

SUPPORTING INFORMATION

Correlation of lipidomic composition of cell lines and tissues of breast cancer patients using hydrophilic interaction liquid chromatography – electrospray ionization mass spectrometry and multivariate data analysis

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Table S1. List of human breast cell lines

Cell line	Medium	Type	Disease	ER ^{*1}	PR ^{*2}	HER2 ^{*3}
MCF 10A	DMEM/F12	Nonmalignant breast tissue	Fibrocystic disease	NA ^{*4}	NA ^{*4}	NA ^{*4}
ZR-75-1	RPMI-1640	Breast cancer	Ductal carcinoma	+	+/-	+
T-74D	HG-DMEM	Breast cancer	Ductal carcinoma	+	+	-
MCF7	HG-DMEM	Breast cancer	Adenocarcinoma	+	+	-
MDA-MB- 231	HG-DMEM	Breast cancer	Adenocarcinoma	-	-	-
MDA-MB- 453	Leibovitz's L- 15	Breast cancer	Metastatic carcinoma	-	-	+/-
MDA-MB- 468	HG-DMEM	Breast cancer	Adenocarcinoma	-	-	-
SK-BR-3	McCoy's 5A	Breast cancer	Adenocarcinoma	-	-	+
BT-474	HG-DMEM	Breast cancer	Ductal carcinoma	+	+/-	+
BT-549	HG-DMEM	Breast cancer	Ductal carcinoma	-	-	-

^{*1} Estrogen receptor.

^{*2} Progesterone receptor.

^{*3} Human epidermal growth factor receptor 2 overexpression.

^{*4} Not announced.

Table S2 Relative abundance (%) of identified lipid species in normal and tumor breast cell lines.

Lipid	MCF1 0A	ZR-75-1	T-47D	MCF7	MDA- MB-231	MDA- MB-453	MDA- MB-468	SK- BR-3	BR-474	BT-549
PI 32:3	0.75	0.32	0.24	0.85	0.40	0.50	0.19	0.38	0.53	0.38
PI 32:2	0.75	0.38	0.26	0.92	0.36	0.69	0.50	1.16	0.61	0.51
PI 32:1	1.04	3.17	1.41	3.68	0.51	3.14	1.82	12.39	1.88	0.76
PI 32:0	0.66	2.34	1.19	2.20	0.59	1.82	0.91	3.50	1.10	0.61
PI 34:3	0.75	0.38	0.26	0.85	0.40	0.82	0.72	0.55	0.65	0.66
PI 34:2	2.26	2.19	2.62	4.32	1.03	4.97	10.04	6.02	2.86	3.61
PI 34:1	6.03	11.26	12.92	18.13	2.81	18.27	11.51	28.95	5.64	6.97
PI 34:0	1.41	2.28	2.34	3.33	1.19	2.61	1.77	2.43	1.59	1.81
PI 36:4	1.23	3.09	3.66	1.63	1.58	1.29	2.15	2.37	1.39	1.07
PI 36:3	4.34	3.12	3.40	1.77	1.46	2.52	4.33	3.42	6.70	2.72
PI 36:2	15.55	4.85	11.49	9.99	6.29	16.13	27.59	6.02	8.91	17.73
PI 36:1	11.12	7.82	10.16	17.78	9.89	16.76	6.82	11.58	5.68	11.19
PI 36:0	1.60	1.21	1.60	2.41	1.70	2.52	0.99	1.36	1.23	1.63
PI 38:6	0.75	1.01	2.06	1.84	0.67	0.94	0.97	2.90	0.74	1.12
PI 38:5	2.45	5.34	6.20	2.76	4.43	2.99	7.95	3.07	2.37	9.72
PI 38:4	14.14	28.86	15.00	6.52	39.57	6.79	8.94	3.91	13.41	17.93
PI 38:3	21.58	10.71	9.28	4.82	8.79	6.60	4.47	3.62	30.13	7.91
PI 38:2	7.16	3.64	3.25	4.82	4.16	3.52	2.92	1.13	7.07	2.77
PI 38:1	1.51	0.66	0.91	2.12	1.19	1.70	0.63	0.58	1.27	0.74
PI 38:0	0.66	0.26	0.46	0.92	0.47	0.50	0.25	0.29	0.37	0.36
PI 40:6	0.85	3.49	4.85	3.54	3.84	1.60	1.74	1.88	1.35	3.54
PI 40:5	1.13	2.05	3.38	1.98	4.95	1.57	1.49	1.62	1.23	3.21
PI 40:4	1.13	1.04	2.17	1.49	2.61	1.04	0.91	0.61	1.43	2.19
PI 40:3	1.13	0.55	0.89	1.35	1.11	0.69	0.39	0.26	1.84	0.86
PE 32:1	1.59	3.66	5.13	5.23	1.41	4.05	3.30	6.29	3.52	1.94
PE P-34:4	0.76	0.50	0.57	0.49	0.76	0.59	0.51	0.76	0.61	0.84
PE P-34:2; O-34:3	2.05	0.40	0.48	0.63	0.82	0.71	0.60	0.76	0.69	0.65
PE P-34:1; O-34:2	4.33	0.71	0.87	0.84	1.76	4.83	2.92	2.12	2.23	1.88
P-34:0; O-34:1	1.06	0.79	2.35	1.05	1.23	2.00	1.43	0.94	1.94	1.16
PE 34:5	0.61	0.37	0.44	0.56	0.47	0.35	0.35	0.53	0.36	0.45
PE 34:3	0.76	0.55	0.44	0.63	0.59	0.47	0.54	0.71	0.61	0.58
PE 34:2	2.20	4.03	6.09	8.22	1.76	5.26	5.78	7.59	2.83	2.07
PE 34:1	6.61	8.83	9.27	8.29	4.10	7.11	8.03	10.59	7.41	6.47
PE 34:0	1.06	1.21	1.44	1.25	1.00	1.06	1.21	1.29	1.21	1.16
PE P-36:4	2.13	1.98	0.48	0.77	2.64	3.14	1.75	2.71	2.51	2.78
PE P-36:3; O-36:4	2.43	0.79	0.61	0.84	1.23	1.53	1.05	1.29	2.83	1.23
PE P-36:2; O-36:3	5.69	0.63	0.65	0.70	1.35	3.57	2.41	1.18	1.17	1.49
PE P-36:1; O-36:2	5.16	0.69	1.39	1.18	2.05	2.28	1.56	0.94	1.38	1.55
PE P-36:0;	1.37	0.98	2.96	1.25	1.76	1.34	1.05	0.94	2.43	1.29

