Electronic Supplementary Material (ESI) for Analyst.

Chicken, beams, and *Campylobacter*: rapid differentiation of foodborne bacteria via vibrational spectroscopy and MALDI-mass spectrometry

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Supplementary information

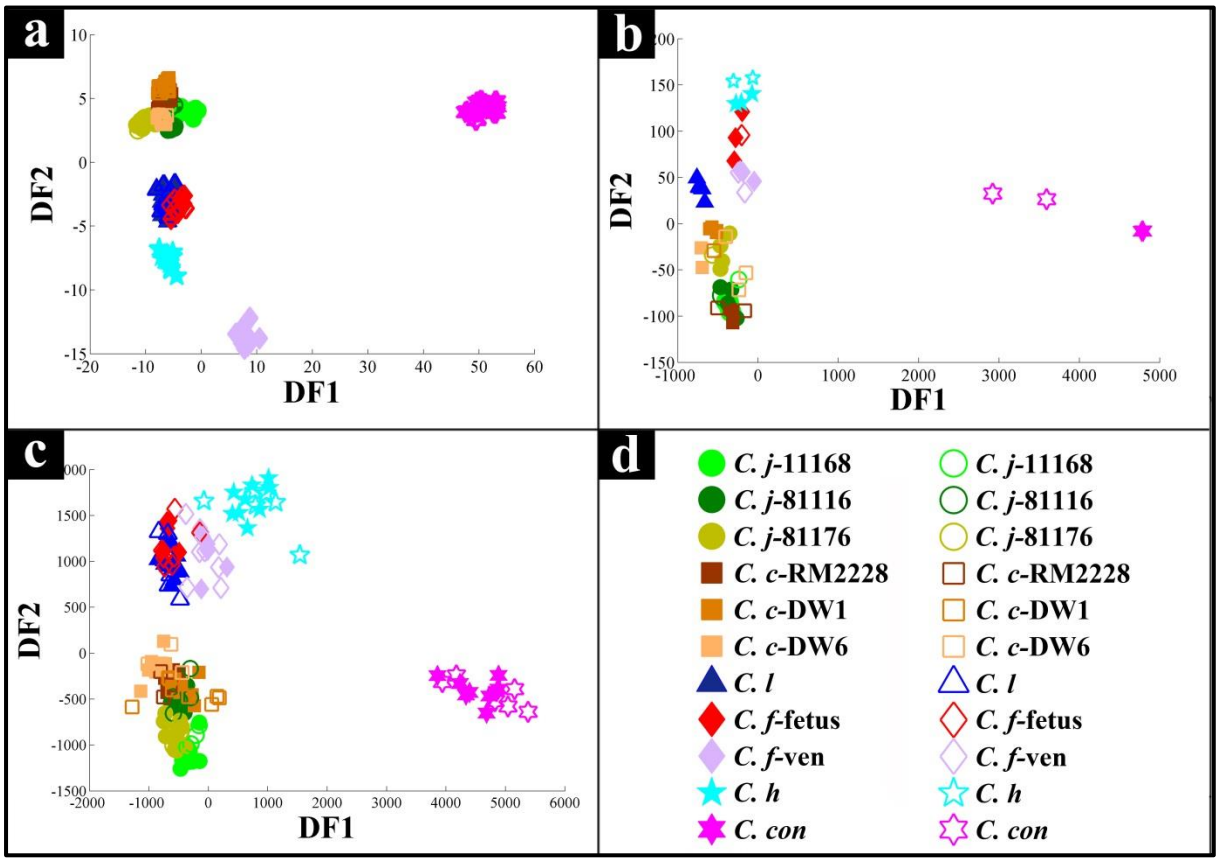

Figure S1. PC-DFA scores biplots of: a) FT-IR, b) Raman, and c) MALDI-TOF-MS data. The PC-DFA of the Raman and FT-IR datasets were carried out using PCs 1-20, while due to the complexity of the MALDI-TOF-MS data the first 40 PCs were employed for discrimination. All generated models were validated using projection of test set spectra not used to construct the PC-DFA model, d) different coloured symbols represent data collected from different strains and used for generating the model (training set), while empty symbols represent the projected samples from these strains (test set).

