

Analytical and Bioanalytical Chemistry

Electronic Supplementary Material

Metabolomic study of human tissue and urine in clear cell renal carcinoma by LC-HRMS and PLS-DA

Joanna Nizioł, Vincent Bonifay, Krzysztof Ossoliński, Tadeusz Ossoliński, Anna Ossolińska,
Jan Sunner, Iwona Beech, Adrian Arendowski, Tomasz Ruman

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Table S1 List of putatively identified metabolites in tissue and urine samples – analysis of water extracts

No.	Formula	Mass ¹	Putative metabolite ²	Average abundances ³							
				Tissue				Urine			
				Normal	Normal SD	Cancer	Cancer SD	Control	Control SD	Cancer	Cancer SD
1	C ₁₂ H ₂₀ O ₁₀	324.1059	Bis-fructose 2',1:2,1'-dianhydride	116	88	34973	24360	-		-	
2	C ₈ H ₁₁ NO ₆ S	249.0309	Norepinephrine sulfate	174	301	999	1285	380	66	630	670
3	C ₅ H ₁₀ N ₂ O ₃	146.0694	Glutamine	23471	20890	31944	17532	15542	7910	12212	8638
4	C ₅ H ₉ NO ₄	147.0532	Glutamate	170025	107354	196812	150964	1451	324	1603	637
5	C ₁₀ H ₂₁ NOS	203.1335	Methylthiononanaloxime	46617	21626	6349	2664	-	-	-	-
6	C ₉ H ₁₇ NO ₃	187.1156	<i>N</i> -Heptanoylglycine	8801	8973	1133	1053	513	301	1021	1443
7	C ₉ H ₁₉ NO ₂	173.1418	Amino-nonanoic acid	6276	2727	427	65	-		-	
8	C ₃₃ H ₄₀ O ₂₂	788.2030	Quercetin sophoroside glucoside	3509	3628	231	199	-	-	-	-
9	C ₁₇ H ₂₀ N ₄ O ₆	376.1384	Riboflavin	11837	11164	682	269	5812	3573	966	1246
10	C ₁₃ H ₁₅ NO ₅	265.0955	<i>N</i> -Phenylacetylglutamic acid	2307	905	119	165	2457	1115	6993	9261
11	C ₁₂ H ₂₁ NO ₅	259.1428	<i>N</i> -(3-oxooctanoyl)homoserine	2039	2555	40	69	4461	2744	4323	5812
12	C ₁₁ H ₁₄ N ₂ O ₃ S	254.0728	Alanyl- α -thiophenylglycine	1480	764	29	50	-	-	-	-
13	C ₁₁ H ₁₆ N ₂ O ₈	304.0905	<i>N</i> -Acetylaspartylglutamate (NAAG)	1546	968	-	-	1176	966	675	687
14	C ₉ H ₁₇ NO ₄	203.1164	Acetylcarnitine	1317	403	119400	154065	-		-	
15	C ₁₇ H ₃₃ NO ₄	315.2413	Decanoylcarnitine	127	167	772	288	724	167	2177	3055
16	C ₁₀ H ₁₉ NO ₄	217.1319	Propanoylcarnitine	3948	1919	13560	7478	5684	1187	10619	13054
17	C ₁₀ H ₁₉ NO ₅	233.1257	Hydroxypropionylcarnitine	592	681	1839	1593	6303	3475	1398	652

18	C ₁₁ H ₂₁ NO ₅	247.1425	Hydroxybutyrylcarnitine	9841	2726	22738	18525	2036	464	11538	19962
19	C ₇ H ₁₅ NO ₃	161.1055	Carnitine	120165	82739	194041	108019	53165	23006	77358	85980
20	C ₁₉ H ₃₅ NO ₄	341.2569	2-Dodecenoylcarnitine	6219	9604	8800	12269	417	59	1728	2769
21	C ₁₈ H ₃₅ NO ₄	329.2570	4,8-Dimethylnonanoylcarnitine	2982	515	2875	355	147	64	1106	1985
22	C ₁₃ H ₂₅ NO ₄	259.1790	Hexanoylcarnitine	4642	2445	2592	1381	-	-	-	-
23	C ₁₃ H ₂₃ NO ₆	289.1527	3-Methylglutarylcarnitine	1888	1100	328	55	4766	1934	16400	15177
24	C ₁₁ H ₁₉ NO ₄	229.1319	Butenylcarnitine	-	-	-	-	1109	485	3383	4212
25	C ₁₄ H ₂₇ NO ₄	273.1947	Heptanoylcarnitine	-	-	-	-	1734	1	3177	3164
26	C ₁₆ H ₃₁ NO ₄	301.2259	2,6-Dimethylheptanoylcarnitine	-	-	-	-	14606	2510	59515	85917
27	C ₁₄ H ₂₅ NO ₆	303.1685	Pimelylcarnitine	-	-	-	-	2036	921	13598	19339
28	C ₁₉ H ₃₅ NO ₆	373.2459	Dodecanedioylcarnitine	-	-	-	-	294	110	2114	3573

¹ Experimental monoisotopic neutral mass; ² putative identification of extracted features with metabolites and other compounds in the IDEOM database; ³ average abundances from all samples of the same type; “-” - peak not detected; PG – glycerophosphoglycerols; PIP – phosphatidylinositol phosphates; PI – phosphatidylinositols; PC – phosphocholines; MG – monoacylglyceride; TG – triacylglyceride; PA – phosphatidylglycerols; PE – glycerophosphoethanolamines; SP – sphingosines; PS – phosphatidylserines

