Electronic Supplementary Material (ESI) for Analyst.

GENE EXPRESSION DATA AND FTIR SPECTRA PROVIDE A SIMILAR PHENOTYPIC DESCRIPTION OF BREAST CANCER CELL LINES IN 2D AND 3D CULTURES

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SUPPLEMENTARY MATERIALS

Negative	Positive
210772_at	219216_at
41553_at	212721_at
216154_at	217725_x_at
207870_at	213225_at
210636_at	209379_s_at
215701_at	202314_at
207696_at	203543_s_at
214920_at	205089_at
216702_x_at	212248_at
216611_s_at	201963_at
216500_at	217936_at
215987_at	209430_at
207496_at	204206_at
216441_at	214314_s_at
211333_s_at	202959_at
213297_at	216713_at
216876_s_at	212179_at
214171_s_at	209632_at
206590_x_at	201407_s_at
213819_s_at	202960_s_at
214052_x_at	222119_s_at
206340_at	208802_at
206365_at	218064_s_at
207150_at	212470_at
202648_at	215936_s_at
213494_s_at	200686_s_at
213999_at	204516_at
221546_at	212507_at
213903_s_at	206095_s_at
211446_at	214683_s_at
217537_x_at	218289_s_at
206948_at	202127_at
221141_x_at	218043_s_at
210279_at	201448_at
220799_at	202861_at
213774_s_at	201737_s_at
216351_x_at	208924_at
207679_at	208671_at
215811_at	212615_at
210322_x_at	212616_at
222259_s_at	220553_s_at
215151_at	218989_x_at
34210_at	218422_s_at
206035_at	212454_x_at
222287_at	201084_s_at
217482_at	203552_at
203161_s_at	200914_x_at
207294_at	212177_at
216834_at	212176_at
213907_at	209571_at

Table S1. List of Affymetrix probe set identifiers representing genes which are differentially expressed in 2D or 3D culture conditions. The left (right) column reports the 50 probe sets with the most downregulated (upregulated) expression levels in a 3D culture if compared to a 2D culture.

2D cultures

	HCC1500	HCC1569	ZR751	BT549	Hs578T	MDAMB231	MDAMB361	MCF7	SKBR3	T47D	MCF12A	MDAMB468	MDAMB436
HCC1500	1.00E+00												
HCC1569	5.60E-14	1.00E+00											
ZR751	0.00E+00	0.00E+00	1.00E+00										
BT549	0.00E+00	4.44E-16	0.00E+00	1.00E+00									
Hs578T	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00								
MDAMB231	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00							
MDAMB361	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00						
MCF7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00					
SKBR3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00				
T47D	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.52E-07	0.00E+00	1.00E+00			
MCF12A	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00		
MDAMB468	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	
MDAMB436	0.00E+00	5.83E-14	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00

3D cultures

HCC1500	1.00E+00												
HCC1569	3.89E-13	1.00E+00											
ZR751	0.00E+00	0.00E+00	1.00E+00										
BT549	0.00E+00	0.00E+00	0.00E+00	1.00E+00									
Hs578T	0.00E+00	0.00E+00	2.22E-16	0.00E+00	1.00E+00								
MDAMB231	0.00E+00	0.00E+00	1.11E-16	0.00E+00	8.89E-07	1.00E+00							
MDAMB361	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00						
MCF7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00					
SKBR3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.65E-04	0.00E+00	1.00E+00				
T47D	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.27E-07	0.00E+00	1.09E-08	1.00E+00			
MCF12A	0.00E+00	0.00E+00	4.98E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00		
MDAMB468	7.10E-08	1.45E-09	4.41E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.78E-12	1.00E+00	
MDAMB436	1.11E-16	4.44E-16	7.33E-15	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.87E-09	1.00E+00

Table S2. Comparison of the FTIR spectra of 13 breast cancer cell lines using multivariate analysis of variance (MANOVA). P-values are reported in the table. For each cell line, 50 spectra were randomly extracted from our spectral library. The MANOVA was calculated from the scores of the spectra projected on the first 6 PCs obtained by PCA applied in the 1800-1000 cm^{-1} region on 650 spectra used to characterize the cell lines either in 2D or 3D culture conditions. Values smaller than 10^{-16} appear as 0. Off-diagonal p-values larger than 10^{-16} are shaded.

