

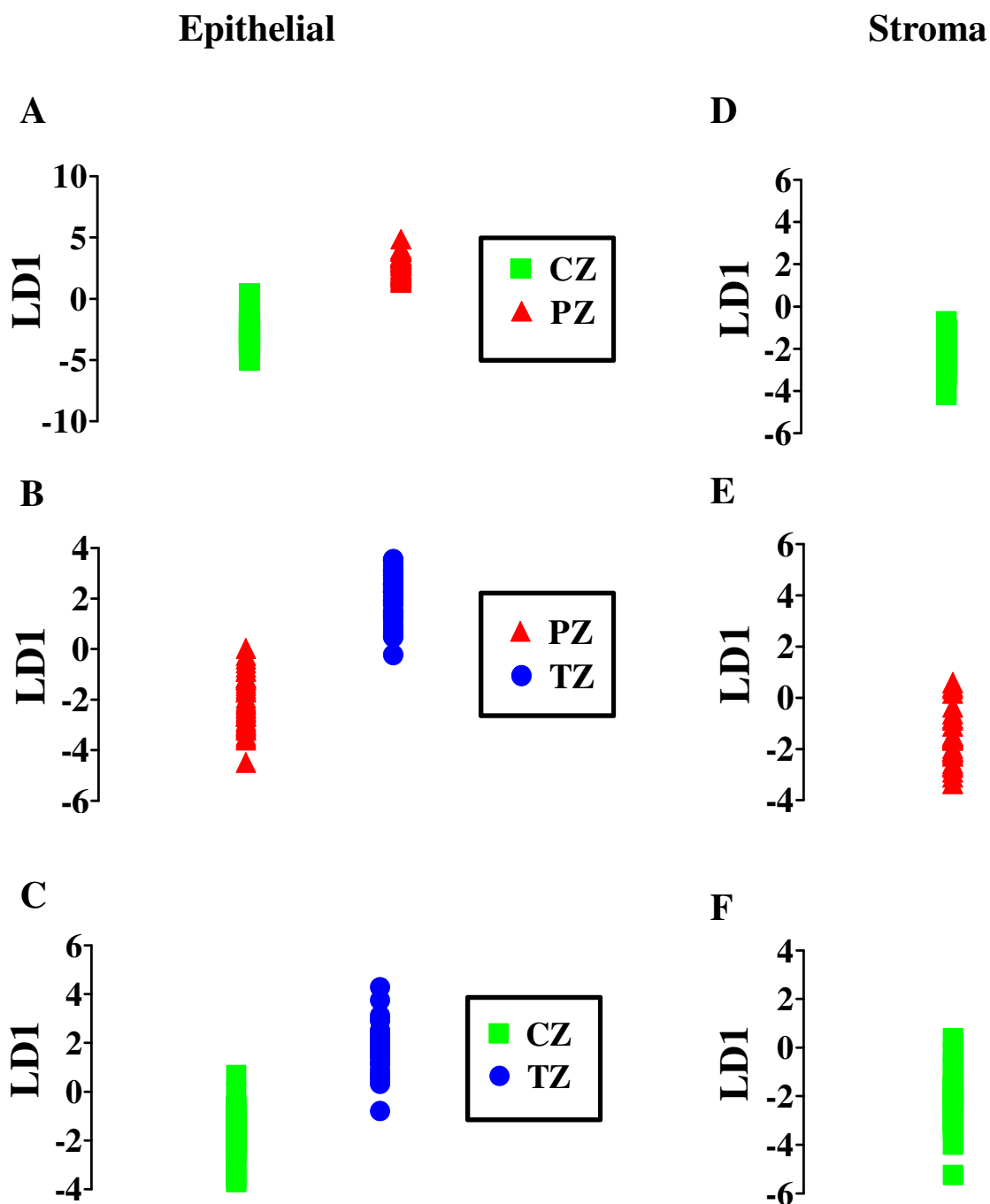
# **Discrimination of zone-specific spectral signatures in normal prostate using Raman spectroscopy**