O-36:1										
PE 36:5	0.84	1.66	1.48	1.18	1.41	0.86	0.60	1.47	1.17	1.03
PE 36:4	0.84	2.45	2.96	2.58	1.41	0.86	0.92	2.24	2.27	1.23
PE 36:3	1.97	2.53	1.09	1.18	1.23	0.75	1.05	1.12	1.98	0.91
PE 36:2	6.91	10.39	13.53	15.26	6.04	12.10	18.16	8.76	6.56	9.70
PE 36:1	8.28	7.20	4.44	4.32	8.73	3.65	3.18	5.12	4.49	5.76
PE 36:0; P-38:6	1.75	2.43	1.31	1.11	2.75	3.65	4.57	3.12	3.12	3.23
PE P-38:5; O-38:6	6.23	2.11	0.91	0.84	3.58	4.95	4.06	2.94	2.47	4.01
PE P-38:4; O-38:5	4.18	2.16	0.96	0.70	5.22	2.63	1.65	1.94	2.71	3.75
PE P-38:3; O-38:4	3.95	0.84	1.13	0.77	1.76	1.10	0.79	0.82	3.12	1.42
PE P-38:2; O-38:3	1.75	0.69	0.74	0.91	1.17	0.79	0.73	0.76	1.46	0.97
PE P-38:1; O-38:2	1.67	0.79	1.39	1.32	1.11	0.94	1.30	0.94	1.25	1.16
PE P-38:0; O-38:1	0.99	0.53	1.22	0.91	0.82	0.67	1.08	0.76	0.77	0.91
PE 38:6	0.76	1.98	2.87	1.67	1.35	1.22	1.11	1.76	1.42	1.55
PE 38:5	2.43	6.12	4.79	4.53	3.34	2.87	2.99	4.65	2.95	3.69
PE 38:4	2.58	11.89	5.61	5.51	7.15	4.44	2.45	7.12	7.81	5.11
PE 38:3	1.67	3.24	1.65	2.30	2.64	1.34	1.49	1.76	4.94	2.72
PE 38:2	1.29	1.08	2.26	3.34	1.35	1.22	1.97	0.88	1.58	1.68
PE 38:1	0.84	0.92	1.17	1.60	1.06	2.40	4.60	1.24	0.93	2.26
PE 38:0; P-40:6	1.37	1.34	0.91	1.05	6.80	2.55	2.51	1.71	2.10	3.88
PE P-40:5; O-40:6	2.66	1.00	1.17	0.84	3.34	1.49	1.33	1.35	1.70	2.98
PE P-40:4; O-40:5	1.21	0.76	1.04	0.63	1.99	0.86	0.67	0.71	1.17	1.75
PE P-40:3; O-40:4	0.99	0.58	0.78	0.70	1.00	0.51	0.44	0.59	1.13	0.78
PE P-40:2; O-40:3	0.99	0.58	0.57	0.77	0.76	0.67	0.48	0.65	0.93	0.71
PE P-40:1; O-40:2	0.91	0.45	0.65	0.91	0.76	0.51	0.57	0.65	0.65	0.71
PE P-40:0; O-40:1	0.68	0.42	0.57	0.70	0.76	0.47	0.54	0.65	0.49	0.71
PE 40:6	0.68	4.98	5.05	3.90	2.75	3.34	3.21	3.35	3.76	3.95
PE 40:5	0.91	2.53	3.05	3.00	2.81	2.28	1.91	1.65	2.14	3.30
PE 40:4	0.91	0.92	1.31	1.74	1.64	1.02	0.95	1.00	1.34	2.01
PE 40:3	0.84	0.58	0.74	1.25	1.00	0.63	0.64	0.71	0.81	1.03
PE 40:2	0.61	0.37	0.87	1.46	0.64	0.51	0.92	0.53	0.57	0.71
PE 40:1	0.53	0.34	0.61	1.11	0.70	0.43	0.64	0.41	0.49	0.84
PC 32:1	4.53	12.46	11.93	11.46	5.32	9.33	6.77	14.71	11.65	6.68
PC 32:0	2.42	3.44	4.38	2.44	3.67	3.25	3.76	3.11	4.40	4.08
PC P-34:2; O-34:3	2.42	1.58	1.81	1.95	2.02	1.83	1.35	1.38	1.76	1.67
PC P-34:1; O-34:2	2.72	1.29	1.51	1.71	1.83	1.62	1.80	1.38	1.76	1.67
PC 34:2	4.23	5.73	4.83	5.37	3.30	4.06	3.91	5.02	5.49	4.64

