Electronic Supplementary Information

ATR-FTIR Spectroscopy with Chemometrics for Analysis of Saliva Samples Obtained in a Lung-Cancer-Screening Programme: Application of Swabs as a Paradigm for High Throughput in a Clinical Setting

Francis L Martin [1,2,*], Andrew W Dickinson [2], Tarek Saba [2], Thomas Bongers [2], Maneesh N Singh [1,3], Danielle Bury [1,*]

1 Biocel UK Ltd., Hull HU10 6TS, UK; mnsingh@biocel.uk
2 Department of Cellular Pathology, Blackpool Teaching Hospitals NHS Foundation Trust, Whinney Heys Road, Blackpool FY3 8NR, UK; aw.dickinson@hotmail.com (A.W.D.); dr.saba@nhs.net (T.S.); thomas.bongers@nhs.net (T.B.)
3 Chesterfield Royal Hospital, Chesterfield Road, Calow, Chesterfield S44 5BL, UK
* Correspondence: flm13@biocel.uk (F.L.M.); danielle.bury@nhs.net (D.B.)

Multivariate linear model

PC2 vs PC3 MANOVA — No Subtraction

Intercept	Value	Num DF	Den DF	F Value	Pr > F
Wilks' lambda	0.9622	2.0000	207.0000	4.0651	0.0185
Pillai's trace	0.0378	2.0000	207.0000	4.0651	0.0185
Hotelling-Lawley trace	0.0393	2.0000	207.0000	4.0651	0.0185
Roy's greatest root	0.0393	2.0000	207.0000	4.0651	0.0185

Diagnosis	Value	Num DF	Den DF	F Value	Pr > F
Wilks' lambda	0.8325	2.0000	207.0000	20.8212	0.0000
Pillai's trace	0.1675	2.0000	207.0000	20.8212	0.0000
Hotelling-Lawley trace	0.2012	2.0000	207.0000	20.8212	0.0000
Roy's greatest root	0.2012	2.0000	207.0000	20.8212	0.0000