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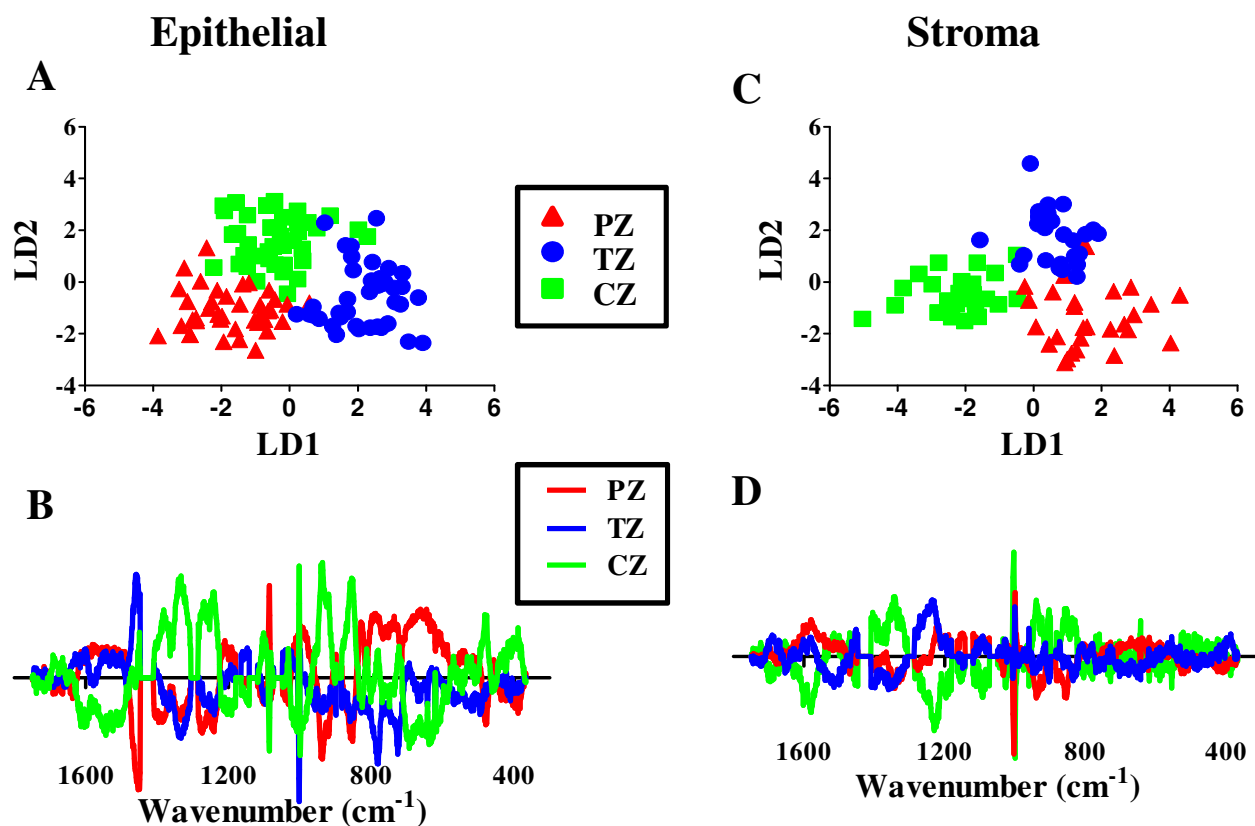
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**Figures = 4**

**Tables = 1**



**Figure 1S.** Principal component analysis with subsequent linear discriminant analysis (PCA-LDA) of prostate epithelial-cell or stromal inter-zone comparisons. Wavenumbers associated with paraffin vibrational modes were excluded. One-D scores plots illustrating segregation between categories are displayed: PZ (red triangles), CZ (green squares), TZ (blue circles). (A) PCA-LDA scores plot of CZ vs. PZ epithelial cells; (B) PCA-LDA scores plot of PZ vs. TZ stroma (C) PCA-LDA scores plot of CZ vs. TZ epithelial cells; (D) PCA-LDA scores plot of CZ vs. PZ stroma (E) PCA-LDA scores plot of PZ vs. TZ epithelial cells; and, (F) PCA-LDA scores plot of CZ vs. TZ stroma. CZ, central zone; LD, linear discriminant; PZ, peripheral zone; TZ, transition zone