PC 34:1	11.48	14.90	15.56	12.20	9.17	14.60	10.98	13.32	11.65	14.10
PC 34:0	2.11	3.15	3.17	2.68	2.94	2.64	2.26	2.60	3.08	2.97
PC P-36:0	1.81	1.29	1.36	1.46	1.83	1.62	1.20	1.38	1.32	1.48
PC P-36:3; O-36:4	1.51	1.00	1.06	1.46	1.65	1.42	1.05	1.04	1.32	1.11
PC P-36:2; O-36:3	2.72	1.15	1.36	1.95	1.47	1.83	1.65	1.38	1.54	1.48
PC P-36:1; O-36:2	3.93	1.58	2.42	2.20	2.39	2.03	1.80	1.38	2.42	2.23
PC P-36:0; O-36:1	3.02	1.58	3.63	1.71	2.57	2.03	1.65	1.38	3.52	1.86
PC O-36:0	1.51	1.15	1.66	1.22	1.65	1.62	3.01	3.63	1.98	1.67
PC 36:4	1.81	2.58	1.66	1.71	2.20	1.62	1.20	2.08	1.98	2.04
PC 36:3	2.72	2.58	1.36	1.95	5.32	1.62	1.35	1.56	2.42	10.76
PC 36:2	9.67	6.02	7.40	7.56	5.69	7.71	6.92	5.54	7.03	4.27
PC 36:1	4.83	5.16	3.02	3.17	2.94	4.46	2.41	4.84	3.52	2.04
PC 36:0; P-38:6	2.72	1.86	1.66	3.17	1.83	3.04	2.56	2.42	2.20	1.48
PC P-38:5; O-38:6	1.81	1.15	1.66	1.71	1.65	1.62	1.50	1.38	1.76	1.11
PC P-38:4; O-38:5	1.21	0.72	1.36	0.98	1.47	1.01	1.05	1.04	1.10	0.93
PC P-38:3; O-38:4	1.21	0.86	0.91	0.98	1.65	1.01	1.05	0.87	1.10	1.86
PC P-38:0; O-38:1	1.81	1.43	2.11	1.46	2.75	1.62	6.62	1.73	1.76	2.60
PC 38:6	1.81	3.15	2.57	2.20	2.75	2.43	2.86	3.11	2.42	2.78
PC 38:5	1.51	3.01	2.11	1.95	2.94	1.83	2.11	2.08	1.98	2.41
PC 38:4	2.11	2.87	1.66	1.95	2.57	1.83	1.65	1.90	2.42	1.67
PC 38:3	2.42	2.72	1.81	2.44	1.47	2.03	1.80	1.90	2.20	1.11
PC 38:1	1.51	0.86	1.06	1.71	3.67	1.62	1.95	1.21	0.88	1.48
PC 38:0; P-40:6	1.81	1.00	1.06	2.93	2.75	2.84	3.76	1.73	1.32	1.86
PC P-40:5; O-40:6	2.11	1.00	1.66	1.95	1.65	1.83	2.71	1.90	1.98	1.30
PC P-40:1; O-40:2	1.81	1.43	1.06	1.46	1.65	1.22	1.80	1.21	1.10	1.67
PC P-40:0; O-40:1	1.81	1.15	1.36	1.71	2.75	1.42	2.71	1.38	1.54	2.78
PC O-40:0	2.11	2.29	2.11	2.20	3.12	2.03	2.86	2.08	2.20	3.15
PC 40:6	1.81	3.01	2.42	2.20	2.20	2.84	3.16	2.77	2.20	1.67
PC 40:5	1.51	1.43	1.36	1.22	2.20	1.22	1.50	1.21	1.32	1.30
PC 40:3	1.81	1.00	1.21	2.20	1.83	2.23	2.11	1.38	1.32	1.30
PC 40:2	1.81	0.86	1.36	1.71	1.83	1.42	1.65	1.21	1.10	1.67
PC 42:6	1.81	1.58	1.36	1.71	1.28	1.62	1.50	1.73	1.32	1.11
SM 34:2	1.56	1.04	1.95	1.63	2.67	1.16	1.41	1.29	2.01	1.23
SM 34:1	13.22	21.66	21.98	10.25	18.42	14.35	12.50	11.04	16.95	8.94
SM 35:1	1.66	1.04	2.33	1.54	1.69	1.39	1.03	0.92	2.16	1.40
SM 36:3	12.07	24.44	21.98	30.31	19.41	34.49	25.09	31.19	37.50	33.83
SM 36:2	2.08	2.60	2.33	3.72	2.11	3.70	3.29	3.22	3.88	3.77
SM 36:1	2.08	2.08	1.95	2.09	1.55	1.39	2.91	1.20	2.73	2.80
SM 37:1	1.46	1.21	1.56	1.63	1.13	1.27	1.41	0.92	1.44	1.40
SM 38:2	1.77	1.39	1.95	1.72	1.55	1.39	1.79	1.01	1.87	1.49