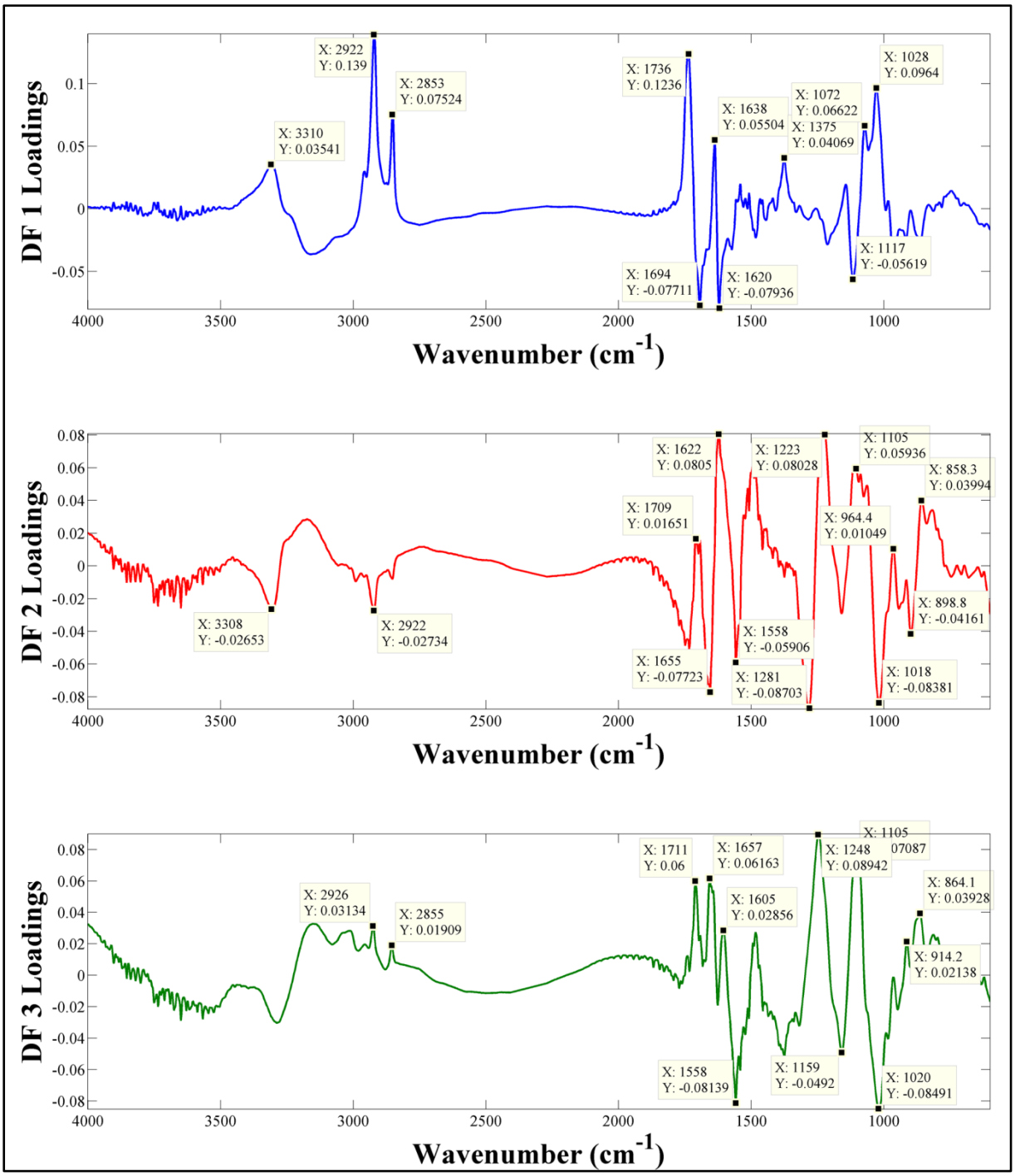

Figure S2. PC-DFA loadings plot of the FT-IR spectral data illustrating the significant vibrational regions that contribute towards the separation on each DF ordinate (axis; positive loadings are of importance in the positive PC-DF score space, while negative loadings have greater importance for samples located in the negative half of the same PC-DF score).

