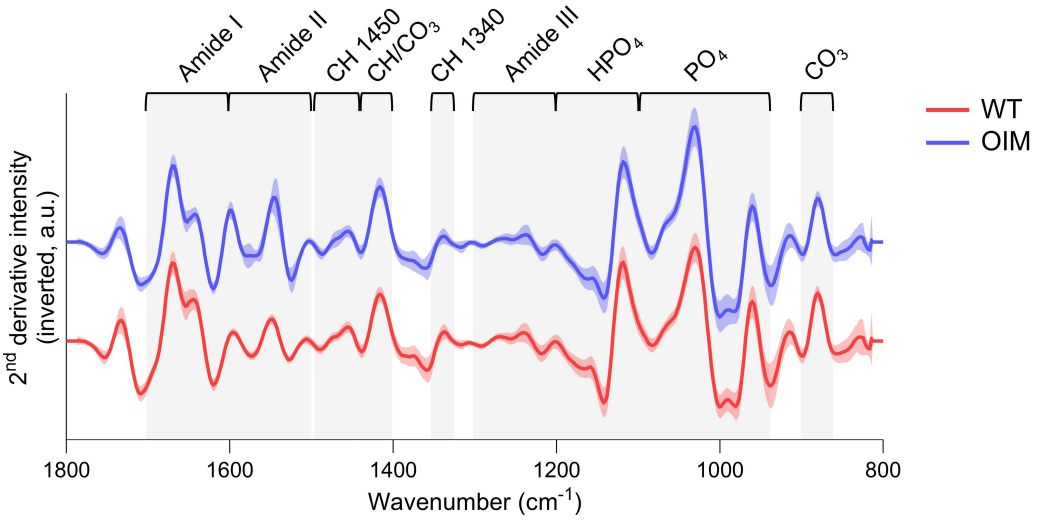
Explainable machine learning for infrared spectral analysis of bone

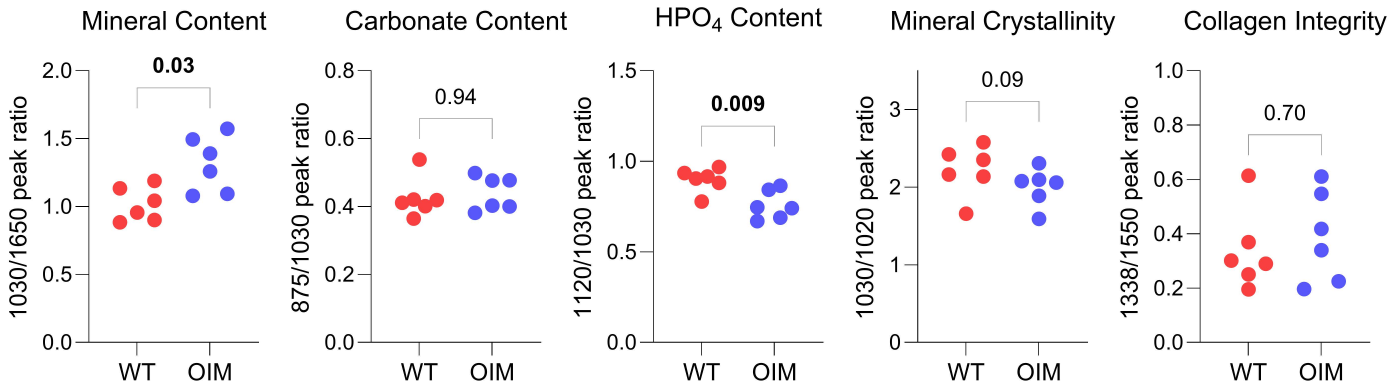
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Supplementary Information



Supplementary Figure S1. Second-derivative O-PTIR spectra of WT and OIM bones. Mean second-derivative-processed spectra, showing enhanced resolution of overlapping spectral features within chemically grounded spectral zones. Spectra are vertically staggered to facilitate visualization.



Supplementary Figure S2. Animal-level conventional O-PTIR compositional parameters in WT and OIM bones. Mean values for each animal are shown for the five peak-ratio parameters reflecting bone tissue compositional properties (6 animals per group). P-values were calculated using the Mann–Whitney test.

(a)

	Raw Spectra Range			2nd Derivative Spectra Range			
	Full	Collagen	Mineral	Full	Collagen	Mineral	Peak Ratios
Logistic Regression	0.90	0.89	0.83	0.89	0.90	0.83	0.61
SVM	0.89	0.87	0.81	0.87	0.84	0.78	0.63
KNN	0.82	0.81	0.69	0.80	0.80	0.60	0.59
Random Forest	0.88	0.86	0.78	0.84	0.83	0.71	0.61
XGBoost	0.89	0.87	0.80	0.83	0.81	0.74	0.61

Full range = 1800–800 cm^{-1}; collagen range = 1800–1200 cm^{-1}; mineral range = 1200–800 cm^{-1}

(b)

	Raw Spectra Range			2nd Derivative Spectra Range			
	Full	Collagen	Mineral	Full	Collagen	Mineral	Peak Ratios
Logistic Regression	0.97	0.97	0.90	0.96	0.96	0.89	0.64
SVM	0.96	0.95	0.89	0.92	0.92	0.84	0.67
KNN	0.88	0.86	0.78	0.86	0.83	0.70	0.63
Random Forest	0.95	0.94	0.85	0.93	0.91	0.75	0.64
XGBoost	0.95	0.93	0.87	0.91	0.91	0.80	0.64

Full range = 1800–800 cm^{-1}; collagen range = 1800–1200 cm^{-1}; mineral range = 1200–800 cm^{-1}

Supplementary Figure S3. Additional classification performance metrics across spectral representations and modeling approaches. (a) F1-score and (b) receiver operating characteristic area under the curve (ROC-AUC) across machine-learning models using different spectral ranges (full fingerprint, collagen-rich, mineral-rich) and conventional peak-ratio representations. Raw and second-derivative spectra are compared for each spectral-range analysis.