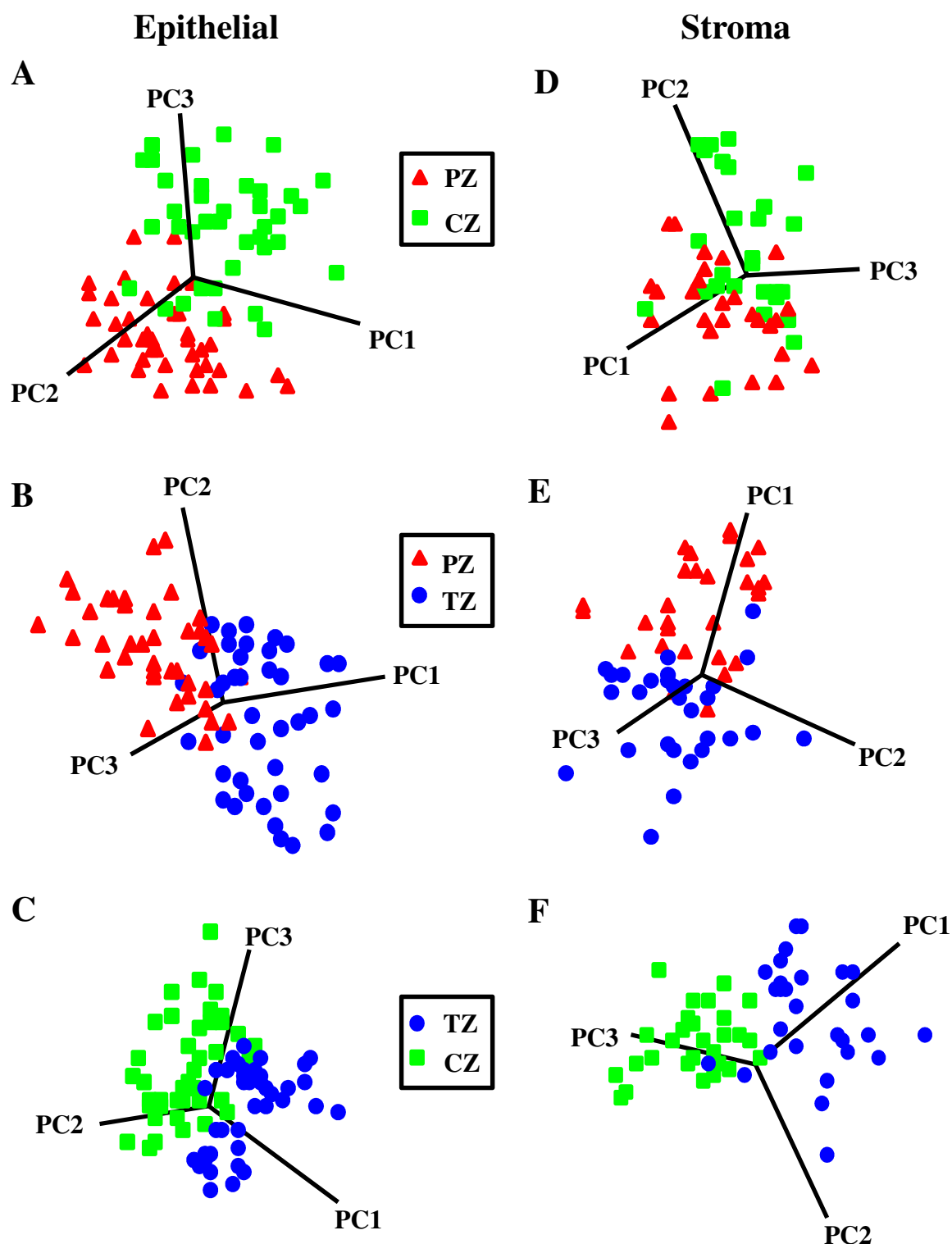
**Figure 2S.** Principal component analysis with subsequent linear discriminant analysis (PCA-LDA) of prostatic inter-zonal epithelial cells and stroma. Wavenumbers associated with paraffin vibrational modes were excluded. Two-D scores plots and corresponding cluster vectors illustrating segregation between categories are displayed: PZ (red triangles), CZ (green squares), TZ (blue circles). (A) PCA-LDA scores plot of PZ vs. CZ vs. TZ epithelial cells; (B) Cluster vectors of PZ vs. CZ vs. TZ epithelial cells; (C) PCA scores plot of PZ vs. CZ vs. TZ stroma; and, (D) Cluster vectors of PZ vs. CZ vs. TZ stroma.

