SUPPORTING INFORMATION

Lipidomic differentiation between human kidney tumors and surrounding normal tissues using HILIC-HPLC/ESI-MS and multivariate data analysis

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Table S1.

Main patient characteristics and tumor histopathological data.

Patient characteristics			**Tumor histopathology**		
No.	**Age at diagnosis**	**BMI**[1]	**Type**	**Size [mm]**	**Stage**[2]
1	67	21	Clear cell	55x55x55	III
2	67	30	Clear cell	170 x 120 x 150	III
3	80	28	Clear cell	30 x 32 x 30	I
4	59	31	Clear cell	68 x 60 x 50	II
5	74	31	Clear cell	50 x 50 x 30	III
6	18	19	Wilms tumor	45x45x45	-
7	74	28	Clear cell	33 x 32 x 30	I
8	76	28	Clear cell	44x44x44	I
9	81	38	Papillary	65 x 65 x 50	I
10	80	27	Clear cell (relapse)	35 x 30 x 22	recurrent
11	59	28	Clear cell	25 x 17 x 38	I
12	75	35	Clear cell	21 x 15 x 40	III
13	66	-	Clear cell	45 x 40 x 33	I
14	80	22	Clear cell	53 x 55 x 30	I
15	36	33	Clear cell	24 x 16 x 18	I
16	64	33	Clear cell	75 x 75 x 75	III
17	52	32	Clear cell	90 x 60 x 60	III
18	66	27	Clear cell	72 x 70 x 45	II
19	70	27	Clear cell	40x40x40	I
20	60	35	Clear cell	105 x 75 x 70	III

[1] Body mass index.

[2] Tumor stage: I – tumor smaller than 70 mm limited to the kidney, no spread to the lymph nodes or distant organs, II – tumor larger than 70 mm limited to the kidney, no spread to the lymph nodes or distant organs, III –kidney tumor of any size, spread to the regional lymph nodes, but not to distant organs.

Table S2.

Models for all identified lipid species, 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).

Method	**Components**	**Samples**	**R^2X(cum)**	**R^2Y(cum)**	**Q^2(cum)**
PCA	2	40	0.451	-	0.270
OPLS	1+1+0	40	0.242	0.422	0.291

Table S3.

Concentrations [μmol/g] of individual lipid classes in normal and tumor tissues of 20 kidney cancer patients with their standard errors determined by the positive-ion HILIC-HPLC/ESI-MS. Statistically significant differences determined by T-test are labeled by an asterisk, where * refers to the significance $p \leq 0.05$ and ** $p \leq 0.01$.

Lipid class	Normal tissue	Tumor tissue
PI	3.13 ± 0.26	2.55 ± 0.33
PE**	6.30 ± 0.42	4.56 ± 0.41
PC	10.53 ± 0.57	10.40 ± 0.57
SM*	2.90 ± 0.18	2.31 ± 0.19
LPC**	0.10 ± 0.01	0.04 ± 0.01

Fig. S1. Comparison of absolute concentrations [µmol/g] of individual species in normal and tumor tissues of 20 kidney cancer patients: (A) PE and (B) PC determined by relative abundances of $[M-H]^-$ and $[M-CH_3]^-$ ions, respectively, in the negative-ion HILIC-HPLC/ESI-MS. Statistically significant differences according to T-test are indicated by an asterisk, where * refers to the significance $p \leq 0.05$, ** $p \leq 0.01$, and *** $p \leq 0.001$.