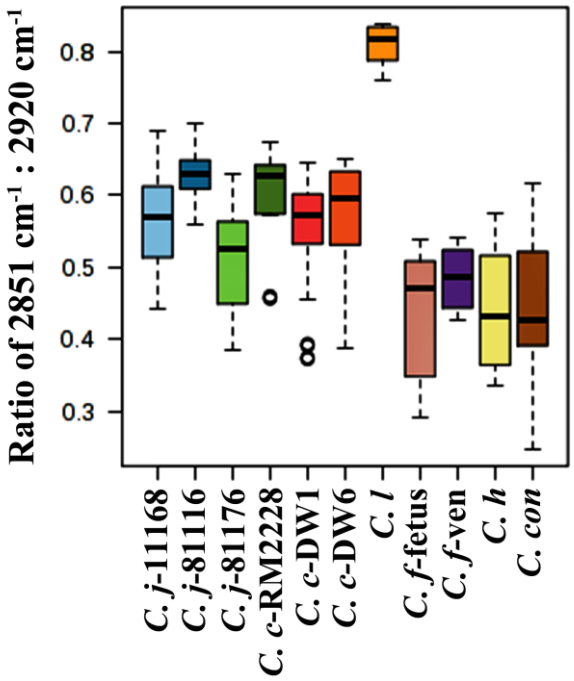

Figure S3. Comparison of the ratio of 2851 cm^{-1} : 2920 cm^{-1} peaks showing the symmetric C-H : asymmetric C-H stretch in lipids, detected in the FT-IR spectra of all the samples. This plot shows box-whiskers where the thick line within the boxes are the median ratios, the top and bottom of the boxes are the 25^{th} and 75^{th} percentiles; the size of the box is the interquartile range (IQR); the whiskers (with the dotted lines) extend to the most extreme data points which are not considered as outliers, defined as no more than 1.5 × IQR outside of the IQR, whilst outliers ratios are shown as open circles.