Table S2 List of putatively identified metabolites in tissue samples – analysis of THF extracts

No.	Formula	Mass ¹	Putative metabolite ²	Average abundances ³			
				Tissue			
				Normal	Normal SD	Cancer	Cancer SD
1	C ₁₂ H ₂₀ O ₁₀	324.1060	Bis-D-fructose 2',1:2,1'-dianhydride	137	173	2221	2047
3	C ₅ H ₁₀ N ₂ O ₃	146.0694	Glutamine	197	202	12938	16883
14	C ₉ H ₁₇ NO ₄	203.1161	Acetylcarnitine	11150	15016	151110	139733
15	C ₁₇ H ₃₃ NO ₄	315.2406	Decanoylcarnitine	446	232	2071	2157
16	C ₁₀ H ₁₉ NO ₄	217.1320	Propanoylcarnitine	2569	3353	10807	14085
19	C ₇ H ₁₅ NO ₃	161.1054	Carnitine	19208	22821	76516	69447
20	C ₁₉ H ₃₅ NO ₄	341.2571	2-Dodecenoylcarnitine	317	212	762	514
21	C ₁₈ H ₃₅ NO ₄	329.2570	4,8-Dimethylnonanoylcarnitine	6005	1251	5657	1463
22	C ₁₃ H ₂₅ NO ₄	259.1789	Hexanoylcarnitine	881	752	2258	2281
25	C ₁₄ H ₂₇ NO ₄	273.1938	Heptanoylcarnitine	1522	1441	874	985
29	C ₄₀ H ₅₂ O ₂	564.3962	Unidentified cancer tissue biomarker	64	64	738	712

¹ Experimental monoisotopic neutral mass; ² putative identification of extracted features with metabolites and other compounds in the IDEOM database; ³ average abundances from all samples of the same type



Fig. S1 Examples of total ion chromatograms for tissue extracts (red/top – cancer tissue, green/bottom – normal tissue)

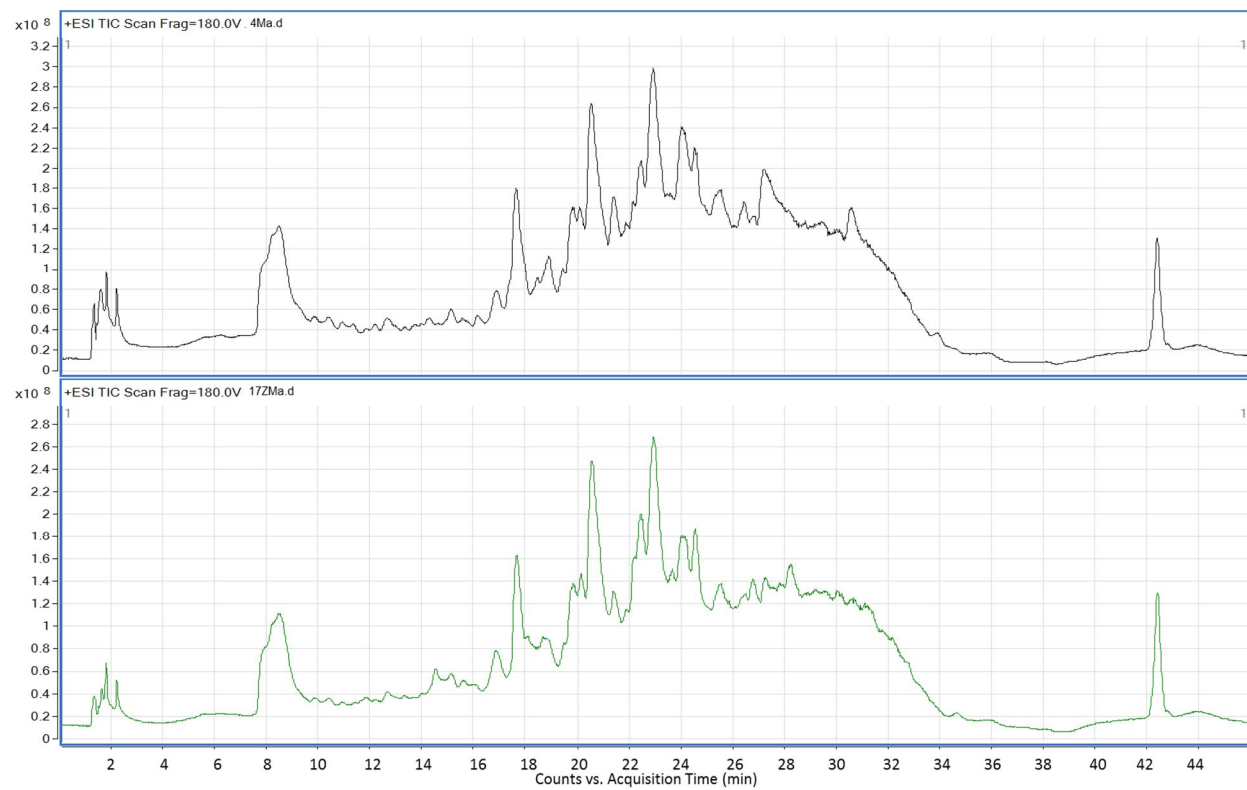


Fig. S2 Examples of total ion chromatograms for urine samples (red/top – cancer patient urine, green/bottom – control urine)