SUPPORTING INFORMATION

Lipidomic differentiation of human breast cancer tissues and surrounding normal tissues using HPLC/ESI-MS and multivariate data analysis

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Table S1 Main patient characteristics and tumor histopathological data

Patient	Patient characteristics				Tumor histopathology					
	Age at diagnosis	BMI *1	Smoking history	Alcohol consump-tion	Type	Size [mm]	Stage	ER [%] *2	PR [%] *3	HER2 [IHC] *4
1	73	31	no	no	IDCA*5	21	IIA	100	90	0
2	67	29	no	yes	IDCA*5	10	IA	100	0	2+
3	46	-	-	-	IDCA*5	70	IIB	90	80	3+
4	71	24	no	no	IDCA*5	10	IIIA	90	90	1+
5	71	33	no	no	IDCA*5	28	IIB	70	0	3+
6	60	29	no	no	IDCA*5	20	IA	100	100	0
7	55	21	yes	yes	IDCA*5	15	IB	90	100	0
8	58	29	yes	yes	IDCA*5	8	IA	100	100	0
9	79	29	no	yes	IDCA*5	17	IA	100	100	0
10	35	35	yes	no	IDCA*5	12	IB	100	100	0

*1 Body mass index

*2 Estrogen receptor

*3 Progesterone receptor

*4 Human epidermal growth factor receptor 2

*5 Invasive ductal carcinoma

Table S2 PCA models for individual lipid classes, 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)

| Title	Components	Number of samples	R^2X(cum)	Q^2(cum)
PI	2	20	0.764	0.475
PE	2	20	558	0.192
PC	2	20	0.827	0.226
SM	2	20	0.713	0.325
All	2	20	0.500	0.158

Table S3 OPLS models for individual lipid classes, 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)

| Title	Components	Number of samples	R^2X(cum)	R^2Y(cum)	Q^2(cum)
PI	1+2+0	20	0.671	0.894	0.543
PE	1+1+0	20	0.479	0.929	0.843
PC	1+1+0	20	0.494	0.83	0.379
SM	1+1+0	20	0.665	0.759	0.510
All	1+3+0	20	0.660	0.983	0.871

Table S4 Concentrations [µmol/g] of individual lipid classes in normal and tumor tissues of ten breast cancer patients with their standard errors obtained using the positive-ion HILIC-HPLC/ESI-MS. Statistically significant differences determined by T-test are labeled by an asterisk

| Lipid class	Normal tissue	Tumor tissue
PI*	1.16 ± 0.23	4.99 ± 0.42
PE*	0.56 ± 0.10	2.40 ± 0.18
PC*	3.40 ± 0.36	7.31 ± 0.49
SM*	1.02 ± 0.14	1.45 ± 0.08
LPC*	0.05 ± 0.01	0.24 ± 0.03

