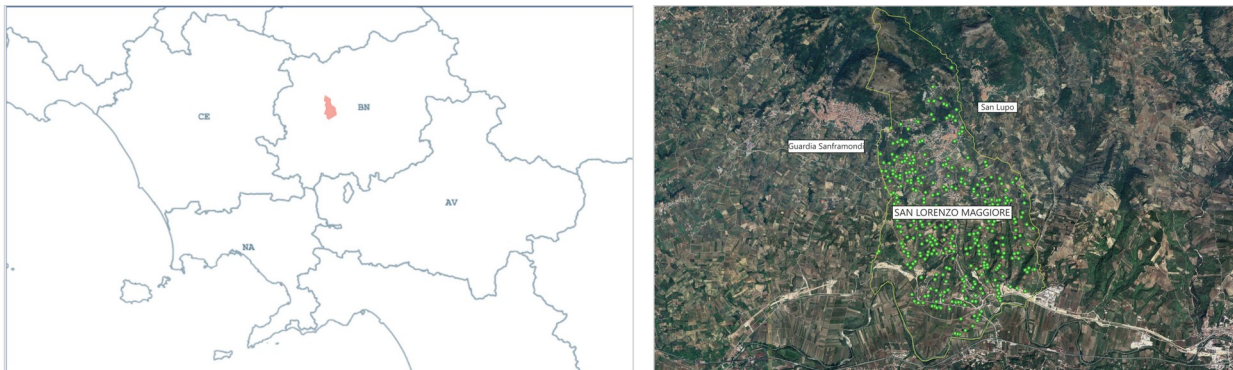


Fig. S1 Geographic context of the study area. Left: location of San Lorenzo Maggiore within Benevento province, Campania, Southern Italy. Right: qualitative representation of the municipal territory and olive-growing features mapped by the authors. The map is provided for orientation; the green points do not represent the 45 analytical samples or a quantitative sampling-density design

