

SUPPORTING INFORMATION

HILIC/ESI-MS determination of gangliosides and other polar lipid classes in renal cell carcinoma and surrounding normal tissues

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Table S-1 List of male RCC patients enrolled in the present study

Patient number	Age	Body-mass-index [kg/m²]
1	50	33.2
2	50	34.5
3	70	32.1
4	50	33.8
5	81	23.7
6	70	25.2
7	45	35.7
8	61	27.6
9	77	24.8
10	75	26.2
11	58	23.7
12	72	21.7
13	41	27.5
14	60	54.5
15	77	31.1
16	58	17.9
17	64	29.1
18	64	22.1
19	63	23.4
20	47	30.1
Mean	61.7±11.8	27.1±4.4

Table S-2 Parameters of method validation for internal standards SulfoHexCer d18:1/12:0, GM3 d18:1/12:0, and PS 14:0/14:0 in pooled sample of kidney tissues for high-level (HL) and low-level (LL) concentrations

Parameters		SulfoHexCer d18:1/12:0	GM3 d18:1/12:0	PS 14:0/14:0
Extraction recovery [%]	HL	70	103	48
	LL	55	106	53
Accuracy [%]	HL	80	83	80
	LL	96	117	63
RSD [%]	HL	5.5	4.4	8.1
	LL	2.7	5.6	5.5
Carry-over [%]		0.5	0.1	2.3
Selectivity [%]		97.9	98.7	98
LOD [pmol/mL]		2.6	64	270
LOQ [pmol/mL]		4.3	110	450
Calibration curve		$210.74x - 0.42$	$5.12x - 0.14$	$20.34x - 7.45$

Table S-3 List of all quantified lipid species (uploaded separately)

Fig. S-1 Confirmation of expected structure and purity of synthesized GM3 d18:1/12:0 IS using HILIC/ESI-MS (conditions in Experimental): **a** reconstructed ion current chromatogram of m/z 1095.6 corresponding to $[M-H]^-$ ion. **B** negative-ion ESI mass spectrum showing $[M-H]^-$ ion m/z 1095.6408 (mass accuracy 2.3 ppm).

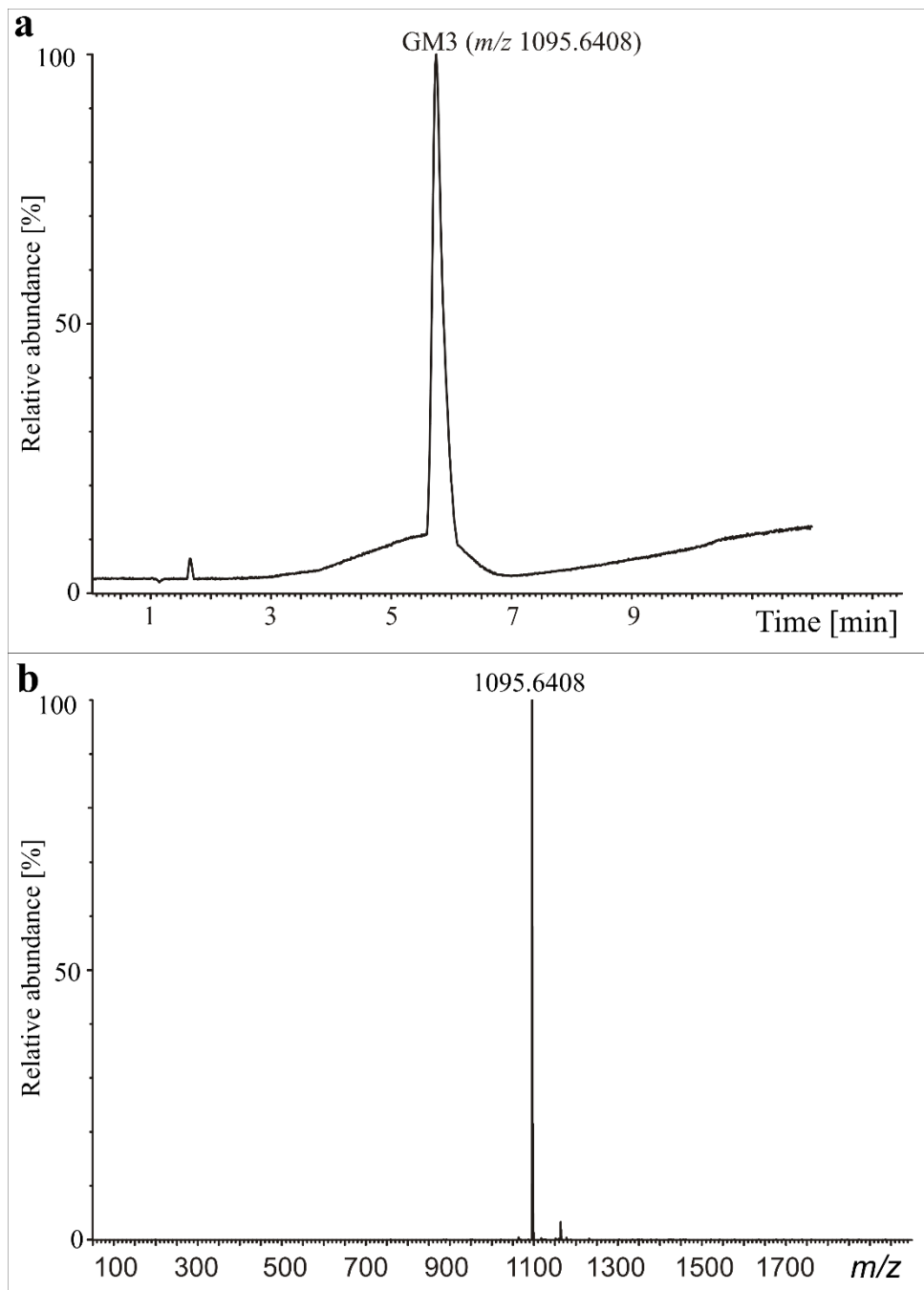


Fig. S-2 Comparison of extracted ion currents (EIC) of selected lipids in surgically removed tumor and surrounding normal tissue parts of selected RCC patient. Blue to red style color visualization was used, and intensity values at minimum and maximum are written above particular images