Fig. S-1 Positive-ion HILIC-HPLC/ESI-MS of total lipid extracts of normal (black line) and tumor (red line) tissues without the reduction of huge amount of nonpolar lipids using the hexane – methanol - water extraction. HPLC conditions: column Spherisorb Si (250 x 4.6 mm, 5 μm), flow rate 1 mL/min, separation temperature 40°C, gradient 0 min - 94% A + 6% B, 60 min - 77% A + 23% B, where A is acetonitrile and B is 5 mM aqueous ammonium acetate
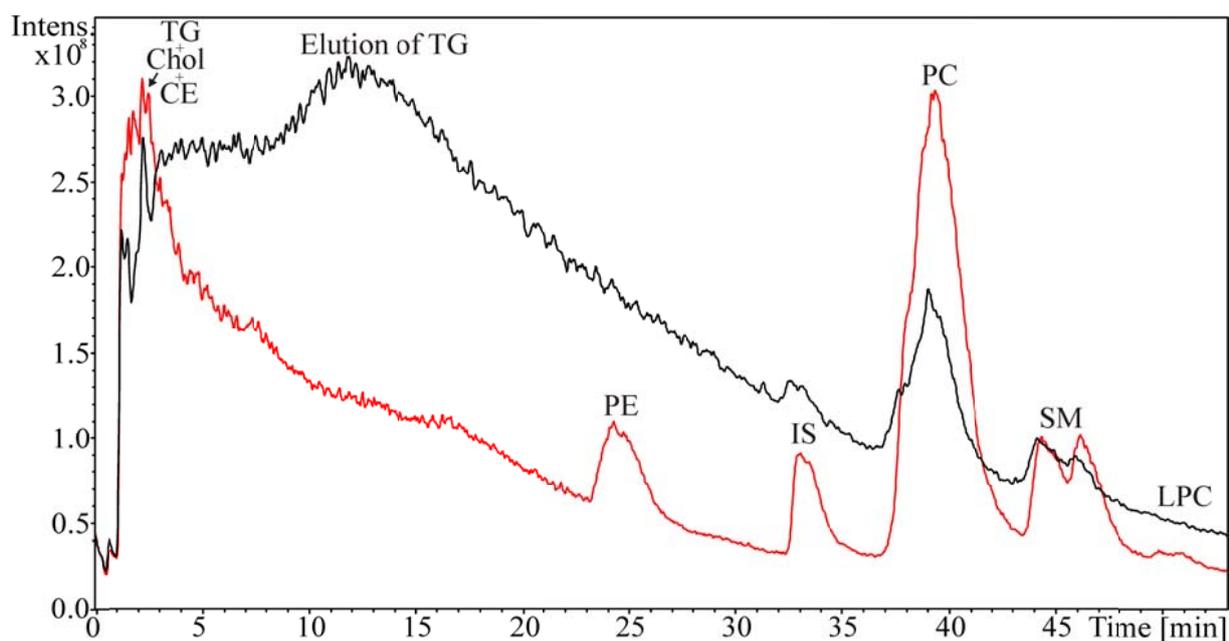
Fig. S-2 Comparison of concentrations [μmol/g] of individual **(a)** PI, **(b)** PE, **(c)** PC and **(d)** SM