SM 38:1	2.19	1.56	1.95	2.00	1.55	1.39	1.97	1.20	2.44	1.49
SM 39:1	1.66	1.21	1.95	1.72	1.41	1.27	1.32	0.92	1.58	1.49
SM 40:2	3.75	2.43	2.92	2.99	2.53	2.08	3.29	2.21	2.44	2.80
SM 40:1	7.08	4.85	4.09	5.54	5.34	3.59	3.57	6.44	4.17	4.82
SM 41:2	2.71	2.08	3.11	2.99	2.67	2.43	3.76	1.93	2.30	2.80
SM 41:1	2.71	2.95	3.89	2.81	3.23	3.01	2.63	2.67	3.02	2.72
SM 42:2	25.81	13.52	10.51	17.42	15.33	15.86	24.53	13.52	7.18	18.23
SM 42:1	18.21	15.94	15.56	11.62	19.41	11.23	9.49	20.33	8.33	10.78

Table S3 PCA models of all lipids in breast cell lines (Fig. 4A) and breast cell lines and tissues of cancer patients (Fig. 5A), numbers of components and samples, fractions of the sum of squares of all X that the model can explain using principle components (R^2X) and fractions of the sum of squares of all X predicted by the model according to the cross validation (Q^2).

Figure	Components	Number of samples	$R^2X(\text{cum})$	$Q^2(\text{cum})$
4A	6	19	0.824	0.244
5A	6	39	0.765	0.460

Table S4 OPLS-DA models of all lipids in breast cell lines (Fig. 4B) and breast cell lines and tissues of cancer patients (Fig. 5B), numbers of components and samples, fractions of the sum of squares of all X that the model can explain using the latent variables (R^2X), fractions of the sum of squares of all Y that the model can explain using the latent variables (R^2Y), and fractions of the sum of squares of all X and Y predicted by the model according to the cross validation (Q^2).