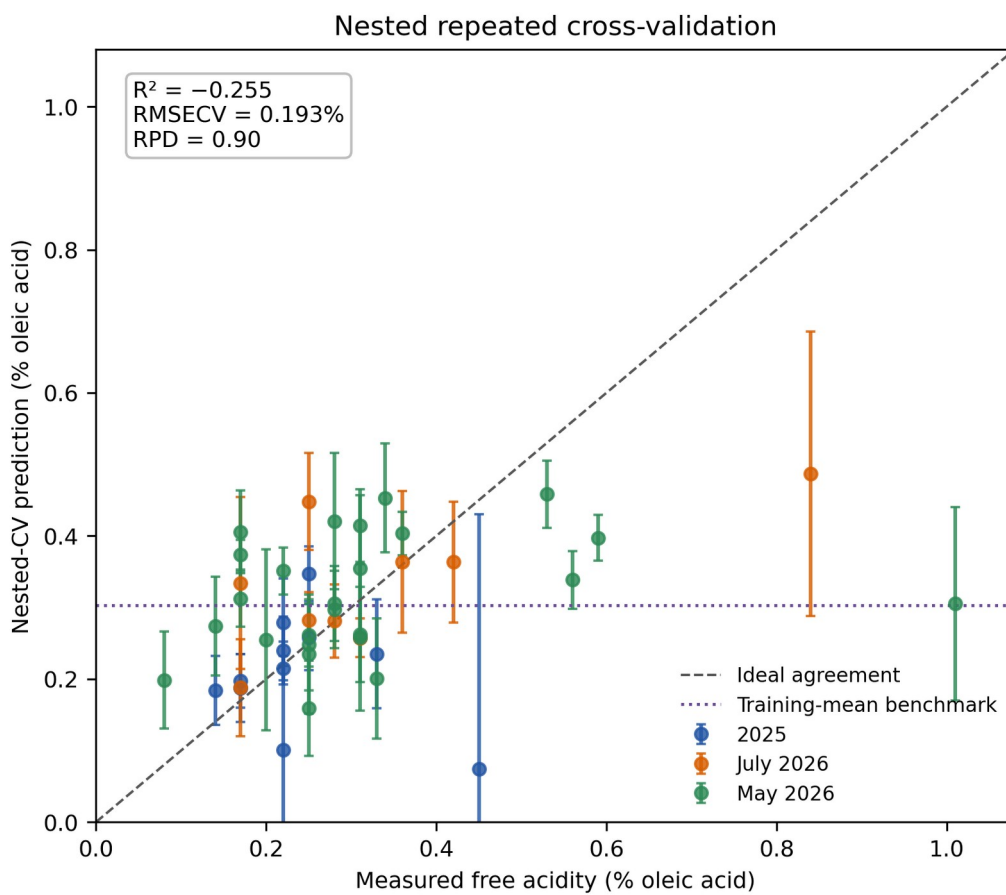


Fig. S2 Measured free acidity and predictions from the ten-repeat nested five-fold procedure. Error bars show the between-repeat standard deviation of each sample's out-of-fold predictions. The dashed line is ideal agreement; the dotted horizontal line is the overall mean benchmark

Supplementary tables

Table S1 Validation hierarchy for the exploratory free-acidity PLSR

Validation design	Model-selection status	R^2	RMSE (%)	MAE (%)	RPD
Repeated 5-fold CV ×20	Prespecified SNV fingerprint, 1 LV	0.032	0.169	0.110	1.03
Repeated 5-fold CV ×20	Best apparent screened model	0.189	0.155	0.123	1.12
Nested repeated 5-fold CV ×10	Selection inside inner folds	-0.255	0.193	0.125	0.90
Leave-acquisition-period-out	Prespecified model	-0.325	0.198	0.149	0.88
Sensitivity: remove IDs 32 and 33	Prespecified model; n = 43	0.045	0.171	0.111	1.04

LV, latent variable; RPD, standard deviation of the reference response divided by the cross-validated RMSE.

Table S2 Chemical measurements for the 45 olive-oil samples

Sample	Free acidity (%)	Peroxide value (meq O ₂ kg ⁻¹)	K232	K272	ΔK
1	0.170	3.9	1.771	0.090	0.002
2	0.280	5.0	1.955	0.075	0.002
3	0.220	5.6	1.637	0.075	0.002
4	0.330	3.7	1.485	0.080	0.001
5	0.220	2.5	2.198	0.095	0.003
6	0.450	4.9	1.732	0.108	0.001
7	0.170	3.1	2.059	0.076	0.003
8	0.220	2.9	1.897	0.086	0.001
9	0.170	2.5	1.577	0.074	0.002
10	0.310	11.2	2.065	0.116	0.003
11	0.250	4.5	1.980	0.065	0.002
12	0.220	3.7	1.752	0.063	0.003
13	0.360	40.5	3.201	0.196	0.003
14	0.250	4.1	1.801	0.184	0.002
15	0.250	6.6	2.339	0.205	0.001
16	0.250	11.0	2.895	0.263	0.002
17	0.420	29.4	3.438	0.295	0.001
18	0.170	4.8	2.405	0.235	0.002
19	0.140	3.8	2.713	0.224	0.002
20	0.840	17.9	3.310	0.236	0.001
21	0.250	6.2	2.752	0.215	0.003
22	0.250	2.9	2.171	0.196	0.003
23	0.080	2.7	2.488	0.200	0.004
24	0.280	5.7	2.682	0.197	0.003
25	0.250	4.0	2.332	0.192	0.003
26	0.170	3.6	1.519	0.101	-0.002
27	0.310	9.0	1.244	0.091	-0.002

Sample	Free acidity (%)	Peroxide value (meq O ₂ kg ⁻¹)	K232	K272	ΔK
28	1.010	6.3	2.546	0.206	0.002
29	0.140	5.4	2.873	0.201	0.003
30	0.250	3.3	1.719	0.167	0.002
31	0.330	10.6	1.837	0.091	-0.001
32	0.170	3.6	1.519	0.101	-0.002
33	0.310	9.0	1.244	0.091	-0.002
34	0.170	3.6	1.519	0.101	-0.002
35	0.280	6.9	1.872	0.089	0.002
36	0.280	5.9	1.556	0.058	0.002
37	0.530	10.7	1.603	0.061	0.002
38	0.590	8.4	1.047	0.039	0.003
39	0.310	8.1	2.297	0.105	0.008
40	0.220	7.9	2.350	0.093	0.002
41	0.200	6.4	2.254	0.151	0.004
42	0.360	5.2	1.905	0.119	0.001
43	0.340	7.1	1.893	0.131	0.009
44	0.560	9.2	2.630	0.150	0.003
45	0.310	14.2	2.398	0.087	0.002

Values are those used for the descriptive statistics and chemical PCA in the main manuscript.