in normal and tumor tissues of ten breast cancer patients (compare with relative abundances shown in **Fig. 2**)
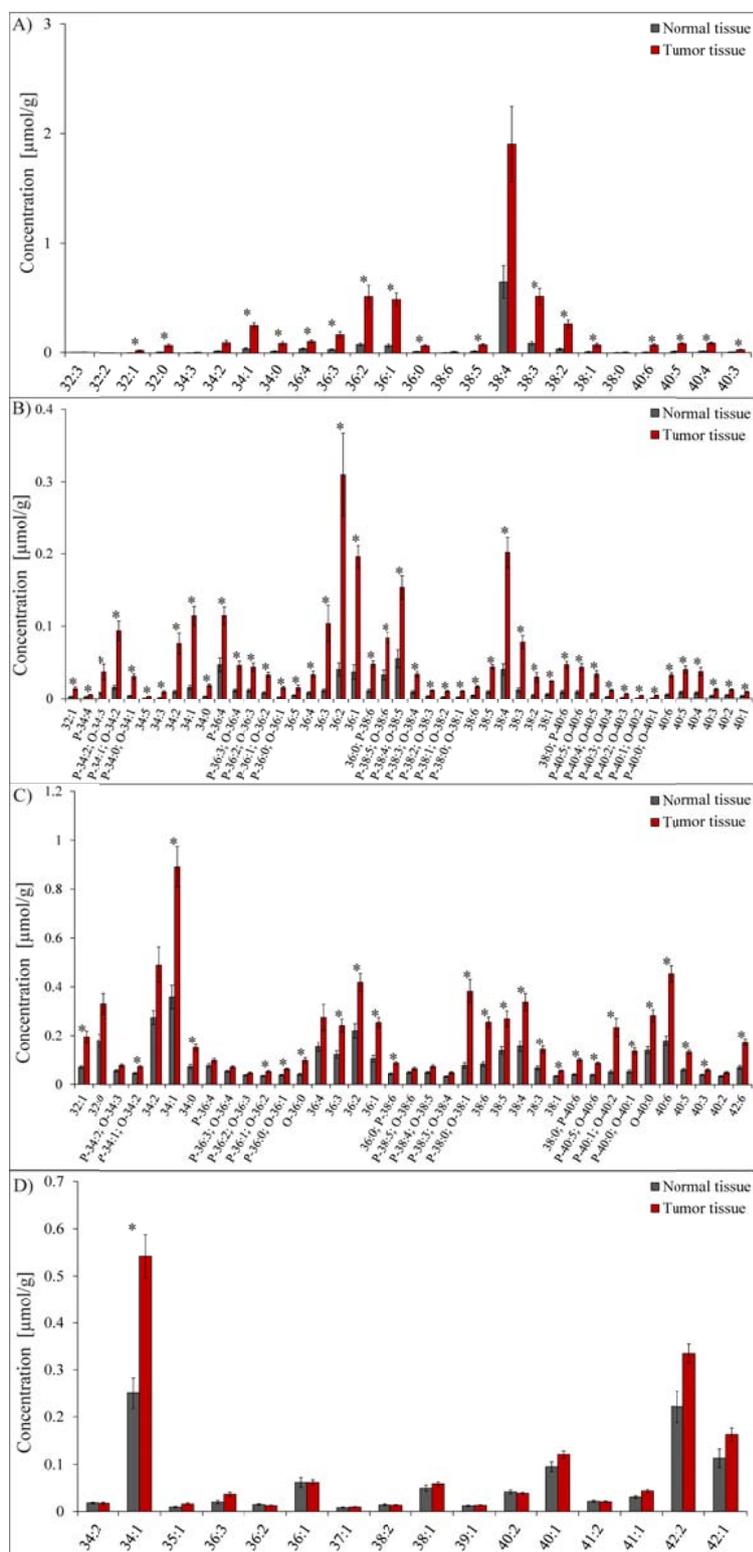
Fig. S-3 Multivariate data analysis of relative abundances [%] of individual PC species in normal (black) and tumor (red) tissues: **(a)** PCA score plot, **(b)** OPLS score plot, **(c)** OPLS S-plot
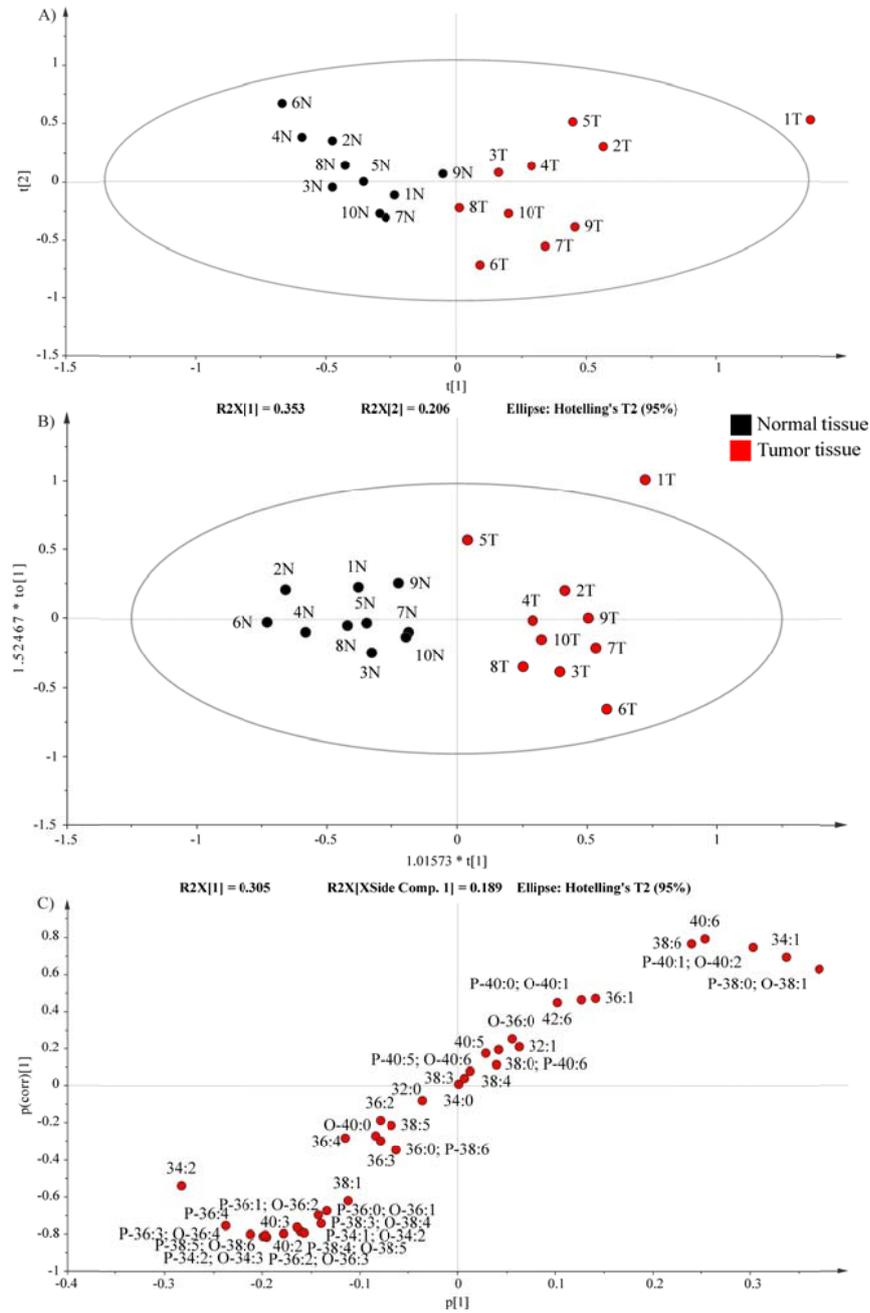
Fig. S-4 Multivariate data analysis of relative abundances [%] of individual SM species in normal (black) and tumor (red) tissues: **(a)** PCA score plot, **(b)** OPLS score plot, **(c)** OPLS S-plot