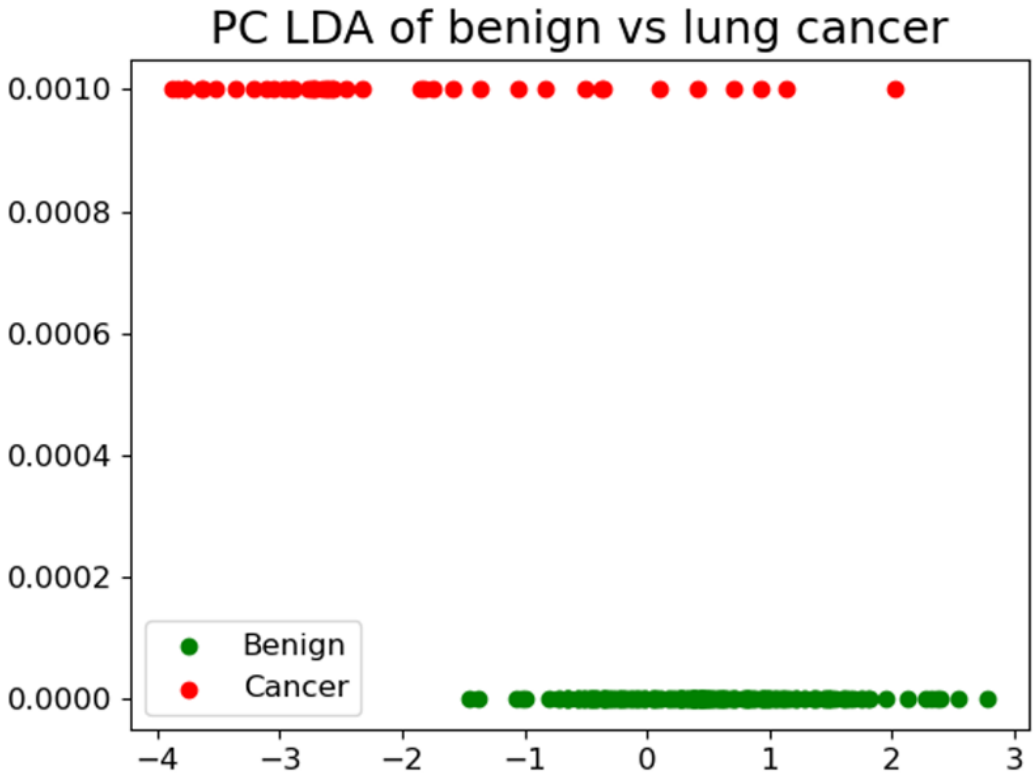

Figure S1 Exploratory analysis of saliva samples on a swab following PCA. Following pairwise comparisons of benign *versus* cancer, four independent multivariate analysis of variance (MANOVA) tests were undertaken to test for significance of segregation. Separation between the categories is also examined employing PCA-LDA (using the first 10 PCs) in a 1-D scores plot.

Multivariate linear model

PC2 vs PC3 MANOVA Dry swab subtracted

Intercept	Value	Num DF	Den DF	F Value	Pr > F
Wilks' lambda	0.9622	2.0000	207.0000	4.0651	0.0185
Pillai's trace	0.0378	2.0000	207.0000	4.0651	0.0185
Hotelling-Lawley trace	0.0393	2.0000	207.0000	4.0651	0.0185
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Roy's greatest root	0.2012	2.0000	207.0000	20.8212	0.0000

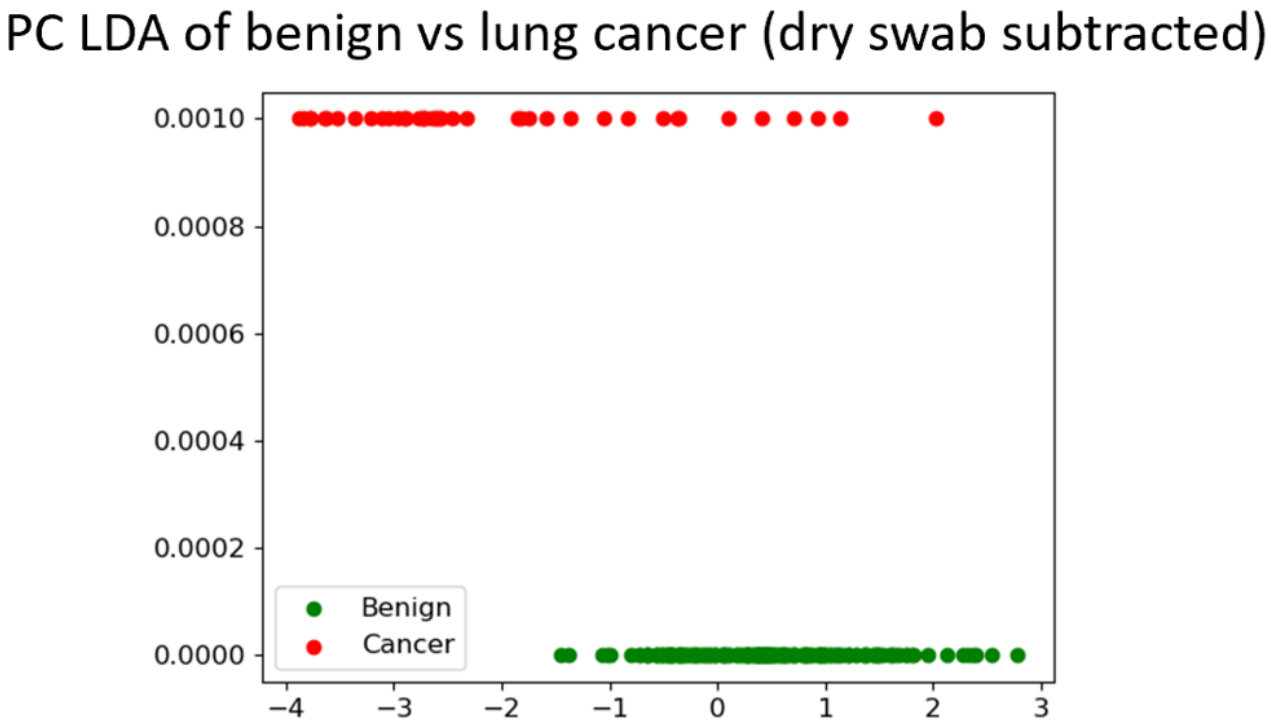


Figure S2 Exploratory analysis of saliva samples minus a dry swab spectral signature following PCA. Following pairwise comparisons of benign *versus* cancer, four independent multivariate analysis of variance (MANOVA) tests were undertaken to test for significance of segregation. Separation between the categories is also examined employing PCA-LDA (using the first 10 PCs) in a 1-D scores plot.