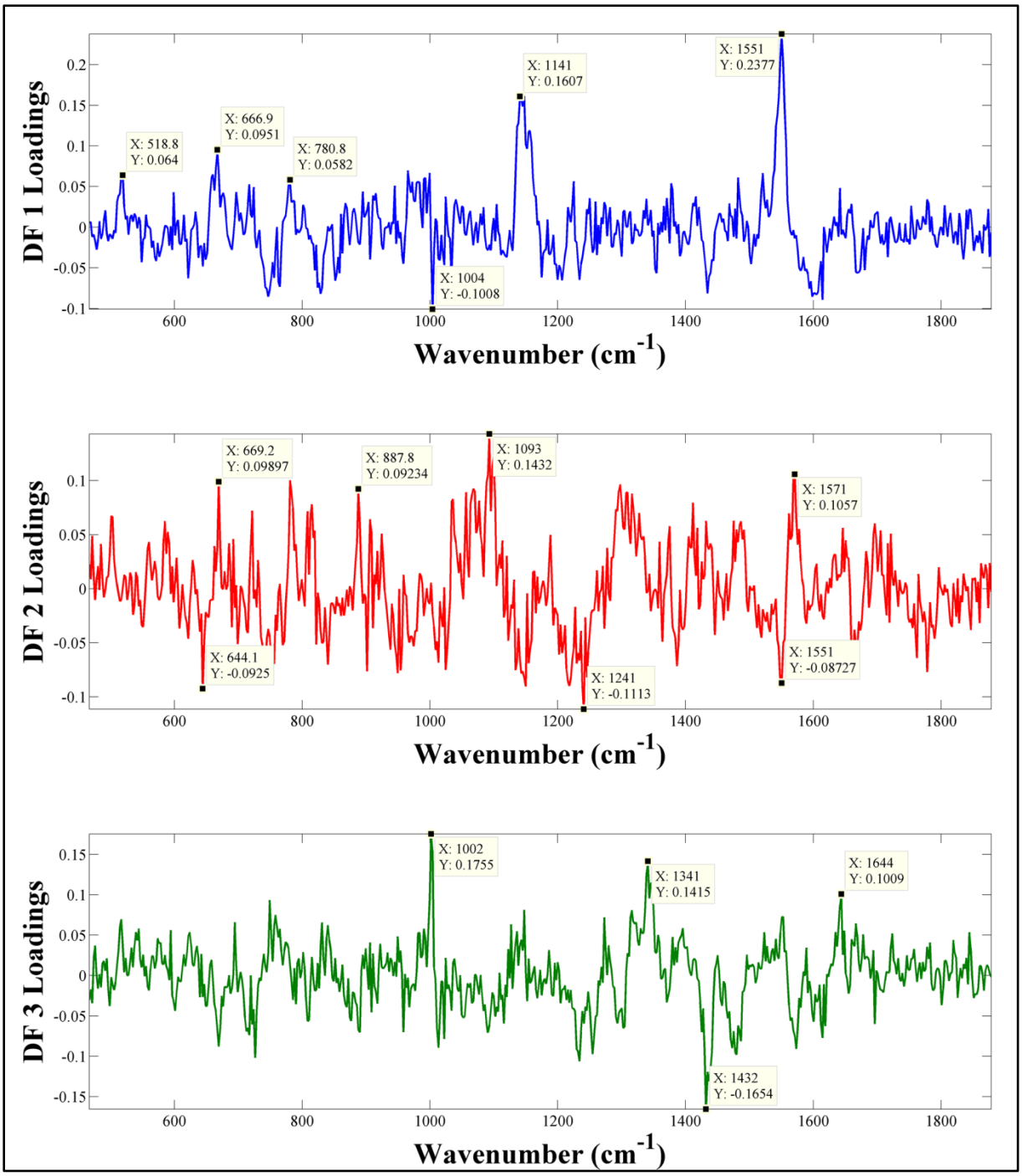

Figure S4. PC-DFA loadings plot of the Raman spectral data, illustrates the significant wavenumbers that contribute towards the separation on each DF ordinate.

