

Evaluation of Raman spectroscopy combined with gate recurrent unit serum detection method in early screening of gastrointestinal cancer

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Table. S1 Peak positions and tentative assignments of the major Raman bands from biological samples

Peak position, cm ⁻¹	Major Assignments
855/856 ^{1, 2}	Proline, hydroxyproline, tyrosine C-C stretching, proline (collagen assignment)
951 ³	$\nu_s(\text{CH}_3)$ of proteins (α -helix)
1000 ⁴	Phenylalanine Bound & free NADH
1002 ^{1, 2}	C-C aromatic ring stretching Phenylalanine
1003 ⁵	Phenylalanine, C-C skeletal
1004 ^{1-3, 6}	Phenylalanine (of collagen) $\nu_s(\text{C-C})$, symmetric ring breathing, phenylalanine (protein assignment) Phenylalanine (collagen assignment) $\nu(\text{C-C})$ phenylalanine
1150 ^{7, 8}	Glycogen Carotenoid
1152 ⁶	$\nu(\text{C-N})$, proteins (protein assignment) $\nu(\text{C-C})$, carotenoid Carotenoid peaks due to C-C & conjugated C=C band stretch
1153 ⁷	Carbohydrates peak for solutions
1155 ^{7, 9-11}	C-C (&C-N) stretching of proteins (also carotenoids) Glycogen $n(\text{C-C})$ Diagnostic for the presence of a carotenoid structure, most likely a cellular pigment
1272/3	CH α' rocking
1275 ¹²	Amide III
1332 ¹³	-C stretch of Phenyl (1) and C ₃ -C ₃ stretch and C ₅ -O ₅ stretch CH α in-plane bend
1333 ¹⁴	Guanine
1335 ^{6, 10, 15, 16}	CH ₃ CH ₂ wagging, collagen (protein assignment)

	<p>CH₃CH₂ wagging, nucleic acid</p> <p>CH₃CH₂ wagging mode of collagen & polynucleotide chain (DNA purine bases)</p> <p>CH₃CH₂ twisting and wagging in collagen</p> <p>Cellular nucleic acids</p> <p>CH₃CH₂ deforming modes of collagen and nucleic acids</p> <p>An unassigned mode</p>
1436 ^{4, 9, 17, 18}	CH ₂ scissoring
1437 ^{4, 9, 17, 18}	<p>CH₂ (lipids in normal tissue)</p> <p>CH₂ deformation (lipid)</p> <p>Acyl chains</p>
1514 ¹¹	$\nu(\text{C}=\text{C})$ diagnostic for the presence of a carotenoid structure, most likely a cellular pigment
1515 ¹⁴	Cytosine
1517 ¹⁹	b-carotene accumulation (C-C stretch mode)
1518 ⁶	<p>$\nu(\text{C}=\text{C})$, porphyrin</p> <p>Carotenoid peaks due to C-C & conjugated C=C band stretch</p>
1520–38 ⁹	-C=C- carotenoid
1602 ^{1, 6}	<p>Phenylalanine</p> <p>$\delta(\text{C}=\text{C})$, phenylalanine (protein assignment)</p>
1603 ^{9, 10, 13}	<p>C=C in-plane bending mode of phenylalanine & tyrosine</p> <p>Ring C-C stretch of phenyl (1)</p>
2913–38 ²⁰	CH stretch of lipids and proteins