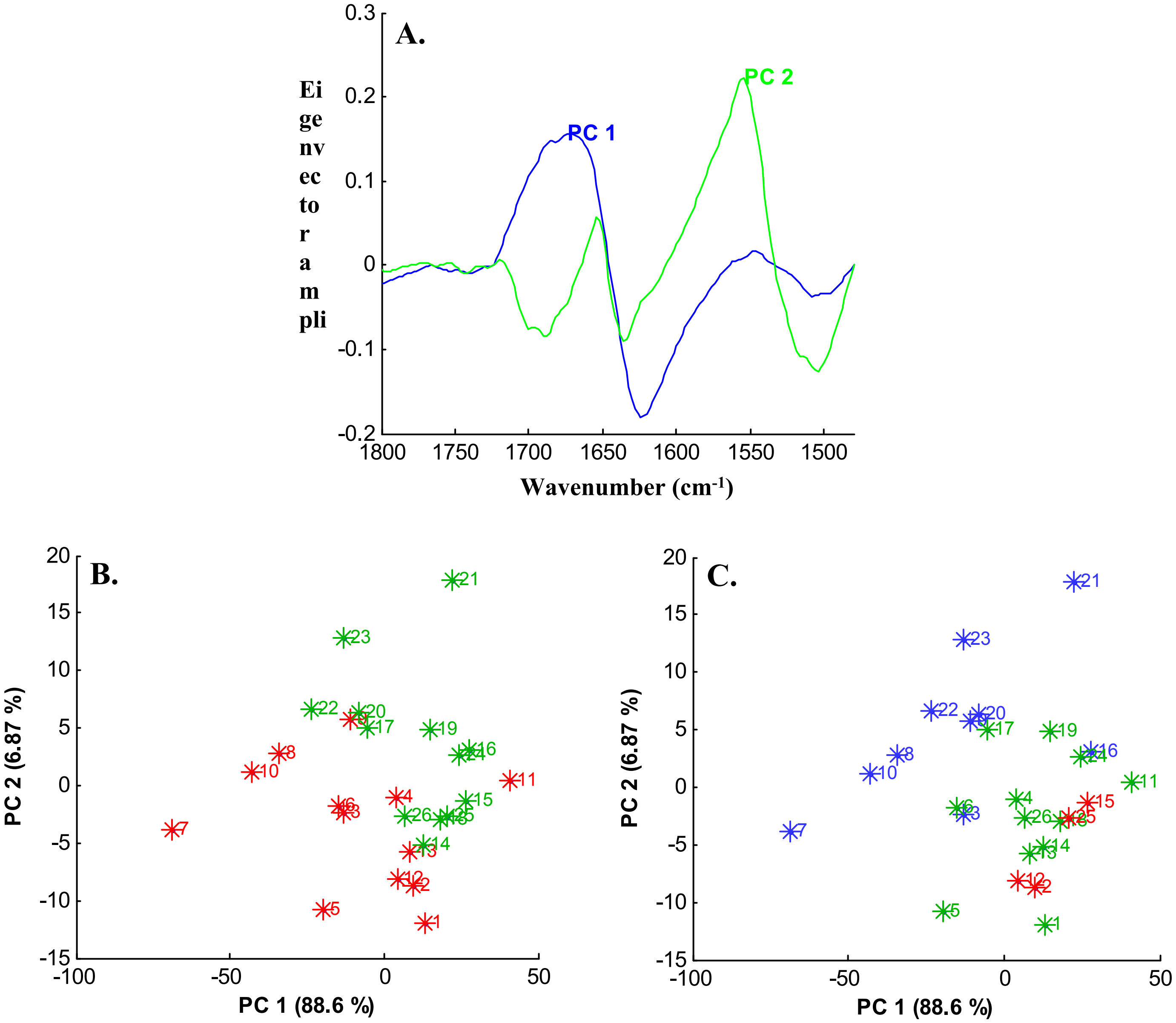

Figure S1. A. Loadings plot for the first 2 PCs obtained by applying PCA on the mean spectra of each cell line grown in 2D and 3D culture conditions. **B.** Score plot representing the projection of the spectra on PC1 and PC2. The numbering and color code of the spectra in the score plot correspond to those reported in Table 1. **C.** Score plot representing the projection of the spectra on PC1 and PC2. The numbering of the spectra in the score plot corresponds to the numbering reported in Table 1. Colors have been modified to group cell lines according to their molecular subtype: basal A (red), basal B (green) and luminal (blue). The variance explained by each PC appears on the axes. PCA has been computed after mean centering in the 1800-1480 cm^{-1} spectral range.