Multivariate linear model

PC2 vs PC3 MANOVA — Wet swab subtracted

Intercept	Value	Num DF	Den DF	F Value	Pr > F
Wilks' lambda	0.9622	2.0000	207.0000	4.0651	0.0185
Pillai's trace	0.0378	2.0000	207.0000	4.0651	0.0185
Hotelling-Lawley trace	0.0393	2.0000	207.0000	4.0651	0.0185
Roy's greatest root	0.0393	2.0000	207.0000	4.0651	0.0185

Diagnosis	Value	Num DF	Den DF	F Value	Pr > F
Wilks' lambda	0.8325	2.0000	207.0000	20.8212	0.0000
Pillai's trace	0.1675	2.0000	207.0000	20.8212	0.0000
Hotelling-Lawley trace	0.2012	2.0000	207.0000	20.8212	0.0000
Roy's greatest root	0.2012	2.0000	207.0000	20.8212	0.0000

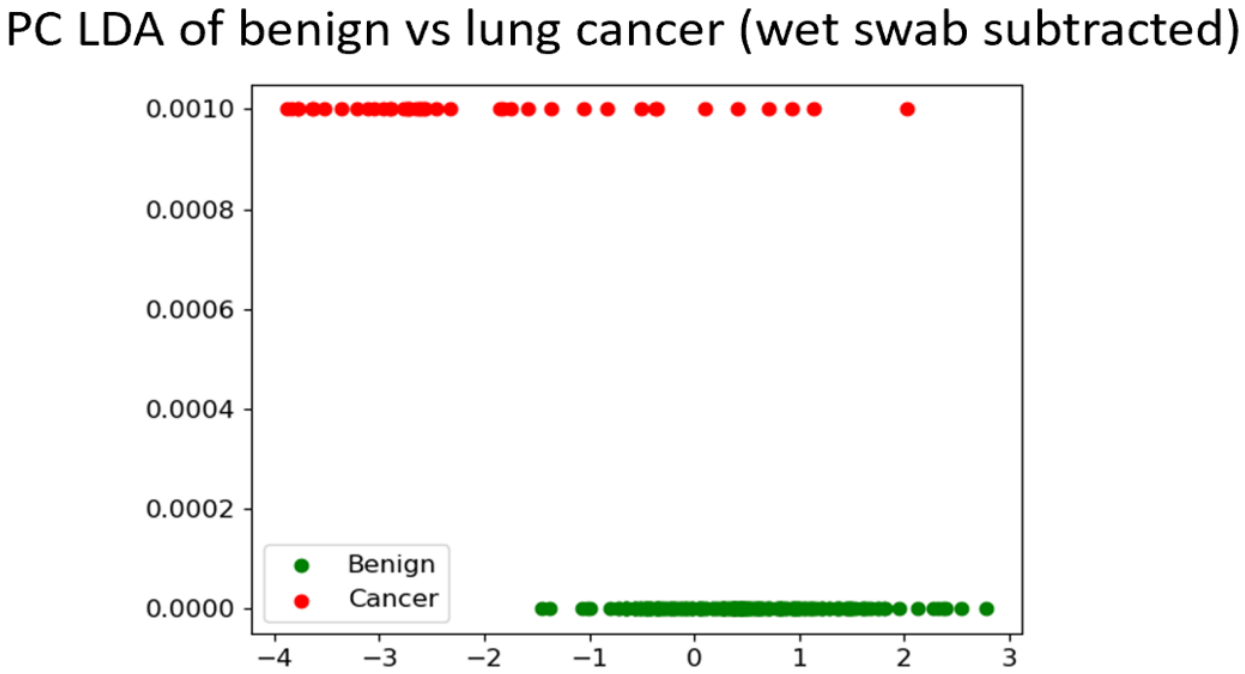


Figure S3 Exploratory analysis of saliva samples minus a wet swab spectral signature following PCA. Following pairwise comparisons of benign *versus* cancer, four independent multivariate analysis of variance (MANOVA) tests were undertaken to test for significance of segregation. Separation between the categories is also examined employing PCA-LDA (using the first 10 PCs) in a 1-D scores plot.