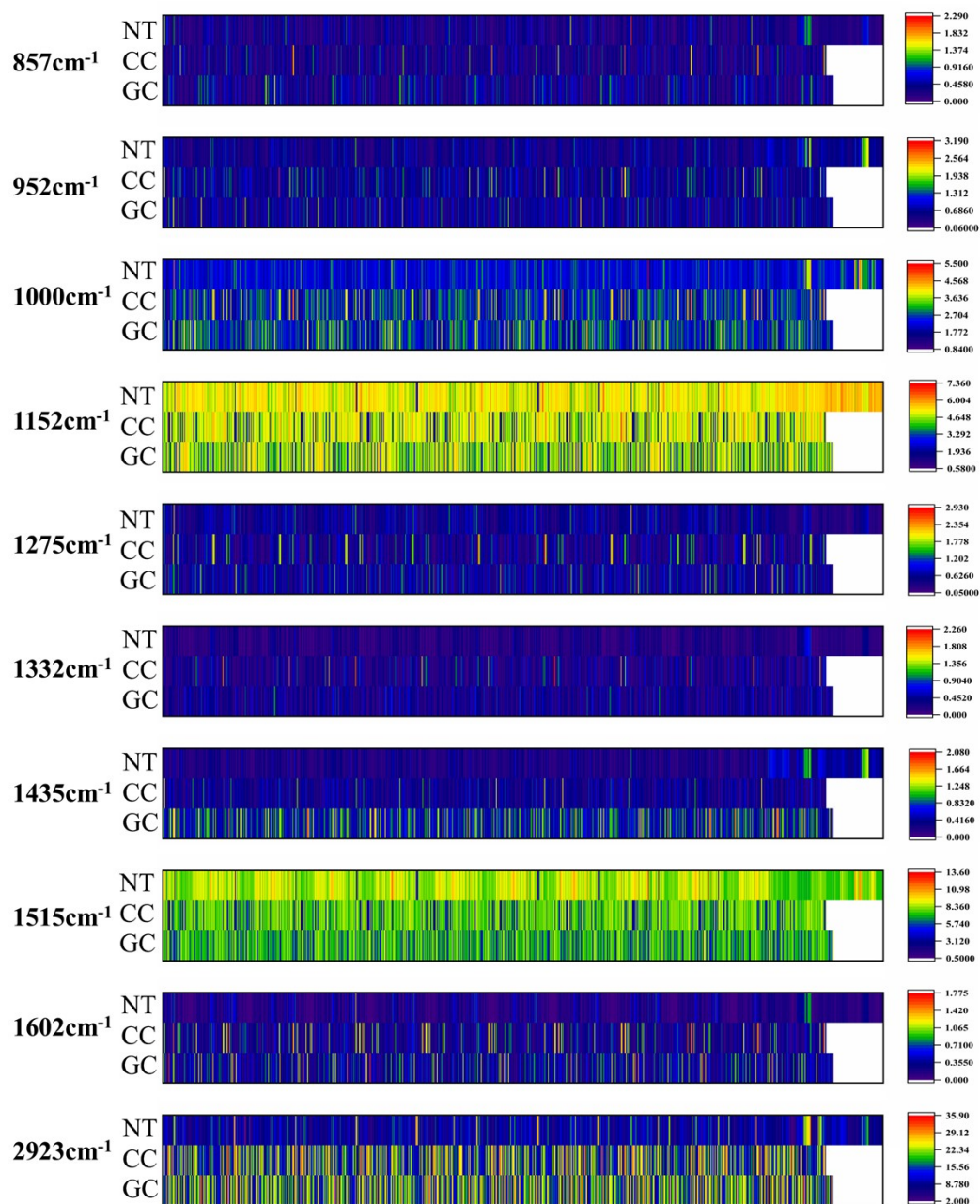


Figure S1 : Heat map of peak areas of different Raman features between patients with gastric cancer, colorectal cancer, and non-tumor. (NT: Non-tumor; CC: Colorectal cancer; GC: Gastric cancer)

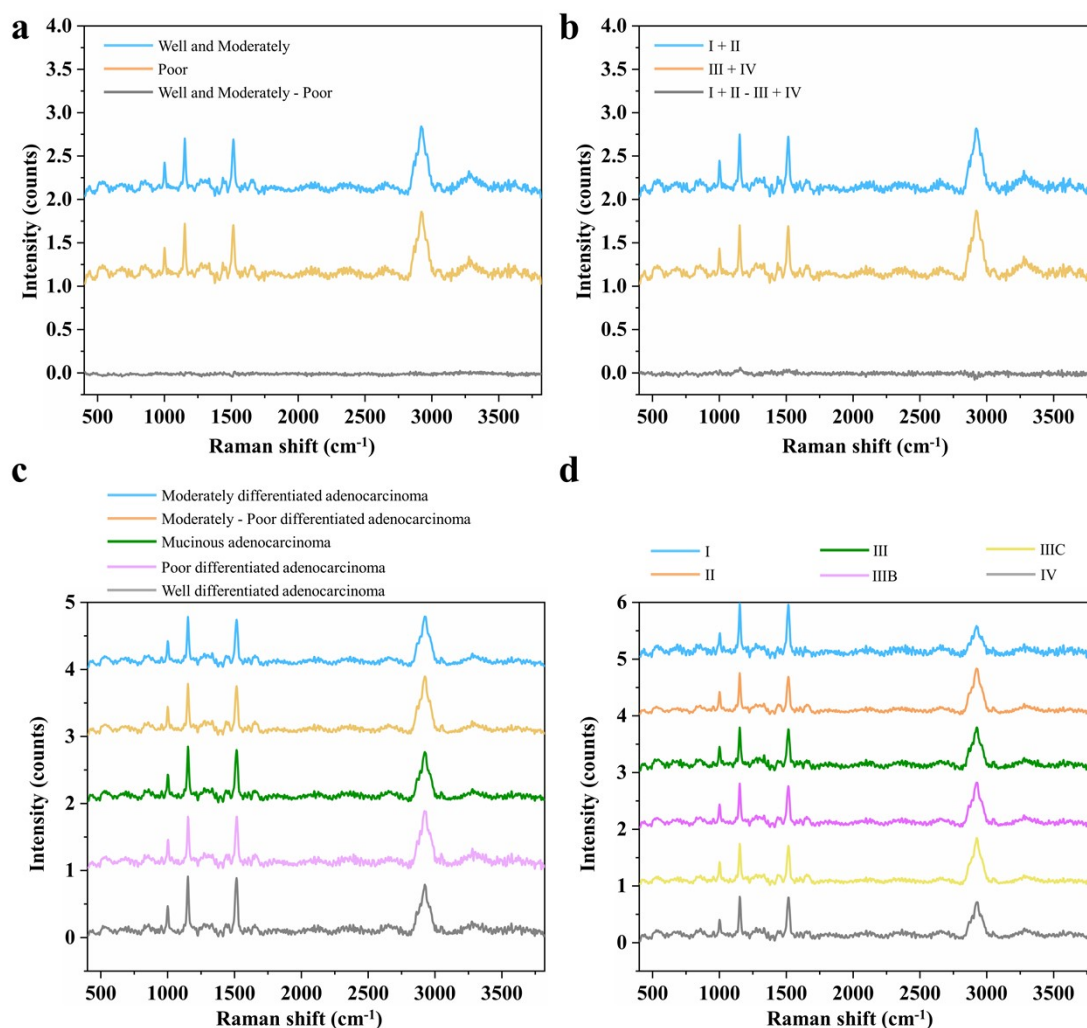


Figure S2 : Mean Raman spectra of patients with different degrees of differentiation and different stages of gastric and colorectal cancers. a). Mean Raman spectra of sera from patients with different degrees of differentiation of gastric cancer. b). Mean Raman spectra of sera from patients with different stages of gastric cancer. c). Average Raman spectra of sera from patients with different differentiation of colorectal cancer. d). Mean Raman spectra of sera from patients with different stages of colorectal cancer.

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