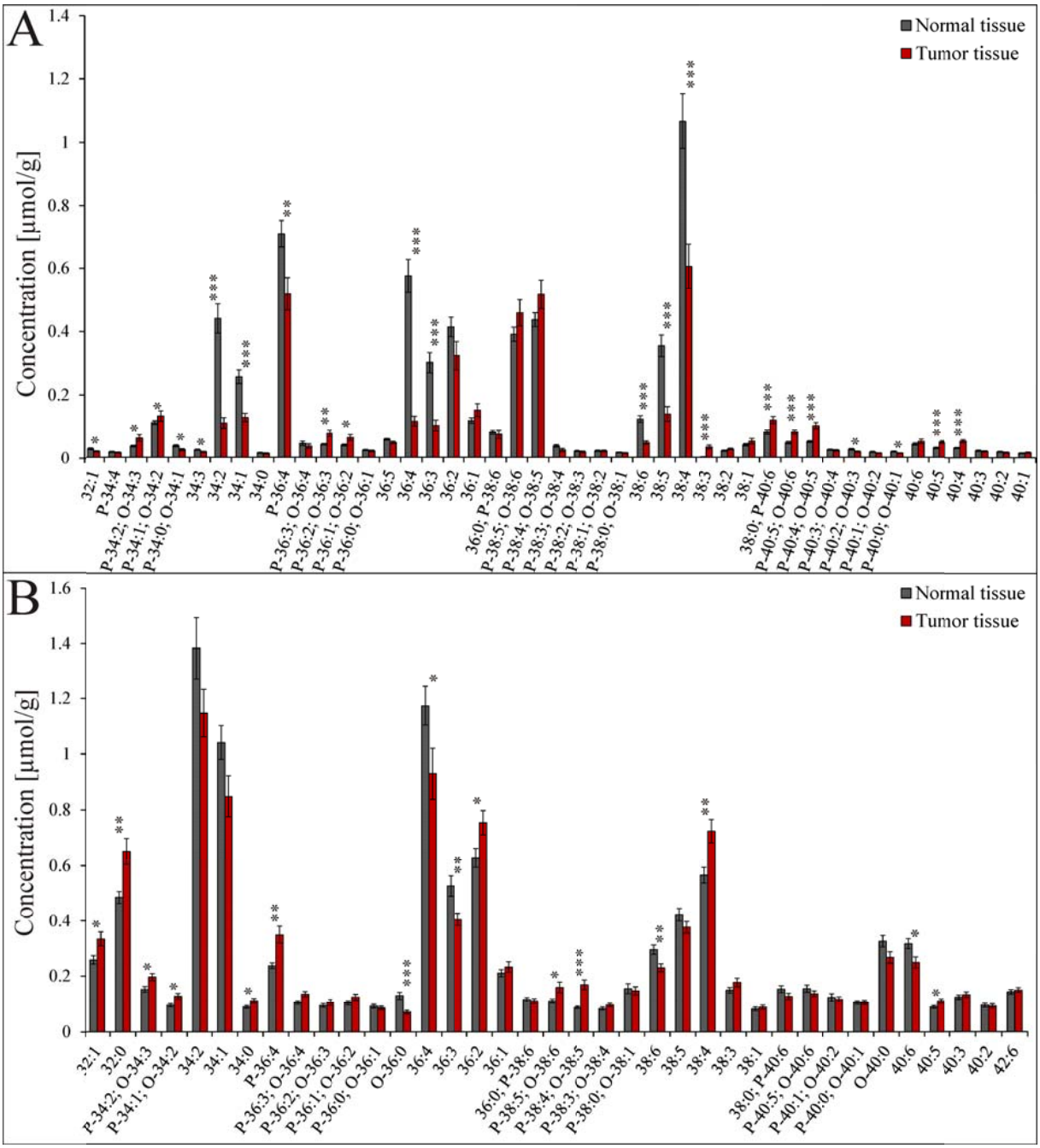

Fig. S2. Comparison of absolute concentrations [µmol/g] of individual species in normal and tumor tissues of 20 kidney cancer patients: (A) PI and (B) SM determined using relative abundances of $[M-H]^-$ and $[M+H]^+$ ions, respectively, in the negative and positive-ion HILIC-HPLC/ESI-MS. Statistically significant differences according to T-test are indicated by an asterisk, where * refers to the significance $p \leq 0.05$, ** $p \leq 0.01$, and *** $p \leq 0.001$.