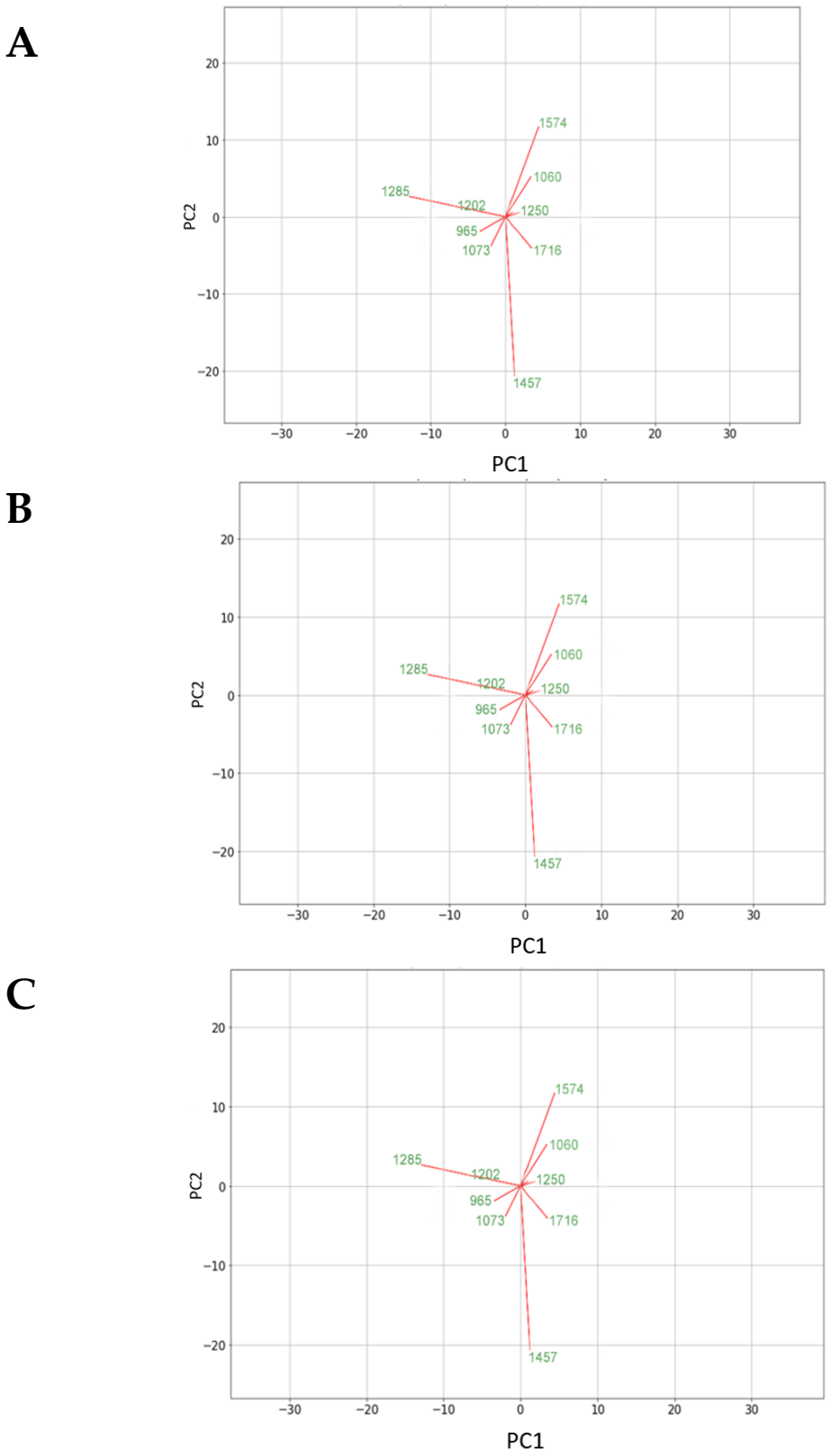
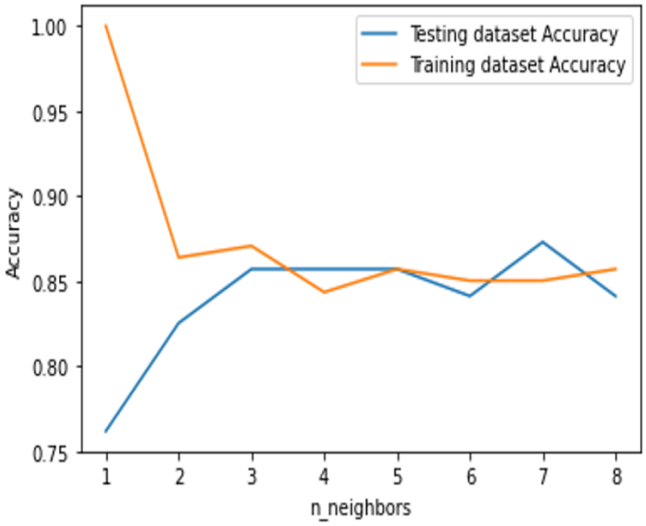
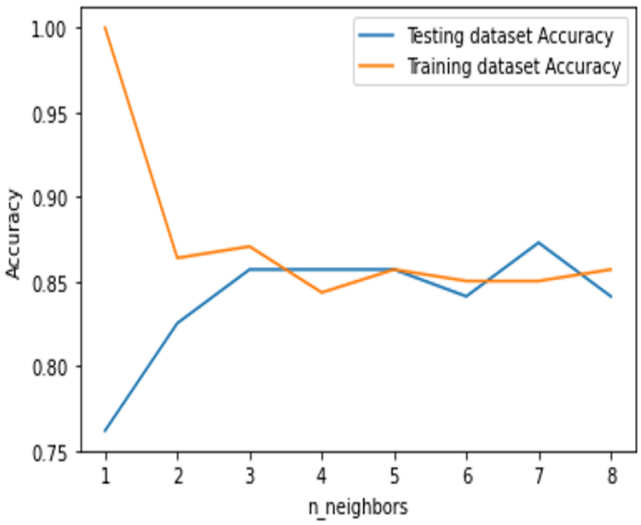


