Supplementary Information
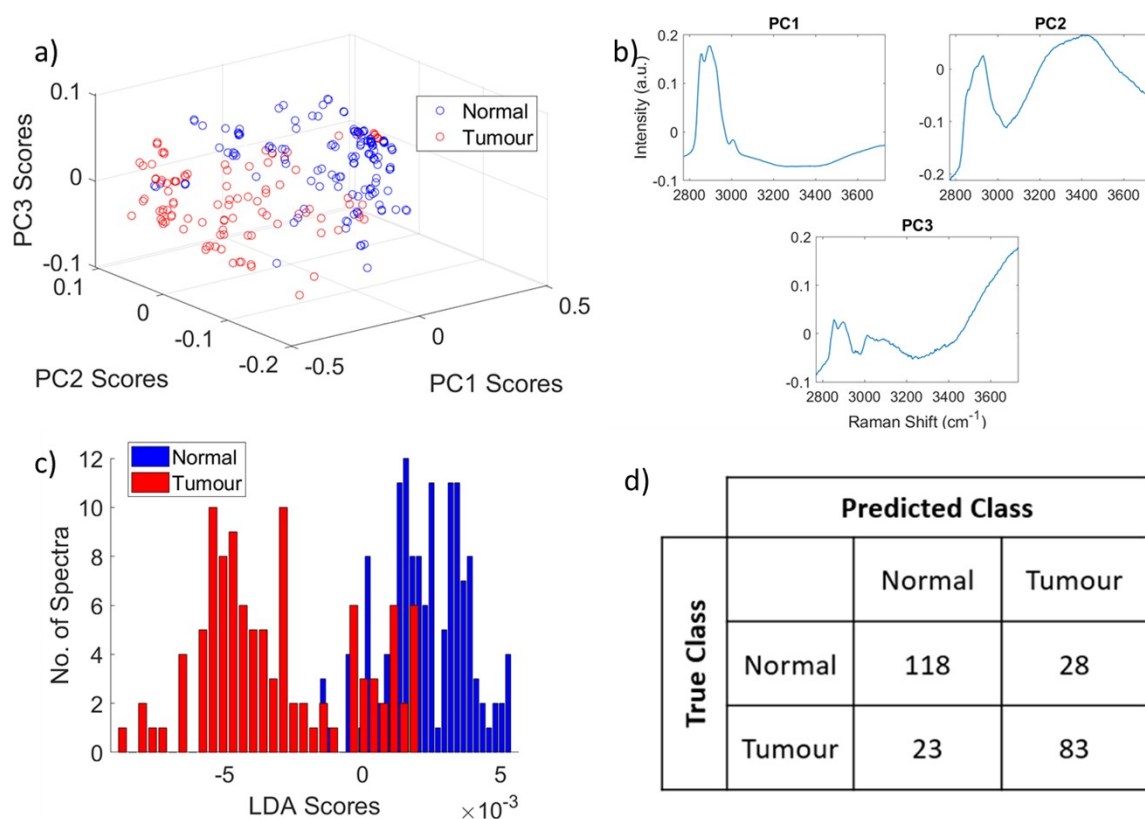

Figure S1. PCA-LDA classification model of pathology confirmed data. (a) Scatter plot of principal component scores from PC1, PC2 and PC3. The scores of normal spectra are blue (146 spectra) and the scores of the tumour spectra are red (106 spectra). b) The loadings of PC1, PC2 and PC3 c) Histogram of the linear discriminant scores; those of normal spectra shown in blue, while those of tumour spectra are shown in red. d) Confusion matrix showing the number of spectra correctly and incorrectly classified as normal and tumour based on the model following leave one sample out cross validation, giving 78.3% sensitivity and 80.8% specificity.