CZ, central zone; PZ, peripheral zone; LD, linear discriminant; TZ, transition zone

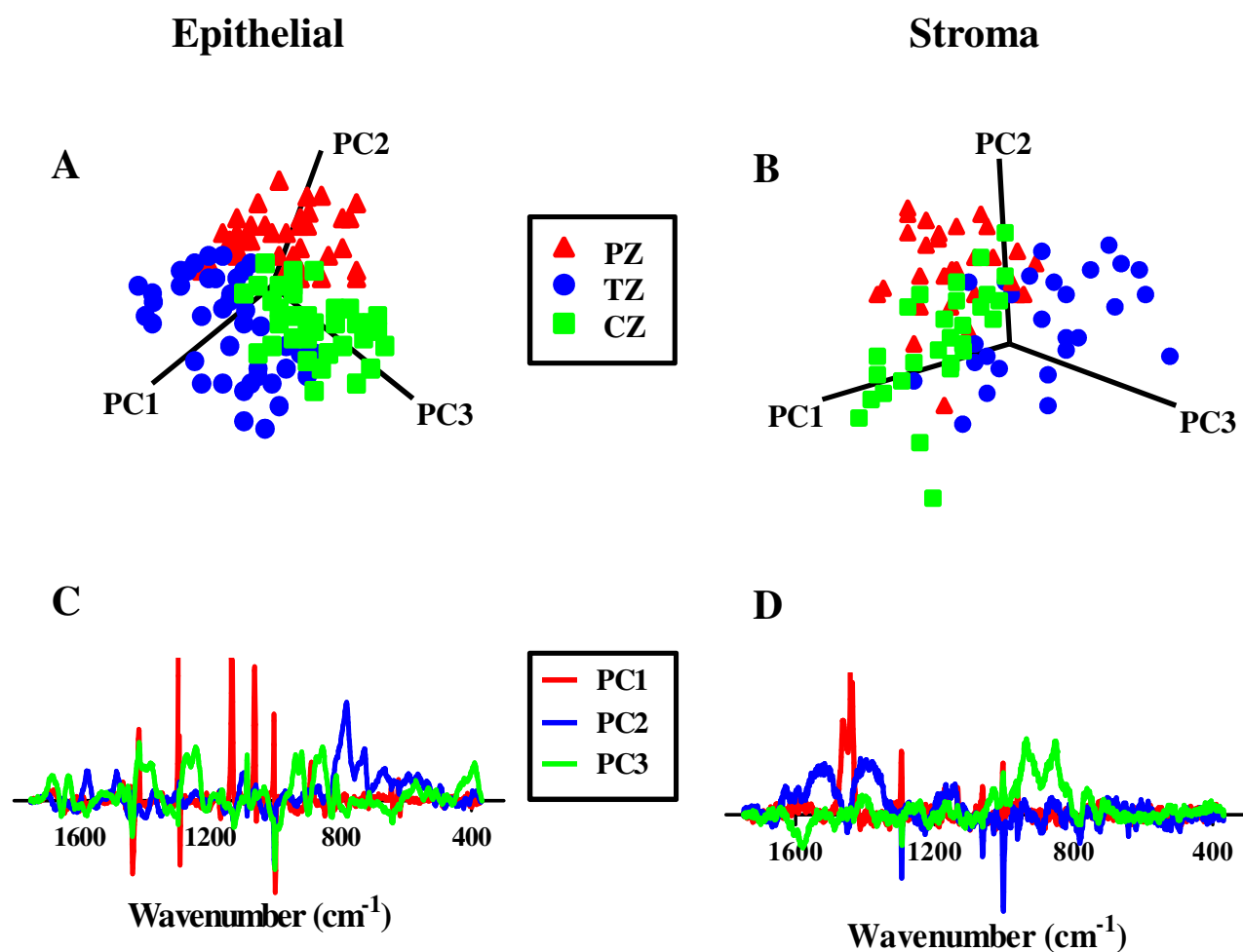
**Table 1S.** Discriminating wavenumbers for inter-category segregation identified by PCA-LDA cluster vectors