Figure	Components	Number of samples	$R^2X(\text{cum})$	$R^2Y(\text{cum})$	$Q^2(\text{cum})$
4B	1+1+0	19	0.316	0.892	0.658
5B	1+2+0	39	0.580	0.906	0.753

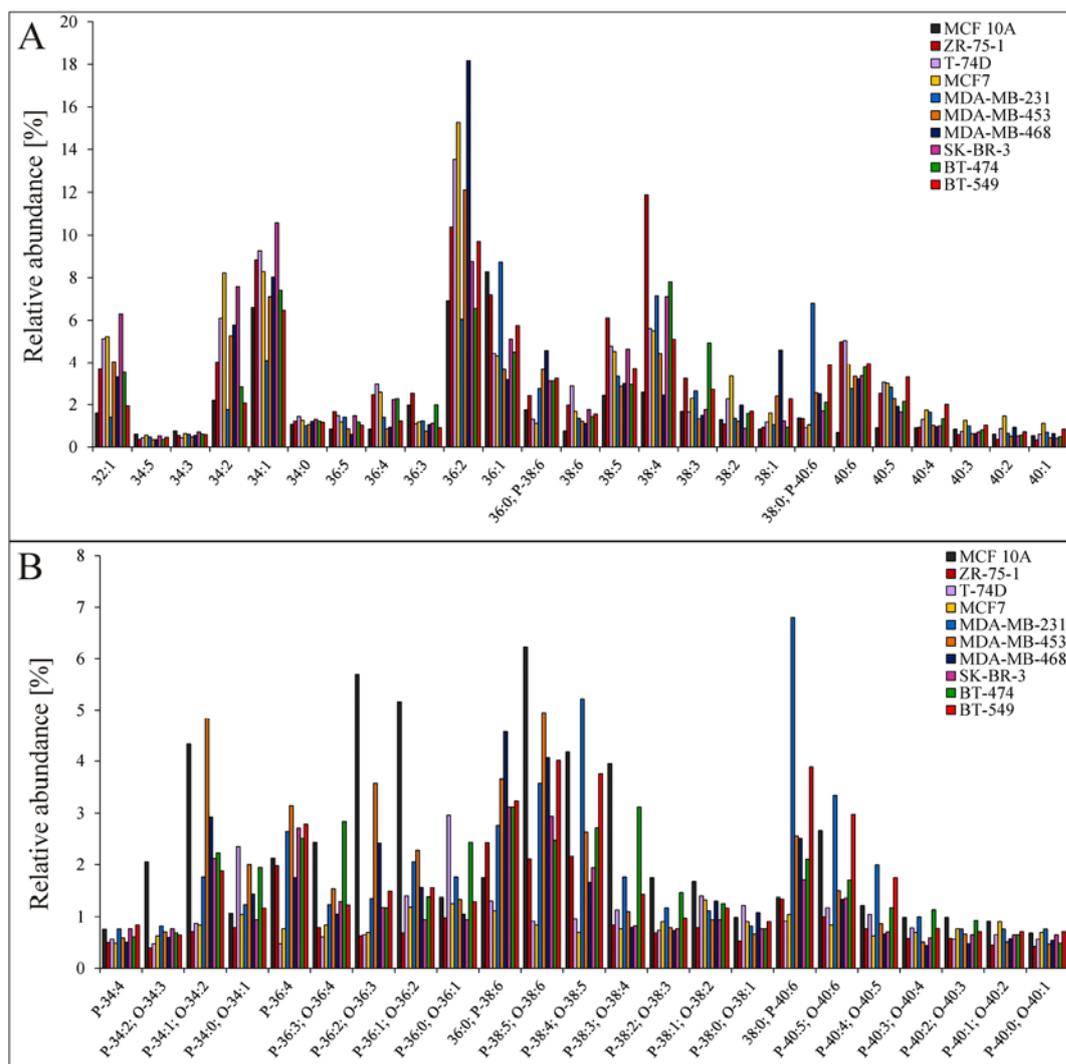


Figure S1. Relative abundance (%) of PE species: (A) diacyls and (B) ethers / plasmalogens in normal and tumor breast cell lines.