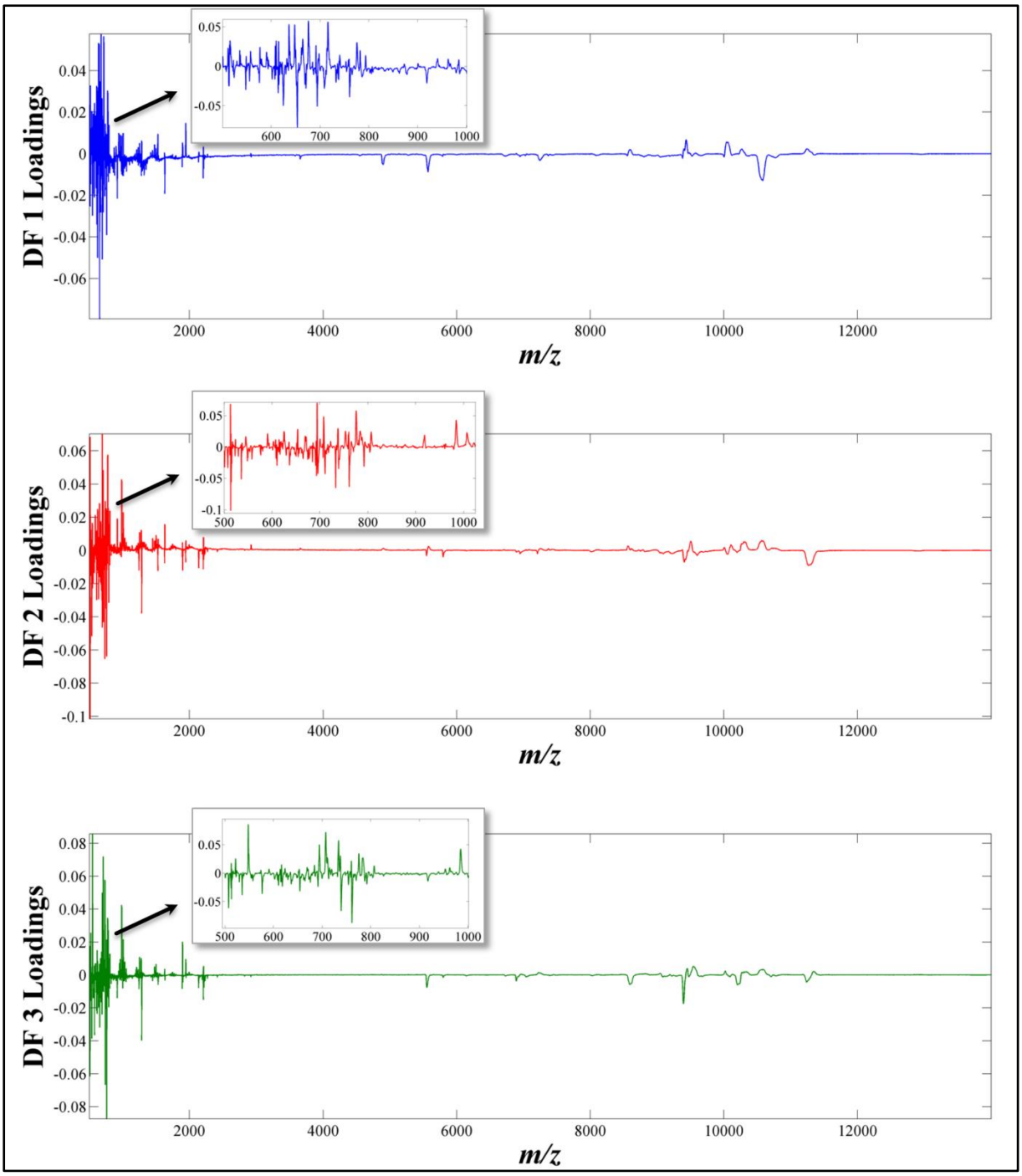

Figure S5. MALDI-TOF-MS PC-DFA loadings plot, illustrates the significant *m/z* that contribute towards the separation on each DF ordinate