Figure S4 The wavenumbers contributing the most to variance along each of the first 10 PCs (87.2% total variance). Obtained following pairwise comparisons: A) benign *versus* cancer following swab analysis; B) benign *versus* cancer following swab analysis with subtraction of dry swab spectra; and, C) benign *versus* cancer following swab analysis with subtraction of wet swab spectra.

A



B



C

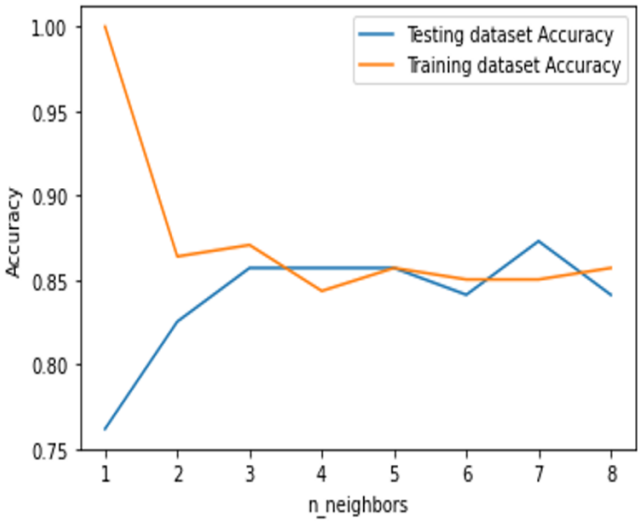


Figure S5 Application of k-nearest neighbours (k-NN). A three nearest neighbours construction was undertaken for each of the three pairwise comparisons undertaken: A) benign *versus* cancer following swab analysis; B) benign *versus* cancer following swab analysis with subtraction of dry swab spectra; and, C) benign *versus* cancer following swab analysis with subtraction of wet swab spectra.