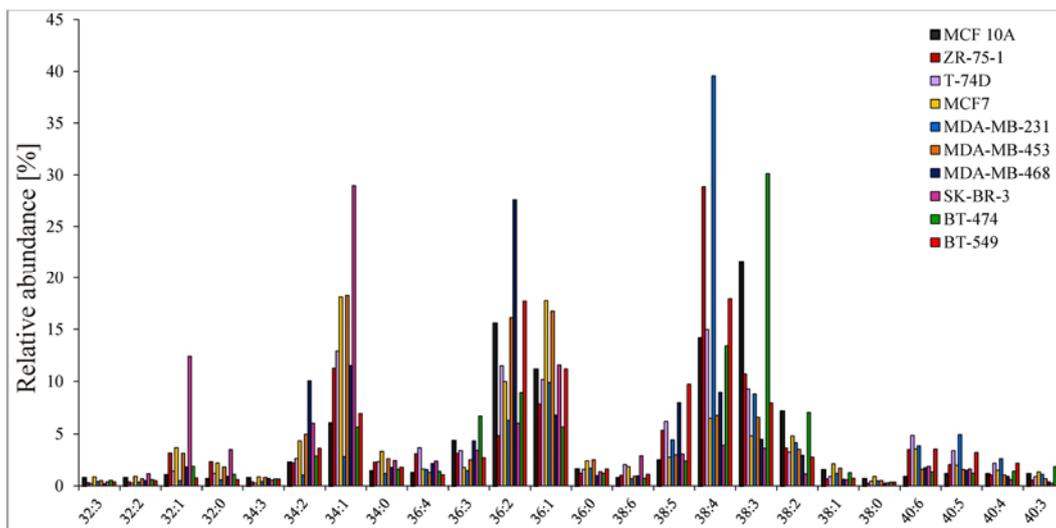


Figure S2. Relative abundance (%) of PI species in normal and tumor breast cell lines.

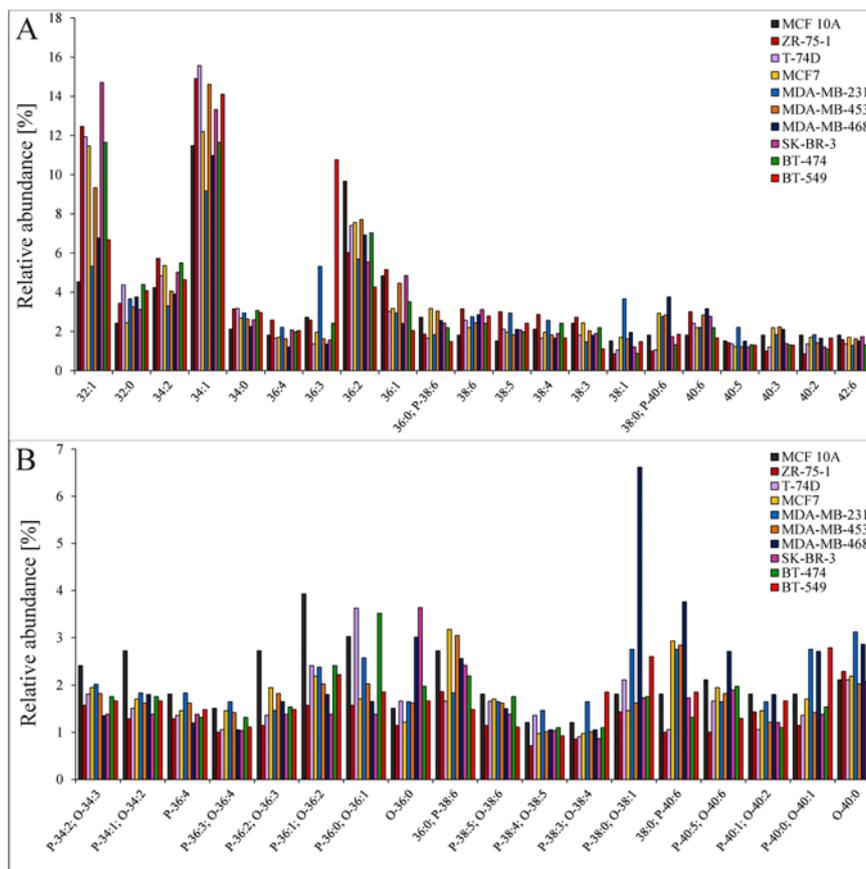


Figure S3. Relative abundance (%) of PC species: (A) diacyls and (B) ethers / plasmalogens in normal and tumor breast cell lines.

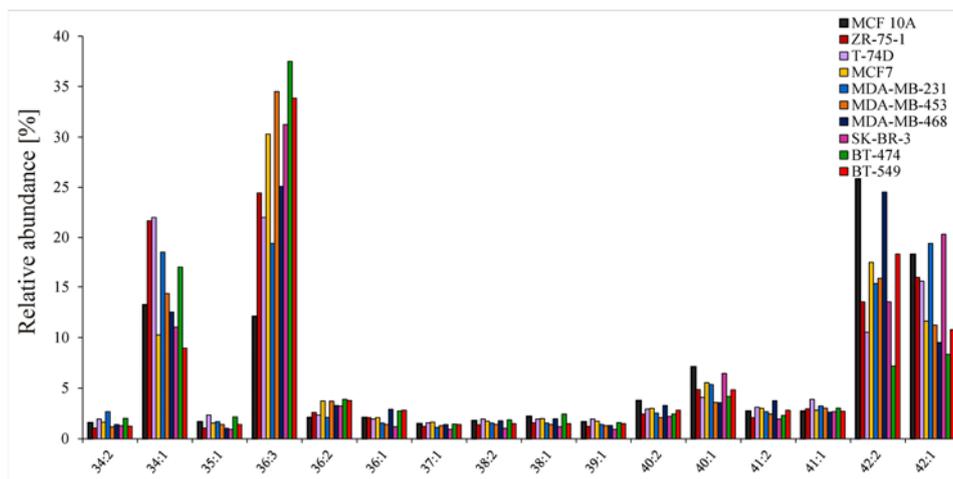


Figure S4. Relative abundance (%) of SM species in normal and tumor breast cell lines.