Tentative wavenumber (cm <sup>-1</sup> ) assignments <sup>13,18,22-24</sup>	Inter-zone comparison					
	PZ versus CZ		PZ versus TZ		CZ versus TZ	
	E	S	E	S	E	S
-1585: lipids (C=C olefinic stretch)			X			
-1575: purine rings			X			
-1548: tryptophan				X		
-1485: purine rings						
-1468		X				
-1459: lipids and proteins (CH <sub>2</sub> deformation)		X	X	X	X	
-1386: CH <sub>3</sub> bend	X					
-1369: guanine, proteins and lipids						
-1346: collagen						X
-1311: collagen/ lipids (CH <sub>3</sub> CH <sub>2</sub> twisting)						
-1269: Amide III (α-helix)				X		
-1223: Amide III (β-helix)		X				X
-1210: phenylalanine and tryptophan (C-C <sub>6</sub> H <sub>5</sub> stretch)						
-1150: proteins (C-C and C-N stretch)						
-1090-1111: lipid and proteins (C-C and C-N stretch)				X		
-1030: phenylalanine (C-H stretch)		X		X		
-1001: phenylalanine (symmetric ring breathing)		X	X	X	X	X
-961						X
-938: protein backbone (C-C stretch)	X	X			X	
-936: protein/ glycogen (C-C stretch)		X				
-921: proline ring/ glucose (C-C stretch)					X	
-905			X			
-859: tyrosine/ glycogen		X				
-853: tyrosine/ proline (ring breathing/ C-C stretch)	X				X	X
-838						X
-787: DNA (O-P-O stretch)	X		X			
-781: cytosine/uracil (ring breathing)	X		X			
-755: tryptophan (ring breathing)				X		
-727: protein (C-S stretch/ CH <sub>2</sub> rocking)						
-718: phospholipid head/ adenine (C-N stretch)				X		
-642: tyrosine (C-C twisting)	X				X	
-621: phenylalanine (C-C twisting)	X		X		X	X
-525: proteins (S-S stretch)						X
-506			X			
-480: starch	X				X	

X, discriminating in this inter-category comparison; E, epithelial cell; S, stroma; CZ, central zone; PZ, peripheral zone; TZ, transition zone



**Figure 3S.** Principal component analysis (PCA) for two-class discrimination of prostate inter zone comparisons of epithelial cells or stroma. Principal components (PCs) determining best segregation of classes are displayed: PZ (red triangles), CZ (green squares), TZ (blue circles). (A) PCA scores plot of epithelial cell PZ vs. CZ; (B) PCA scores plot of epithelial cell PZ vs. TZ; (C) PCA scores plot of epithelial cell TZ vs. CZ; (D) PCA scores plot of stromal PZ vs. CZ; (E) PCA scores plot of stromal PZ vs. TZ; and, (F) PCA scores plot of stromal TZ vs. CZ. CZ, central zone; PZ, peripheral zone; TZ, transition zone



**Figure 4S.** Principal component analysis (PCA) analysis of prostate inter-zone comparisons of epithelial cells or stroma. Principal components (PCs) determining best segregation of classes are displayed: PZ (red triangles), CZ (green squares), TZ (blue circles). **(A)** PCA scores plot of PZ vs. CZ vs. TZ epithelial cells; **(B)** PCA scores plot of PZ vs. CZ vs. TZ stroma; **(C)** PCA loadings plot of PZ vs. CZ vs. TZ epithelial cells; and, **(D)** PCA loadings plot of PZ vs. CZ vs. TZ stroma. CZ, central zone; PZ, peripheral zone; TZ, transition zone