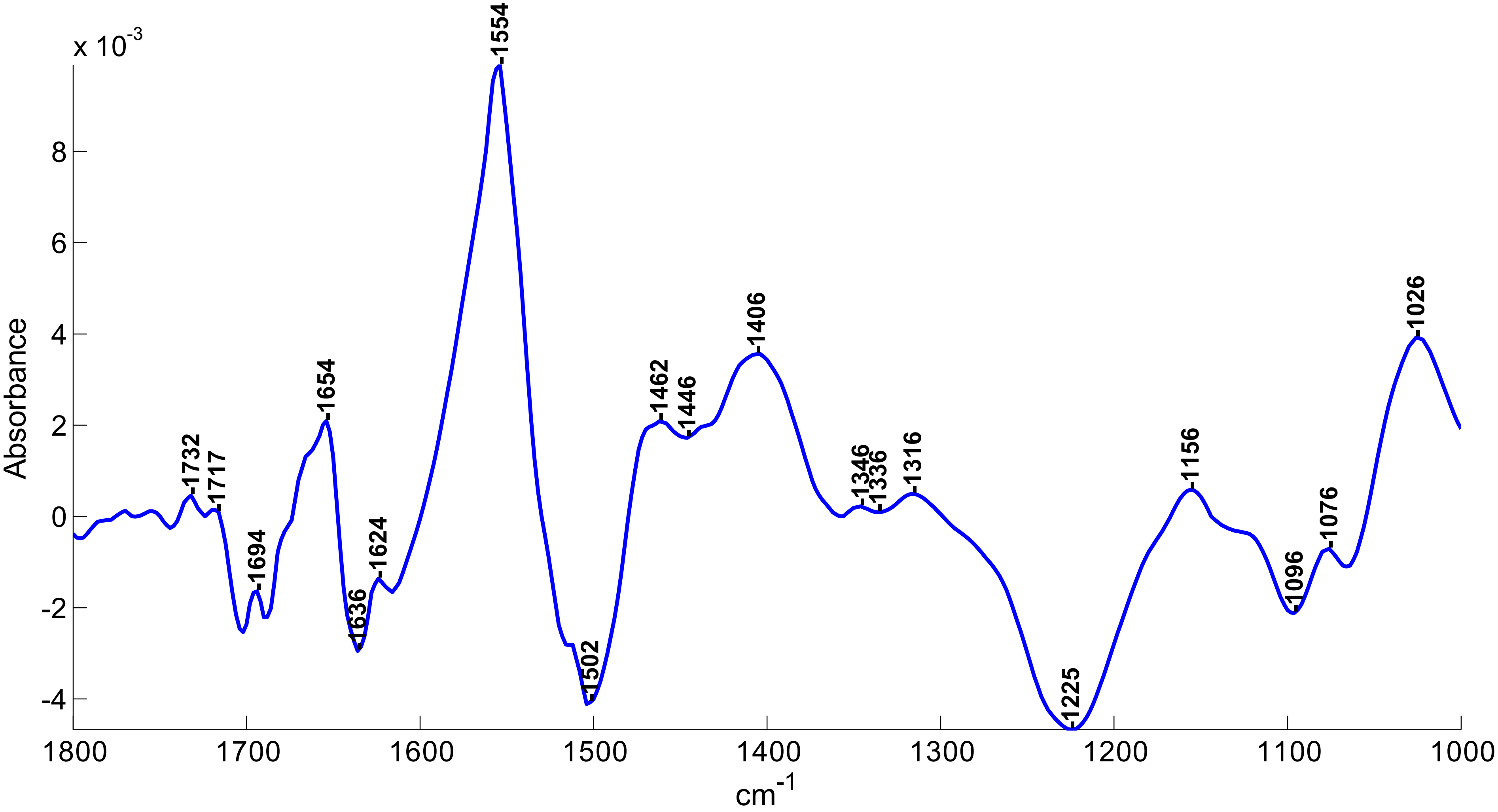

Figure S2. Discriminant vector obtained by linear combination of the first 6 PCs to achieve the best discrimination between 2D and 3D cell cultures based on the FTIR spectral signatures. Wavenumber values are assigned to the main maxima and minima of the vector.