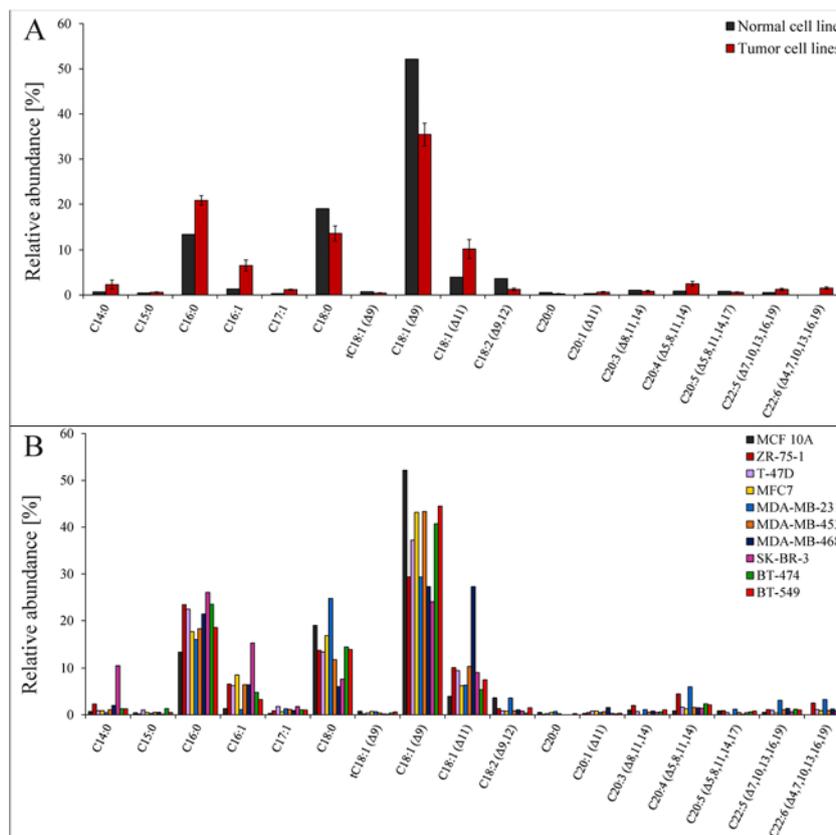


Figure S5. Relative abundance (%) of fatty acyls after the transesterification of total lipid extracts measured by GC/MS in normal and tumor cell lines: (A) comparison of normal cell line (black columns) and average relative abundances from nine tumor cell lines including standard errors of average value (red columns), and (B) relative abundance of individual tumor cell lines. GC/MS conditions are described in the Experimental part.

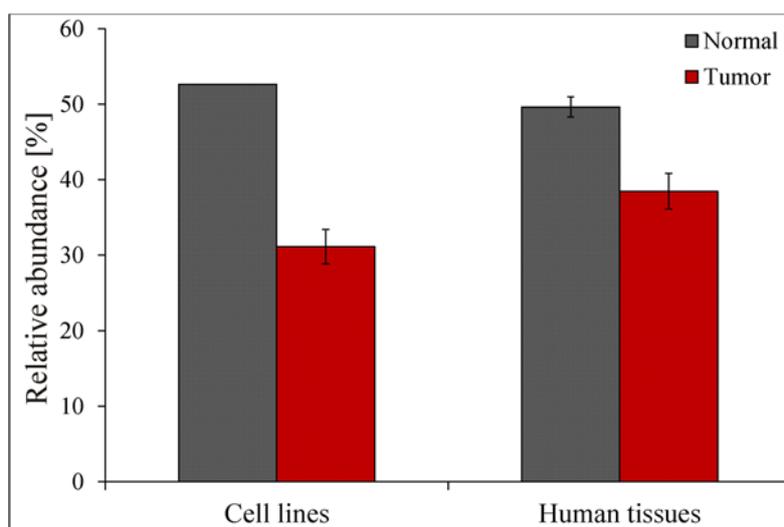


Figure S6. Comparison of total relative abundances of PE ethers and plasmalogens in normal cell line (black columns) and tumor human tissue and nine tumor cell lines and tumor human tissues (red columns, including standard errors of average value).

