

Supporting Information

Raman spectroscopy in colorectal cancer diagnostics: Comparison of PCA-LDA and PLS-DA
models

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Table S1. Peak assignments of vibrational bands of human colorectal tissue from Raman spectra.

Colorectal tissues		Peak Assignment
Wavenumber/cm ⁻¹		
Normal	Tumor	
	890	Lipids/carbohydrates/collagen C–C–N ⁺ , C–O–C ring, C–C
	1002	Phenylalanine
1063	1063	Lipids/collagen, C–C str
1134	1134	Fatty acid (C–C str.)/proteins (C–C/C–N str.)
1174	1172	L-Tryptophan
	1243	Phospholipid, O–P–O antisym. str
1297	1297	Lipids, phospholipids, C–H ₂ twist
	1371	Lipids CH ₃ sym. bend, lipids
1414	1419	Lipids N ⁺ (CH ₃) ₃ sym. bend
1442	1442	Fatty acids, triglycerides, CH ₂ or CH ₃ deformations
1461	1461	Lipids/proteins C–H wag, CH ₂ or CH ₃ def.
	1663	Proteins Amide I α helix, C=O
2726	2729	C–H stretching
2847	2847	Fatty acids, triglycerides, C–H ₂ sym. str
2879	2879	Lipids, C–H ₂ antisym. str.
2927	2927	Proteins/lipids, CH ₃ sym. str
	2966	C–H ₂ stretching
	3068	Nucleic acids/proteins, C–H aromatic

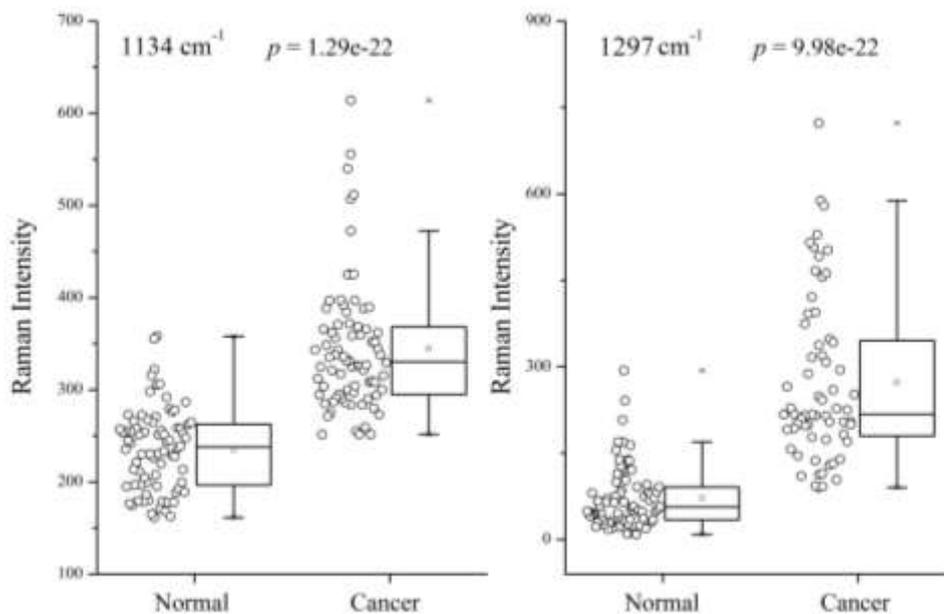


Figure S1. Box charts of the intensity of Raman bands at 1134 and 1297 cm^{-1} from normal and cancerous tissues. The line within each box represents the median, while the lower and upper boundaries of the box indicate the first (25th percentile) and the third (75th percentile) quartiles, respectively. Error bars (whiskers) represent the 1.5-fold interquartile range.

The intensity of Raman bands at 1134 cm^{-1} (C–C/C–N stretching vibration) and 1297 cm^{-1} (C–H₂ twisting vibration) was measured for normal and cancer groups. The independent-sample t-test was performed to evaluate the intensity change between these two groups. As shown in Figure S1, the average values of peak intensities at 1134 cm^{-1} (314.96) and 1297 cm^{-1} (272.79) in the cancer group are higher than those in the control group (235.15 and 72.22), respectively. The *p* values of peak intensities at 1134 ($p_{1134}= 1.29\text{e-}22$) and 1297 cm^{-1} ($p_{1297}= 9.98\text{e-}22$) are less than 0.05. Thus, the peak intensities at 1134 and 1297 cm^{-1} increased significantly in cancerous tissue, relative to the normal tissue.

Table S2. Comparison of diagnostic performance of PCA-LDA and PLS-DA models for differentiating cancerous from normal colorectal tissues.

Raman spectroscopy model	Accuracy	Sensitivity	Specificity
PCA-LDA	79.2%	72.8%	85.9%
PLS-DA	84.3%	77.7%	91.0%