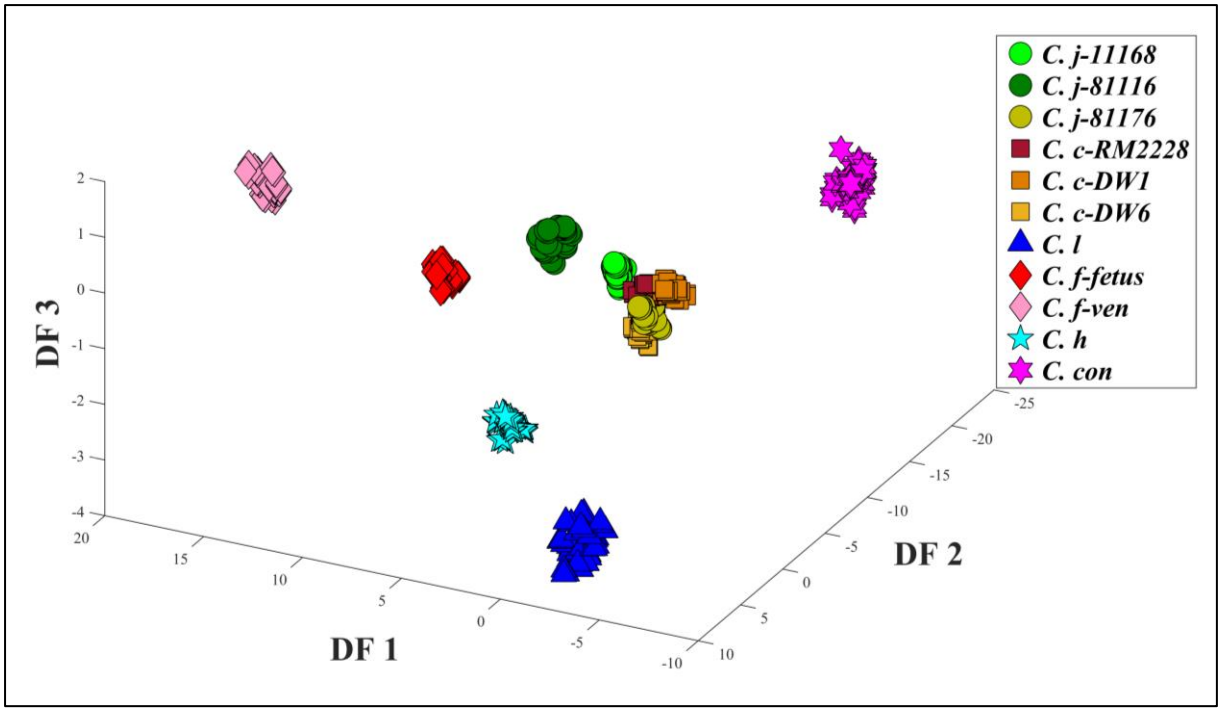

Figure S6. PC-DFA scores plots of the FT-IR spectral data collected in 1878-600 cm^{-1} range. Different coloured symbols represent different *Campylobacter* strains.

Table S1. UHPLC-FTMS solvent gradient used for reverse phase analysis.

Time (min)	Flow Rate (µL min^{-1})	Mobile Phase A (H_20%)	Mobile Phase B (MeOH%)
Initial	400	95	5
5	400	95	5
10	400	5	95
18	400	5	95
25	400	95	5

Table S2. List of significant lipids detected by LC-MS analysis, and contributing to differentiation of *C. fetus* subsp. *fetus* from *C. fetus* subsp. *venerealis*. All detected lipids are putatively identified.

Significant peaks (ID)	*m/z*	RT (s)	Lipid name	Formula
712	259.6426	746.7656	Convolvulinolic acid	$C_{15}H_{31}O_3$
1364	426.3751	711.0585	PC(O-6:0/O-6:0)	$C_{20}H_{45}NO_6P$
1403	446.2731	535.3593	PC(6:2(2E,4E)/6:2(2E,4E))	$C_{20}H_{33}NO_8P$
1423	454.3107	741.7547	LysoPE(0:0/16:0)	$C_{21}H_{45}NO_7P$
1488	481.3333	749.0329	PA(21:0/0:0)	$C_{24}H_{50}O_7P$
1528	502.3121	743.1266	LysoPE(0:0/20:4(5Z,8Z,11Z,14Z))	$C_{25}H_{45}NO_7P$
1556	518.3447	746.8688	PC(18:3(6Z,9Z,12Z)/0:0)	$C_{26}H_{49}NO_7P$
1790	659.3157	745.9508	PA(13:0/20:2(11Z,14Z))	$C_{36}H_{68}O_8P$
1842	684.5027	714.2172	PE(12:0/20:4(5Z,8Z,11Z,14Z))	$C_{37}H_{67}NO_8P$

Code: ID, identifier on plots; RT, retention time; *m/z*, mass-to-charge ratio; PC, phosphatidylcholine; PA, phosphatidic acid; PE, phosphatidylethanolamine.