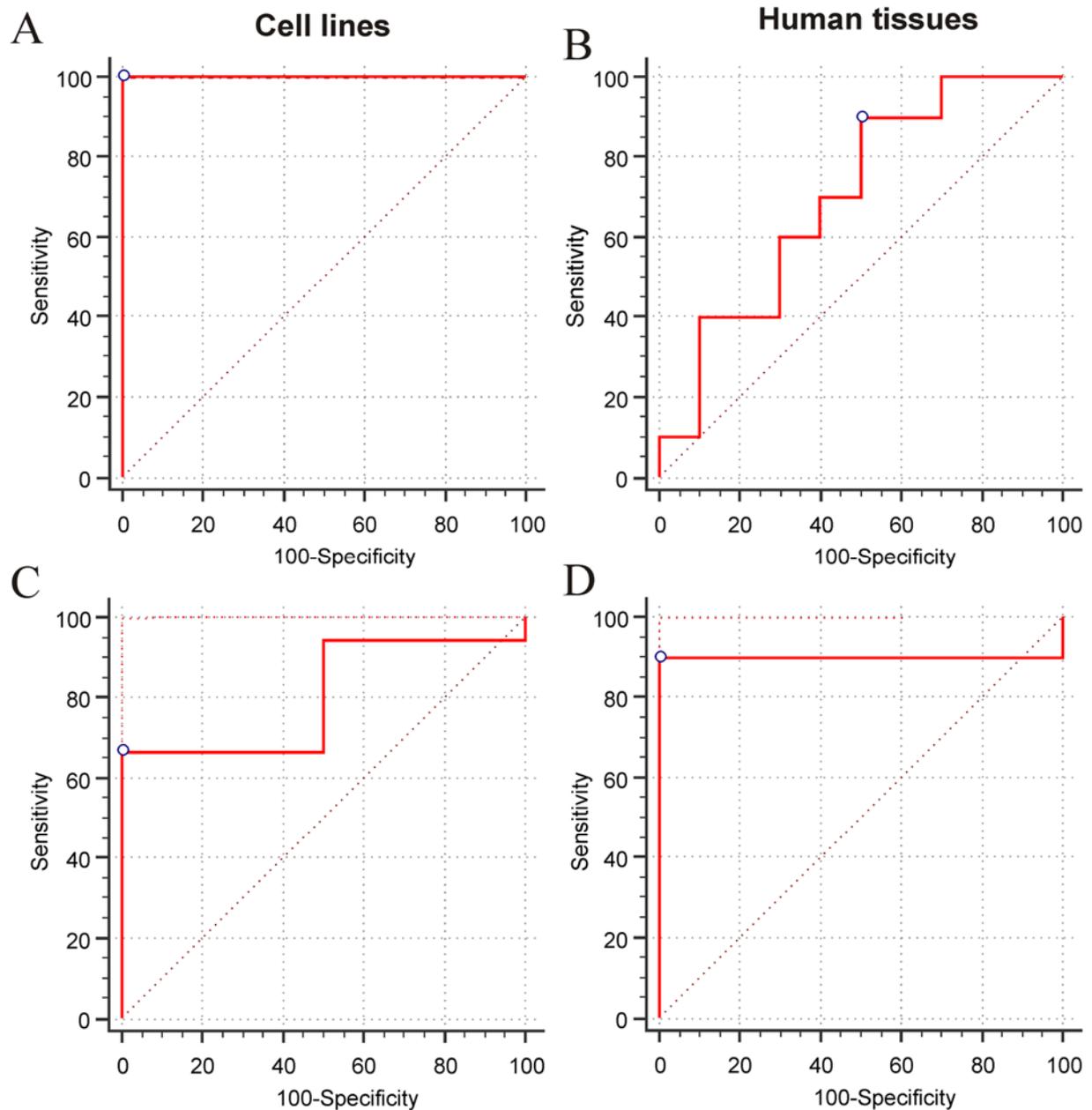


Figure S7. ROC curves constructed for the sum of relative abundances of: A/ PE 32:1, PI 32:1 and PC 32:1 in cell lines, area under curve (AUC) = 1.00, B/ PE 32:1, PI 32:1 and PC 32:1 in human tissues, AUC = 0.70, C/ PE 36:4, PI 36:4 and PC 36:4 in cell lines, AUC = 0.81, and D/ PE 36:4, PI 36:4 and PC 36:4 in human tissues, AUC = 0.90.