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RESEARCH ARTICLE **OPEN ACCESS**

FTIR ATR Fingerprinting Coupled with Hybrid Physics-Informed Neural Networks for Olive Oil Quality Prediction

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Supplementary Materials

Additional data and extended statistical validations supporting the findings of this study are provided in the accompanying Supplementary Statistical Analyses document. This includes:

Table 1: Experimental Design and Sample Distribution, describing the 2 × 3 × 3 factorial structure, three biological replicate plots per treatment combination, and the relationship between biological oil samples and technical FTIR spectra.

Table 2: ANOVA Effect Sizes (η^2, partial η^2, ω^2, and Cohen's f).

Table 3: Temporal Holdout Validation, detailing the cross year predictive performance (2023 *vs.* 2024).

Table 4: Permutation Test Results, establishing the statistical significance of the Leave-One-Treatment-Out predictions against 500 randomized null distributions.

Supplementary Statistical Analyses

Table 1. Experimental Design and Sample Distribution. The design is a fully balanced 2 × 3 × 3 factorial with 18 replicate FTIR scans per treatment cell (total N = 324).

Year	Irrigation (W %ETc)	Fertilization (F %NPK)	Number of Replicates
2023	50	50	18
2023	50	75	18
2023	50	100	18
2023	75	50	18
2023	75	75	18
2023	75	100	18
2023	100	50	18
2023	100	75	18
2023	100	100	18
2024	50	50	18
2024	50	75	18

Year	Irrigation (W %ETc)	Fertilization (F %NPK)	Number of Replicates
2024	50	100	18
2024	75	50	18
2024	75	75	18
2024	75	100	18
2024	100	50	18
2024	100	75	18
2024	100	100	18

Table 2. ANOVA Effect Sizes. Magnitude of differences for primary effects (Year, Irrigation, Fertilization) computed as η^2, partial η^2, ω^2, and Cohen's f.

Trait	Factor	n_groups	F_statistic	p_value	p_sig	η^2	partial_η^2	ω^2	Cohen's_f	Effect_size	SS_between	SS_within	df_between	df_within	MS_between	MS_within
TPC	Year	2	3426.3400	0.0000	***	0.3702	0.3702	0.3700	0.7670	Large	31541.0787	53667.8616	1	5830	31541.0787	9.2055
TPC	W	3	167.9500	0.0000	***	0.0545	0.0545	0.0542	0.2400	Small	4642.7340	80566.2063	2	5829	2321.3670	13.8216
TPC	F	3	69.6200	0.0000	***	0.0233	0.0233	0.0230	0.1550	Small	1987.9726	83220.9677	2	5829	993.9863	14.2771
TFC	Year	2	1626.8600	0.0000	***	0.2182	0.2182	0.2180	0.5280	Large	36.2692	129.9739	1	5830	36.2692	0.0223
TFC	W	3	334.6500	0.0000	***	0.1030	0.1030	0.1027	0.3390	Medium	17.1224	149.1207	2	5829	8.5612	0.0256
TFC	F	3	216.8700	0.0000	***	0.0693	0.0693	0.0689	0.2730	Medium	11.5135	154.7296	2	5829	5.7568	0.0265
DPPH	Year	2	1165.8000	0.0000	***	0.1666	0.1666	0.1665	0.4470	Large	112733.3472	563761.5556	1	5830	112733.3472	96.7001
DPPH	W	3	31.1500	0.0000	***	0.0106	0.0106	0.0102	0.1030	Small	7154.5278	669340.3750	2	5829	3577.2639	114.8294
DPPH	F	3	866.1500	0.0000	***	0.2291	0.2291	0.2288	0.5450	Large	154985.1944	521509.7083	2	5829	77492.5972	89.4681
Carotenoid	Year	2	7386.8800	0.0000	***	0.5589	0.5589	0.5588	1.1260	Large	2455.6971	1938.1277	1	5830	2455.6971	0.3324
Carotenoid	W	3	21.0100	0.0000	***	0.0072	0.0072	0.0068	0.0850	Negligible	31.4481	4362.3767	2	5829	15.7241	0.7484
Carotenoid	F	3	80.3800	0.0000	***	0.0268	0.0268	0.0265	0.1660	Small	117.9258	4275.8990	2	5829	58.9629	0.7336

Table 3. Temporal Holdout Validation. Cross-year predictive performance of the baseline PLSR-PCA model when trained exclusively on 2023 data and tested on 2024 data.

Trait	Method	Level	n_train	n_test	PCA_var_exp	Spearman_rho	rho^2	R^2	RMSE	Bias	p_rho
TPC	PLSR-PCA (n_comp=5)	replicate	2916	2916	0.9688	0.0261	0.0007	-48.4002	5.2462	4.9319	0.1586
TPC	PLSR-PCA (n_comp=3)	treatment-mean	9	9	1.0000	-0.5333	0.2844	-390.0882	12.2312	9.7549	0.1392
TFC	PLSR-PCA (n_comp=5)	replicate	2916	2916	0.9688	0.0866	0.0075	-12.8506	0.1679	0.0914	0.0000
TFC	PLSR-PCA (n_comp=3)	treatment-mean	9	9	1.0000	-0.5500	0.3025	-16.6869	0.1409	-0.0308	0.1250
DPPH	PLSR-PCA (n_comp=5)	replicate	2916	2916	0.9688	0.5292	0.2801	-0.2039	11.7011	6.2149	0.0000
DPPH	PLSR-PCA (n_comp=3)	treatment-mean	9	9	1.0000	0.8000	0.6400	0.2886	8.2136	-4.6877	0.0096
Carotenoid	PLSR-PCA (n_comp=5)	replicate	2916	2916	0.9688	0.0930	0.0086	-84.4754	1.6521	1.5685	0.0000
Carotenoid	PLSR-PCA (n_comp=3)	treatment-mean	9	9	1.0000	-0.4000	0.1600	-361.3283	2.9448	2.6932	0.2861

Table 4. Permutation Test Results. Statistical significance of the Leave-One-Treatment-Out (LOTO) cross-validation predictions derived from 500 random permutations of the target variables.

Trait	n_treatment_cells	n_permutations	Observed_LOTO_rho2	Null_mean_rho2	Null_sd_rho2	Null_95pct_rho2	p_permutation	Significant_p05	Effect_over_null
TPC	18	500	0.1530	0.0628	0.0877	0.2366	0.1160	False	0.0901
TFC	18	500	0.1764	0.0641	0.0857	0.2425	0.0980	False	0.1123
DPPH	18	500	0.3976	0.0590	0.0793	0.2225	0.0100	True	0.3386
Carotenoid	18	500	0.3280	0.0611	0.0798	0.2283	0.0160	True	0.2669

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